DROP: Dimensionality Reduction Optimization for Time Series

Sahaana Suri, Peter Bailis
Stanford InfoLab

ABSTRACT

Dimensionality reduction is critical in analyzing increasingly high-volume, high-dimensional time series. In this paper, we revisit a now-classic study of time series dimensionality reduction operators and find that for a given quality constraint, Principal Component Analysis (PCA) uncovers representations that are over 2× smaller than those obtained via alternative techniques favored in the literature. However, as classically implemented via Singular Value Decomposition (SVD), PCA is incredibly expensive for large datasets. Therefore, we present DROP, a dimensionality reduction optimizer for high-dimensional analytics pipelines that greatly reduces the cost of the PCA operation over time series datasets. We show that many time series are highly structured, hence a small number of data points are sufficient to characterize the data set, which permits aggressive sampling during dimensionality reduction. This sampling allows DROP to uncover high quality low-dimensional bases in running time proportional to the dataset's intrinsic dimensionality—*independent* of the actual dataset size—without requiring the user to specify this intrinsic dimensionality a priori. DROP further enables downstream-operation-aware optimization by coupling sampling with online progress estimation, trading-off degree of dimensionality reduction with the combined runtime of DROP and downstream analytics tasks. By progressively sampling its input, computing a candidate basis for transformation, and terminating once it finds a sufficiently high quality basis in a reasonable running time, DROP provides speedups of up to 50× over PCA via SVD and 33× in end-to-end high-dimensional analytics pipelines.

1 INTRODUCTION

As high-volume, high-dimensional time series become increasingly common [5, 6, 36, 40], dimensionality reduction techniques offer a powerful toolkit for assisting in their efficient analysis [16, 26, 66]. These reduction techniques transform high-dimensional data into a lower-dimensional subspace while still preserving data properties important for downstream analytics tasks, such as variance, pairwise distances, or correlations. Projecting to a lower-dimensional basis while preserving these properties accelerates common analyses including clustering, classification, anomaly detection, and similarity search [3, 22, 24, 34, 42, 43, 45, 61] while preserving accuracy.

In this paper, we begin with a study of dimensionality reduction for high-dimensional time series. We find that when maintaining pairwise distances over a gold standard set of high-dimensional time series [13], Principal Component Analysis (PCA) [16] delivers time series transformations that are on average of 2× lower dimension than alternatives. This constrasts with a recent highly-cited [19] study of the same data that did not consider PCA, which suggested that the choice of reduction technique is immaterial to result quality.

In addition, we find that over time series data, PCA uncovers bases that are of *far* smaller dimension than classical theory predicts. As an example, we ran PCA on a dataset containing 5000 140-dimensional ECG heartbeat readings. The classic Johnson-Lindenstrauss (JL) lemma [1, 16] predicts that to preserve pairwise distances to even 25%, a 137-dimensional basis is required in the worst case. In contrast, PCA finds a 3-dimensional subspace that preserves average distances within 25% in this dataset—a 46× reduction. The reason for this phenomenon is that many time series are highly structured. Our ECG time series measuring heartbeats is periodic and has a high degree of structural repetition. Unlike data-independent approaches like JL, PCA is able to identify this structure within the data and identify a basis that captures this smaller, intrinsic dimensionality.

Unfortunately, while PCA is incredibly effective at reducing the dimensionality of time series, as in [19], it is often overlooked due to its slow speed—as classically implemented via SVD, up to 245 times slower than alternatives from [19], with runtime $O(\min\{m^2d, md^2\})$ for a d-dimensional dataset containing m points. This is prohibitively slow, especially at scale.

Subsequently, we ask: can we take advantage of the low intrinsic dimensionality of highly structured time series to avoid the computational overhead of PCA via SVD while still retaining its utility? Our insight is that the low intrinsic dimensionality of these highly structured datasets leads to *redundancy* that can be exploited via sampling. Instead of running PCA via SVD on the full dataset, we can frequently achieve the same quality basis by performing PCA via SVD on a small subset. We empirically demonstrate that samples as small as 0.39% of the dataset (average: 4.15% over the 18 largest datasets in [13]) are sufficient, yielding speedups of up to 100× (average: 5.5×) over naïve computation over the full dataset.

To exploit this opportunity for sample-based PCA, we develop DROP (Dimensionality Reduction OPtimizer), a new progressive sampling strategy for efficiently computing a high-quality low-dimensional basis for a given time series dataset. Given a time series, distance metric, and accuracy target (e.g.,"preserve average pairwise Euclidean distance within 5%"), DROP returns a low-dimensional basis that achieves the accuracy target. DROP's core contribution is in finding this basis efficiently, by adopting techniques from online aggregation and progressive sampling to iteratively improve an estimate of the true basis, thus performing PCA on a series of increasingly large samples until convergence.

There are three key challenges in realizing this functionality:

First, PCA is guaranteed to find the optimal orthogonal basis with respect to the *Frobenius norm*, an element-wise $\mathcal{L}_2$-norm over matrices [66], whereas many popular analytics and data mining tasks (e.g., k-NN [22], k-Means [34], Kernel Density Estimation [69]),

ACM ISBN 978-x-xxxx-xxxx-x/YY/MM.
https://doi.org/10.1145/nnnnnnn.nnnnnnn

require preservation of pairwise distances of data points, referred to in [19] as the Tightness of Lower Bounds, or *TLB* (Equation 1). Thus, even if we find a good low-dimensional basis that preserves the Frobenius norm, this basis is not guaranteed to preserve the *TLB*. Naïvely computing the *TLB* requires $O(m^2 d)$ computation over the entire dataset—the same as PCA via SVD if $m < d$. To circumvent this overhead while still providing statistical guarantees, DROP adapts techniques from approximate query processing and computes a faster, novel sample-based *TLB* approximation.

Second, there are two ways to sample from a given time series dataset: sampling dimensions from each data point, and sampling data points from the entire dataset. The theoretical statistics and computer science literature offers suggestions for each type of sampling in isolation [33, 52]. DROP combines both for maximum effect, both performing random projections of each data point while also sampling from the full dataset. Beyond combining these approaches, DROP's key innovation is in determining *how much* to sample via progressive sampling. DROP also reuses work across samples via biased sampling, ensuring that data points with particularly poor fit are represented in future samples.

Third, DROP must balance dimensionality and runtime. Dimensionality reduction is typically employed as a pre-processing step in analytics pipelines, and downstream operators are often willing to trade a slightly higher-dimensional basis for faster pre-processing. For example, covariance matrix estimation runs in time quadratic in dimension [7]. Therefore, if DROP is used prior to covariance estimation, and DROP can find a 10% smaller dimensional suitable basis by running twice as long (i.e., processing more samples), then it may be faster overall to spend the time computing this smaller basis. However, if DROP's downstream task is similarity search, which exhibits runtime linear in dimension [34], then running twice as long may in fact *increase* total runtime. To navigate this trade-off, DROP accepts a workload-specific utility function and adapts techniques from progress estimation to perform online optimization of the entire, end-to-end analytics pipeline runtime.

In adapting techniques from approximate query processing for the problem of dimensionality reduction, DROP offers a practical and powerful tool for dimensionality reduction of time series data. For highly structured time series, DROP can uncover the optimal basis in running time that is *independent* of the actual dataset size and without requiring the user to specify the intrinsic dimensionality of the dataset a priori; instead, DROP discovers it. In summary, we make the following contributions in this work:

- We extend the study of [19] to consider PCA. We find that classical methods for PCA provide bases that are often over 2× more effective at dimensionality reduction but are up to 713× slower to compute than alternatives from [19].
- We present DROP, an online optimizer for dimensionality reduction that uses sample-based techniques to automatically determine the intrinsic dimensionality of and obtain an accurate low-dimensional representation of a given time series dataset. We show that as little as 2% of time series data suffices to preserve pairwise distances within 2%, providing a 55.6× reduction in dimension.
- We present optimizations based on online aggregation and progress estimation that enable order of magnitude speedups over classic methods for PCA via SVD and faster end-to-end execution than these techniques on real analytics pipelines.

The remainder of the paper is structured as follows. Section 2 provides a formal introduction to dimensionality reduction and performs an empirical comparison of existing dimensionality reduction operators. Section 3 presents the DROP optimizer and optimizations. Section 4 evaluates DROP's result quality and execution time. Section 5 discusses related work, and Section 6 concludes.

2 BACKGROUND AND COMPARISON

In this section, we provide background on the problem of dimensionality reduction, the *tightness of lower bounds* (*TLB*)—the distance metric we focus on for the majority of this paper (§ 2.1)—and Principal Component Analysis (§ 2.2). We revisit a prior empirical comparison of several dimensionality reduction methods [19] with respect to both runtime and *TLB* (§ 2.3) to motivate our study of efficient dimensionality reduction methods.

2.1 Dimensionality Reduction

Dimensionality reduction is a classic problem in statistics, machine learning, and data mining, and refers to finding a low-dimensional subspace within a dataset that preserves properties of interest, such as distance or similarity between data points [16, 26].

More formally, consider a set of m real-valued, d-dimensional vectors, $x_i \in \mathbb{R}^d$. We can represent this dataset as a matrix $X \in \mathbb{R}^{m \times d}$, where each row i corresponds to vector x_i. Our goal in dimensionality reduction is to compute a transformation function that maps each point x_i to a new *basis*, $\tilde{x}_i \in \mathbb{R}^k$ where $k \leq d$, or $T : \mathbb{R}^d \rightarrow \mathbb{R}^k$, such that the data contained in this basis preserves some *metric*, or property of interest P, e.g., pairwise Euclidean distance (as below). By applying the transformation T to all points in X, we obtain a matrix $\tilde{X}$ in the new basis, or $\mathbb{R}^{m \times k}$. All transformations we consider are contractive, in that pairwise distances in the new basis are always less than or equal to those in the original basis.

As an example transformation, one of the simplest methods for performing dimensionality reduction is to employ *random projections*. To transform from dimension d to dimension k, first choose a set of k d-dimensional vectors at random (e.g., from the unit ball) to form a projection matrix $T \in \mathbb{R}^{k \times d}$. Then transform the data matrix as $\tilde{X} = XT^\intercal$ [1]. Each randomly-chosen d-dimensional vector specifies a linear measurement, or combination, of each vector x_i; taking k of these measurements per data point yields a k-dimensional vector. Classical results from statistics [1] show that random projections can preserve pairwise distances between vectors. In this work, we will focus on a different dimensionality reduction technique (Principal Component Analysis, PCA [7]) that also applies a linear transformation to the input data. However, PCA's transformation matrix is not chosen randomly, but is instead chosen in a data-dependent manner.

Dimensionality reduction techniques are optimized for various choices of properties.Techniques such as Locality Sensitive Hashing [30] can preserve distance metrics such as Hamming distance and Jaccard similarity. PCA seeks to preserve a data matrix property known as the Frobenius norm; however, we will show how to adapt PCA to a specific metric from the time series literature.

We focus on a property that is extremely popular in the time series similarity search: the *tightness of lower bounds* (*TLB*) [19, 24, 42]. The *TLB* measures the average pairwise Euclidean ($\mathcal{L}_2$) distance between pairs of points in the transformed space compared to pairs of points in the original space. Thus, *TLB* measures how well a given dimensionality reduction transformation preserves pairwise distances across points:

$$TLB = \frac{2}{m(m-1)} \sum_{i<j} \frac{\|\tilde{x}_i, \tilde{x}_j\|_2}{\|x_i, x_j\|_2} \quad (1)$$

Intuitively, as we consider contractive transformations, if *TLB* is preserved (close to 1), then nearby points remain nearby and far away points remain far away. A *TLB* of 0.99 means that on average, distances in the low-dimensional space are within 1% of the distances in the original space. Exact *TLB* computation requires computing all-pairs distance—or $O(m^2)$ distance computations—which rivals or exceeds the computational complexity of many downstream analytics tasks. Therefore, in this paper (like [19]), we consider an approximate *TLB*; we measure *TLB* at a given confidence level (e.g., *TLB* at 95% confidence).

In tasks such as similarity search, we can first apply a *TLB*-preserving dimensionality reduction technique to reduce the dimension of input data, then build an index in this lower dimensional space to run similarity search queries. This methodology, which dates to the 1990s in the GEMINI framework [24], is the basis for a wide range of popular similarity search procedures and extensions in the data mining and machine learning communities [3, 9, 34, 41, 43, 47, 61, 75]; several empirical studies including [19] illustrate the relationship between *TLB* and similarity search performance and accuracy.

2.2 Principal Component Analysis

Principal Component Analysis (PCA) is a core analytics task in statistics, machine learning, and data mining (§ 5) PCA identifies a new orthogonal basis for a given dataset—i.e., a set of vectors that are orthogonal to one another—that optimally captures its directions of highest variance. In this work, we focus on dimensionality reduction via PCA, as PCA empirically finds a lower-dimensional *TLB*-preserving representation than conventional alternatives.

Naïvely implemented, PCA often relies on a black-box Singular Value Decomposition (SVD) routine [66], which provides the matrix decomposition $X = U\Sigma V^\top$. Given a data matrix X, PCA via SVD forms the PCA transformation matrix $T : \mathbb{R}^d \to \mathbb{R}^k$ by first subtracting each column in X by the column's mean to obtain C_X ($\mathbf{1}^\top C_X = \mathbf{0}$). The first k right singular vectors of C_X (first k columns of V from computing the SVD of C_X) comprise T. Many implementations of SVD provide a *truncated SVD* routine that performs this truncation to the first k columns [66]. A sample implementation of PCA using a truncated SVD operator is provided in Algorithm 1.

Algorithm 1 PCA via truncated SVD

Inputs:
$X \in \mathbb{R}^{m_1 \times d}$: training data matrix
$Y \in \mathbb{R}^{m_2 \times d}$: data matrix to transform
$k \in \mathbb{Z}_+$: desired dimensionality of transformed data
SVD-T: any truncated SVD algorithm

function FIT(X):
  $\bar{X}$ = columnMeans(X)
  $C_X = X - \bar{X}$ ▷ $C_X \in \mathbb{R}^{m_1 \times d}$
  Store: $\bar{X}, C_A$
function TRANSFORM(Y, k, SVD-T):
  U, Σ, V^T = SVD-T(C_X, k) ▷ $V \in \mathbb{R}^{d \times k}$
  $C_Y = Y - \bar{X}$ ▷ $C_Y \in \mathbb{R}^{m_2 \times d}$
  Store: V ▷ Cache for repeated use
return $C_Y V$

2.3 Measurement Study

To motivate our study of practical methods for dimensionality reduction, we revisit an influential study of time series dimensionality reduction techniques appearing in VLDB 2008 [19]. Via empirical evaluation of eight dimensionality reduction techniques on a suite of datasets from the gold standard UCR Time Series Classification Archive [13], the authors conclude that "the tightness of lower bounding... of the different representation methods for time series data have, for the most part, very little difference on various data sets." The study found that these eight dimensionality reduction methods were equally powerful in reducing the dimensionality of the time series data. This implies that for a given target dimensionality k, all methods achieve similar *TLB*, and, equivalently, for a given target *TLB*, all methods require similar number of dimensions.

While this prior study provides a useful comparison of several dimensionality reduction techniques, the authors left two aspects of dimensionality reduction for future investigation, which we revisit here. First, running time was not a focus of the prior study, which, as the authors note, is critical as data volumes and data dimension continue to increase. Second, the authors did not consider the use of PCA, on the grounds that PCA is "untenable for large data sets." While this second concern is valid, we sought to understand the gap between the quality of techniques explored in [19] and PCA.

To investigate these aspects, we repeated a subset of the experimental evaluation of [19] while also measuring runtime and including results from PCA. In addition to PCA, we report results using two methods from [19]; as the remainder exhibited "very little difference," we chose two of the fastest: Fast Fourier Transform (FFT) and Piecewise Aggregate Approximation (PAA). Section 4 provides additional details regarding experimental setup.

We report the minimum dimensionality (k) achieved by each technique subject to a constraint on *TLB* in Table 6; Figure 1 illustrates this graphically. On average, across 80 datasets, for *TLB*s of 0.99, 0.90, and 0.75, PCA provides bases that are over twice as small as FFT and PAA. For a *TLB* of 0.75, PCA is able to reduce the average dimensionality to just 4% of the original input space. As Table 6 illustrates, the exact margin between PCA and alternatives was dataset-dependent, but PCA was more effective at dimensionality reduction than PAA and FFT across all datasets. That is, by extracting the directions of highest variance first, PCA is able to preserve more of the pairwise distances within a dataset using fewer dimensions. To better understand this phenomenon, Figure 3 depicts the normalized spectrum (set of eigenvalues) of the data (Figure 3). Data with a rapid drop-off in spectrum (as in a majority of the 80 time series we

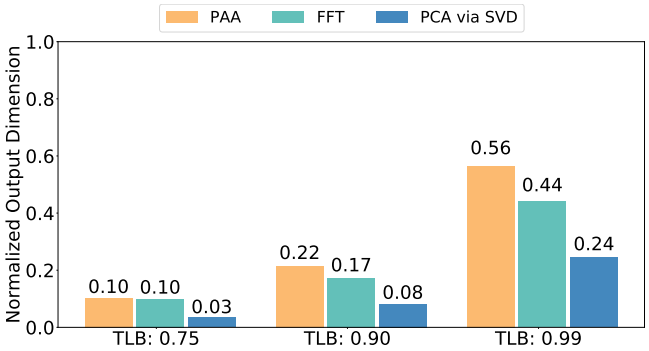

Figure 1: Required output dimension for target TLB, normalized by input dimension. Average over all datasets (N=80).

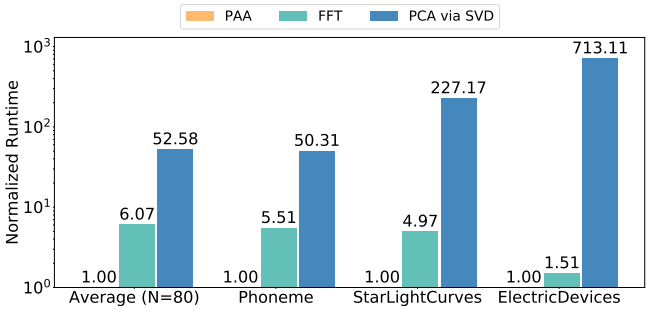

Figure 2: Runtime Comparison of PAA, FFT, PCA, each normalized to PAA runtime

study) implies the data is intrinsically low-dimensional, and PCA is able to identify this low-dimensional basis.

However, PCA's accuracy comes at a price: as Figure 2 illustrates, PCA is on average over 52 times slowerllclahan PAA and over 8 times slower than FFT. This substantiates [19]'s observation that, as classically implemented, PCA is in fact incredibly slow to run compared to alternatives. Theory also agrees: PCA via SVD requires an expensive $O(\min\{m^2d, md^2\})$ running time, which scales poorly with input data size, particularly when compared to methods such as PAA ($O(md)$) and FFT ($O(md \log d)$).

In summary, PCA offers substantially more effective dimensionality reduction than alternative techniques, but with a substantial computational overhead. Therefore, in this paper, we ask: is it possible to retain PCA's ability to provide effective TLB-preserving dimensionality reduction without incurring such an expensive computational overhead? By combining techniques from online query processing and progressive sampling, we can.

3 DROP

While PCA consistently uncovers high-quality low-dimensional subspaces for most time series, conventional implementations of PCA (via SVD) are prohibitively expensive for large, high-dimensional datasets. To bridge this gap between quality and efficiency, we present DROP, a Dimensionality Reduction OPtimizer. Given a time series and desired accuracy (in terms of TLB), DROP automatically produces a low-dimensional transformation that maintains the

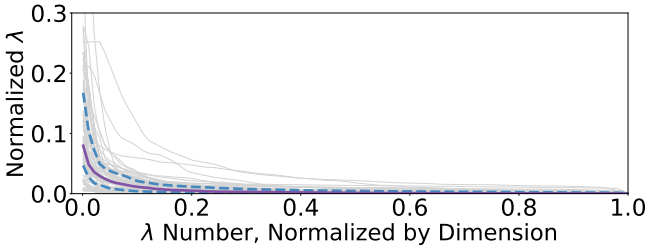

Figure 3: Normalized Time Series Data Spectrum: Spectrum of each of the considered 80 UCR time series, normalized by their data length, along with the 50^{th}, 25^{th}, and 75^{th} percentiles. A data's spectrum refers to its eigenvalues plotted in order of decreasing magnitude, normalized by the sum of all eigenvalues. A rapid falloff in spectrum indicates low intrinsic dimensionality, as most of the data's variance is "captured" by the first few eigenvalues.

Symbol	Description	Type
X	Input dataset	$\mathbb{R}^{m\times d}$
m	Number of input data points	$\mathbb{Z}_+$
d	Input data dimension	$\mathbb{Z}_+$
B	Target TLB preservation	$0 < \mathbb{R} \leq 1$
$C_m(d)$	Downstream cost function	$\mathbb{Z}_+ \rightarrow \mathbb{R}_+$
R	Total DROP runtime	$\mathbb{R}_+$
c	Confidence level for TLB preservation	$\mathbb{R}$
T_k	DROP output k-dimensional transformation	$\mathbb{R}^{m\times k}$
i	Current DROP iteration	$\mathbb{Z}_+$

Table 1: DROP Algorithm Notation.

TLB bound without the computational expense of classical PCA via SVD. DROP allows users to smoothly trade off between reduced dimensionality and runtime by specifying a cost function that relates dimensionality and time; one user may wish to obtain a low-quality basis quickly for exploratory analysis, weighing time much more than dimensionality, while another may wish to obtain a high-quality basis for downstream analytics, weighing dimensionality much more than time. DROP subsequently optimizes the user-specified utility function subject to the TLB constraint.

DROP's key insight is that techniques from approximate query processing and progressive sampling can help avoid the cost of computing a full SVD for PCA. While running SVD over a large dataset is incredibly expensive, computing an SVD over a small subset of this data can be quadratically cheaper. Further, as many time series datasets possess low intrinsic dimensionality, they are amenable to aggressive sample-based approximation—a small number of samples suffices to capture much of the "interesting" behavior in the data. Hence, just as computing an average over a sample is often "good enough" in relational analytics such as online aggregation, we can often compute a TLB-preserving low-dimensional basis using a sample (or, as in DROP, a sequence of increasingly large samples).

We now provide DROP's formal problem statement (§ 3.1) and overall design (§ 3.2), then describe each component in detail (§§ 3.3-3.5). An overview of notation used in this section is in Table 1.

3.1 DROP Problem Statement

DROP is an optimizer that automatically produces a dimensionality reduction transformation tuned to both a given dataset and a given accuracy constraint. As input, DROP takes a set of data points, each representing an interval of time from a time series, as well as a TLB constraint, B. DROP then produces a dimensionality reduction function in the form of a transformation matrix that satisfies the TLB constraint to a specified degree of confidence (default 95%) when applied to the input data. In this way, DROP acts as an analytics preprocessor that reduces a dataset's dimensionality while preserving distances to a specified level.

The highest-quality dimensionality reduction (lowest dimensionality for a target TLB) is almost always the most computationally expensive: running PCA via SVD over all of the data will produce a high-quality reduction but will be expensive. In some cases, such a high-quality reduction is desired. In many other cases, such as when DROP is used as a component of larger analytics workflows, it can be advantageous to return a transformation of a higher dimension than would be achieved with full SVD, but completes faster.

DROP captures this trade-off between reduced dimensionality and runtime using a third input parameter: a cost function that trades-off dimension and time. Users specify a cost function that weights time and dimensionality based on how sensitive to each their downstream application may be. DROP provides a default cost function tuned to the runtime of k-NN classification, relating runtime as $C_m = O(m^2 d)$, hence seeking to equalize the time taken by DROP's dimensionality reduction, and projected k-NN runtime.

More formally, denoting DROP's runtime as R, we define the DROP optimization problem as follows:

Problem 3.1. *Given a dataset $X \in \mathbb{R}^{m \times d}$, TLB constraint $B \in (0, 1]$ with confidence c, and cost function $C_m : \mathbb{Z}_+ \to \mathbb{R}_+$, find a transformation matrix $T_k \in \mathbb{R}^{d \times k}$ that minimizes $R + C_m(k)$ s.t. $TLB(XT_k) \geq B$ with confidence c.*

Intuitively, DROP's goal is to minimize the cost incurred by the cost function ($C_m(k)$, monotonically increasing in k) by finding the best possible transformation (T_k), while accounting for the time required to compute the transformation (R). In this way, DROP balances user preferences between dimensionality and runtime.

We now describe how DROP optimizes this objective.

3.2 DROP Architecture

DROP is composed of the following three steps:

Step 1: Sample (Figure 4A): In its i^{th} iteration, DROP samples a variable proportion p_i of the input data set. DROP performs importance sampling based on the results of prior steps, thus reusing work across iterations (§3.3, Algorithm 2 Line 5).

Step 2: Compute Basis (Figure 4B): DROP computes a candidate low-dimensional basis for the sample. To evaluate the quality of the basis, DROP computes an estimate of the TLB using a confidence-interval-based approximation (§3.4, Algorithm 2 Line 6). Instead of computing each candidate basis with a standard SVD subroutine, DROP exploits the highly structured nature of time series by using a fast, randomized SVD method (§3.4.1).

Step 3: Check Progress (Figure 4C): DROP determines whether to terminate and return the best basis found thus far, or continue iterating to find a better metric-preserving basis. In order to enable this, DROP performs progress estimation to minimize the objective function (§3.5, Algorithm 2 Line 8).

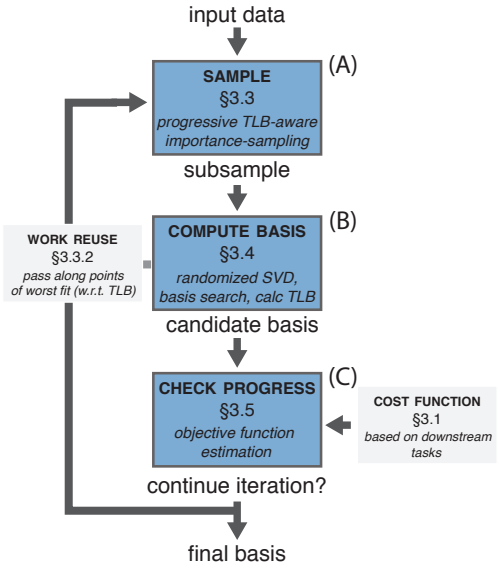

Figure 4: High-level DROP Architecture

Algorithm 2 DROP Algorithm

Input:
X: data matrix
B: target metric preservation level; default $TLB = 0.98$
C_m: cost of downstream operations; default tuned to k-NN

Output:
T_k: k-dimensional transformation matrix

```
1: function DROP(X, B, C_m):
2:     Initialize: i = 0; k_0 = ∞        ▷ iteration and current basis size
3:     do
4:         CLOCK.RESTART
5:         X_i = SAMPLE(X, SAMPLE-SCHEDULE(i))          ▷ § 3.3
6:         T_{k_i} = COMPUTE-BASIS(X, X_i, B)           ▷ § 3.4
7:         r_i = CLOCK.ELAPSED                          ▷ R = ∑_i r_i
8:     while CHECK-PROGRESS(C_m, k_i, r_i, i++)         ▷ § 3.5
9: return T_{k_i}
```

3.3 Step 1: Sample

Instead of processing all of the input data at once as in conventional PCA via SVD, DROP seeks to compute a high-quality basis using a sample of the data. If the sample is sufficient to compute a high-quality basis, DROP can terminate. If not, DROP samples additional data from the input data and computes a new basis. Thus, DROP iteratively samples increasing subsets of the input data.

This iterative approach leads to two design decisions. First, how much should DROP sample at each iteration; second, how can DROP

utilize information from prior iterations in sampling? DROP addresses these questions in turn by employing progressive sampling (§3.3.1) and importance sampling (§3.3.2)

3.3.1 Progressive Sampling. How large a sample suffices to compute a high-quality basis? It is difficult to determine a priori how many samples are required. For example, consider the following two scenarios, where the input time series are generated from room temperature readings. In a first scenario, the temperature is precisely controlled by a heating system to remain at 73 degrees at all times. In this scenario, a single sample is sufficient to characterize all data points. However, consider a second scenario, in which we are given temperature readings from a room that fluctuates based on external weather conditions. Many more samples will be required to effectively characterize the set of all points; however, the dataset will likely contain a small number of data points that are sufficient to characterize general behavior. For instance, within the span of a few weeks, temperature may follow similar daily cycles.

In the worst case, the input data will have no implicit or regular structure, and all data points and dimensions may be required to fully capture the data variance (and appropriate *TLB*-preserving basis). For example, effectively characterizing the data set will require near all data points if a sensor malfunctions and records random, independent values. DROP progressively samples larger and larger samples with each iteration according to a specified schedule; in Section 4, we find that a single schedule of ten steps, in which data is processed no more than twice, works well across all datasets.

3.3.2 Sampling Technique. As a baseline, DROP samples uniformly without replacement from the input data. However, as DROP is an iterative algorithm, a natural opportunity for optimization arises: information learned from previous iterations can provide insight into the underlying data distribution.

Therefore, as DROP computes PCA over a sample of the input data and generates a candidate low-dimensional basis at each iteration, DROP can determine which points are most misrepresented with respect to the transformation generated by the current data sample. Concretely, given a candidate basis and *TLB* estimate, DROP ensures the points in the bottom q^{th} percentile of *TLB* (i.e., worst fit) are passed along to the next iteration's sample (by default, $q = 10$).

DROP then populates the remainder of the sample with points drawn uniformly from the rest of the population.

DROP's method of sampling, where misrepresented points are more likely to appear in future samples, is a form of *importance sampling* [60], or a method that helps reduce variance when estimating a quantity via sampling (here, most closely related to *hard example mining* [64]), adapted to the *TLB*-preservation setting. We considered more exotic sampling procedures (e.g., using coresets [14]) but found that the lightweight computational footprint of this importance sampling struck a balance for many DROP cost functions. We quantify the benefit of importance sampling in Section 4.

3.4 Step 2: Compute Basis

Given a data sample from the first step (§ 3.3), DROP uses PCA to compute a candidate basis that is as low-dimensional as possible while still preserving the specified *TLB* constraint. There are two main design decisions DROP must address in this step: first, how should DROP compute candidate transformations; second, how should DROP efficiently search the space of all PCA transformations to identify the lowest-dimensional *TLB*-preserving basis.

We adopt state-of-the-art randomized methods for PCA to address the former problem of computing candidate transformations (§3.4.1). However, the latter—efficient basis validation—is a point of concern: as we have discussed, naïvely computing the full *TLB* is as expensive as full SVD. Therefore, DROP adopts a novel *TLB* calculation (§3.4.2) and search procedure (§3.4.3) that circumvents this cost by employing adaptive sampling.

3.4.1 Basis Fitting. Recall that PCA via SVD is remarkably effective at producing high-quality bases for time series (§ 2). Hence, DROP's core time series dimensionality reduction operator is PCA.

The most straightforward means of implementing PCA is to perform SVD over the sample (§2.2). There are many suitable libraries for this task—many of which are highly optimized—and therefore this strategy is easy to implement.

However, over the past several years, the theoretical computer science and statistics communities have developed a variety of optimized PCA implementations that improve performance by exploiting randomization (§5). One of the most advanced of these methods is a randomized SVD algorithm (SVD-Halko) by Halko, Martinsson, and Tropp that computes an approximate rank-k factorization (truncated SVD) of a data matrix (Algorithm 3). SVD-Halko computes a $d \times k$ random projection matrix Ω, multiplies this matrix by the centered data matrix C_X, and then runs SVD on $C_X\Omega$ (optionally running power iteration to reduce error) . Perhaps surprisingly, theoretical and empirical studies show that SVD-Halko achieves a high-quality approximation of the best k-dimensional subspace, as produced by full SVD, without the expense—for a matrix $C_X \in \mathbb{R}^{m\times d}$, only $O(mdk + k^2(m + d))$ time. DROP combines SVD-Halko's column-level sampling *with* row-level sampling to further reduce its runtime; we are unaware of such a combination in the literature.

Algorithm 3 SVD-HALKO

Input:
C_X: centered data matrix
k: size of low-dimensional subspace
p: small increase in subspace size; default: 5
q: number of power iteration steps; default: 1

function SVD-HALKO(C_X, k, p, q):
  $\Omega \in \mathbb{R}^{d\times(k+p)}$ ▷ Random Gaussian matrix
  $Y = (C_X C_X^\top)^q C_X \Omega$ ▷ Power iteration to reduce error
  $Q, R \leftarrow \text{QR}(Y)$ ▷ QR-Factorization
  $B = Q^T C_X$
  $\tilde{U}\Sigma V^T \leftarrow \text{SVD}(B)$
return first k columns of V ▷ PCA projection matrix

3.4.2 Basis Evaluation. Given a candidate k-dimensional basis, how can we efficiently determine if the basis preserves the desired *TLB*? As discussed, computing pairwise *TLB* for all data points requires $O(m^2 d)$ time. This computational overhead would overwhelm DROP's runtime: the runtime of brute-force *TLB* computation will dominate the runtime of computing PCA on a sample.

To mitigate this overhead, DROP adapts techniques from online aggregation and approximate query processing [35, 57]: instead of computing an exact *TLB*, DROP uses statistical sampling and confidence intervals to compute the *TLB* to arbitrary confidences. Given a candidate basis, DROP iteratively refines an estimate of the basis' *TLB* by repeatedly sampling pairs from the input data, transforming each pair into the new basis, then measuring the distortion of $\mathcal{L}_2$ distance between the pairs. By repeatedly computing this distortion for independently sampled pairs, DROP can iteratively refine its estimate until it is confident that the candidate basis satisfies the provided *TLB* constraint.

As the *TLB* is an average of random variables bounded from 0 to 1, DROP can rely on standard statistical bounds to perform this iterative estimation of the true *TLB*. Bounds that apply to the *TLB* and DROP's sampling procedure include Markov's inequality, Chebyshev's inequality, and Chernoff bounds, each offering tighter bounds [55]. DROP instead uses a computationally inexpensive estimate of the average *TLB* obtained via the Central Limit Theorem (similar to online aggregation [35]), computing the standard deviation of the sampled pairs' *TLB* measures and applying a Gaussian-based confidence interval to the sample according to the desired confidence. Concretely, if the lower bound of the computed confidence interval is greater than the target *TLB*, DROP concludes that the basis is a sufficiently good fit; if the upper bound of the computed confidence interval is less than the the target *TLB*, DROP concludes that the basis is not a sufficiently good fit. If the confidence interval overlaps the target *TLB*, DROP samples more pairs. This occurs in function EVALUATE-TLB, line 11 of Algorithm 4.

Therefore, for datasets with low variance, DROP is able to evaluate a candidate basis with few samples from the dataset. In practice, and especially for our target time series datasets, we found that DROP rarely uses more than 300 pairs in its *TLB* estimates (and often uses far fewer sampled pairs).

A related benefit of this *TLB* calculation is that DROP can use the computed *TLB*s for each pair in its *TLB* estimation routine for future iterations' basis sampling (§3.3.2). DROP can promote pairs with low *TLB* (and therefore poor fit) in this iteration's basis such that the pairs are more likely to appear in future basis computation samples; i.e., the worst pairs from the current iteration are passed on to future iterations as examples of "hard to fit" data points.

3.4.3 Basis Search. Given the sampled data, PCA routine, and *TLB* evaluation procedure, DROP must find the lowest-dimensional basis that achieves the target *TLB*. Per the previous section, DROP first computes a d-dimensional basis (i.e., of dimension equal to the input dimension) with PCA via SVD or SVD-Halko. With this basis, DROP must determine how many dimensions must be retained to preserve *TLB*. A naïve strategy would evaluate the *TLB* for every combination of the d basis vectors, requiring $d + \binom{d}{2} + \cdots + \binom{d}{d-1} + 1$ *TLB* evaluations. Instead, DROP exploits two key properties of PCA via SVD that allow it to avoid so many evaluations.

First, PCA via SVD produces an orthogonal linear transformation; that is, the first principal component explains the most variance in the dataset, the second explains the second most—subject to being orthogonal to the first—and so on. This means that once the transformation matrix for dimension d has been computed, the transformations for all dimensions k less than d are obtained by truncating the matrix. That is, given a PCA transformation matrix $V_1 \in \mathbb{R}^{d \times k_1}$, that that projects d-dimensional data to dimension k_1, the transformation matrix $V_1 \in \mathbb{R}^{d \times k_2}$ for $k_2 < k_1$ over the same training dataset is formed by taking the first k_2 columns of V_1.

Second, with respect to *TLB* preservation, the more principal components that are retained, the better the lower-dimensional representation in terms of *TLB*. Orthogonal transformations such as PCA preserve inner products. Therefore, a full PCA (where no dimensions are omitted) perfectly preserves $\mathcal{L}_2$-distance between data points. As the $\mathcal{L}_2$-distance is defined to be the squared sum of point-to-point differences (all positive terms), the more principal components retained, the closer the representation is to preserving the $\mathcal{L}_2$-distance.

Using the first property (i.e., of orthogonal linear transformations), DROP obtains all low-dimensional transformations for the sample from the previously computed d-dimensional basis. Using the second property (i.e., of monotonicity of principal components), DROP then runs binary search over these transformations to find the lowest-dimensional basis that attains the desired *TLB*. This occurs in function COMPUTE-BASIS, line 1 of Algorithm 4.

One concern with this approach is that computing the entire d-dimensional basis nullifies the benefit of using SVD-Halko (column-wise sampling). Ideally, the dimension of the best basis is known, obviating the need for binary search, and a d-dimensional SVD

Algorithm 4 Basis Evaluation and Search

Input:
X: sampled data matrix
B: target metric preservation level; default $TLB = 0.98$

1: **function** COMPUTE-BASIS(X, X_iB):
2: PCA.FIT(X_i) ▷ as in Algorithm 1
3: Initialize: high = k_{i-1}; low = 0; $k_i = \frac{1}{2}$(low + high); $B_i = 0$
4: **while** (low ! = high) **do**
5: T_{k_i}, B_i = EVALUATE-TLB(X, B, k_i)
6: **if** $B_i \leq B$ **then** low = $k_i + 1$
7: **else** high = k_i
8: $k_i = \frac{1}{2}$(low + high)
9: T_{k_i} = cached k_i-dimensional PCA transform
10: **return** T_{k_i}

11: **function** EVALUATE-TLB(X, B, k):
12: numPairs = $\frac{1}{2}M(M-1)$
13: $p = 100$ ▷ number of pairs to check metric preservation
14: **while** ($p <$ numPairs) **do**
15: B_i, B_{lo}, B_{hi} = TLB(X, p, k) ▷ Mean and 95%-CI *TLB*
16: **if** ($B_{lo} > B$ or $B_{hi} < B$) **then break**
17: **else** pairs ×= 2
18: **return** B_i

19: **function** TLB(X, p, k):
20: **return** mean and 95%-CI of the *TLB* after transforming p d-dimensional pairs of points from X to dimension k. PCA.TRANSFORM caches the highest transformation computed thus far to limit recomputation of the transformation matrix.

computation—but in practice, this information is rarely known a priori. To overcome this need to compute a d-dimensional basis with each iteration, as with importance sampling (§3.3.2), DROP's iterative architecture allows us to exploit information from previous iterations. If DROP has previously found a candidate TLB-preserving basis of size $d' < d$ in prior iterations, then DROP performs SVD-Halko to only compute d' components. This both reduces the space of low-dimensional bases to consider, and allows for more efficient SVD computation for future iterations with more samples (via truncated SVD methods, such as SVD-Halko).

3.5 Step 3: Check Progress

Given a basis computed and validated in step two, DROP determines whether to continue searching for a better basis by drawing a larger sample and performing another iteration of steps one through three, or to terminate, returning the basis it has already found. To do so, DROP employs the objective function defined in its problem statement (Problem 3.1), which balances DROP computation overhead with achieved dimensionality of the lowest-dimensional TLB-preserving basis. To minimize this objective function, DROP must address two design decisions. First, how should DROP estimate the cost and benefit of future iterations—measured in terms of runtime and dimensionality—compared to early termination; and, second, how can DROP use these estimates to perform online optimization of its objective function? In this section, we describe DROP's approach to each, which combines online progress estimation and convex optimization.

3.5.1 Progress Estimation. Recall that DROP's objective function minimizes $R + C_m(k)$ s.t. $TLB(XT_k) \geq B$, with R denoting DROP's total runtime, T_k the k-dimensional TLB-preserving transformation of data X returned by DROP, and $C_m(k)$ the dimensionality-runtime cost function. Therefore, given a basis T_k^i computed in step two of DROP's i^{th}, DROP evaluates the value of this objective function by substituting its elapsed runtime for R and T_k^i for T_k. We denote the value of the objective at the end of iteration i as obj_i. To decide whether to continue iterating to find an improved basis, DROP determine if $obj_{i+1} < obj_i$ (and, more generally, as we discuss below, $obj_j < obj_i$ for $j > i$). If the objective function will decrease in the next iteration, DROP should continue iterating.

However, the value of obj_{i+1} depends on two unknown quantities: the runtime required for iteration $i+1$ (r_{i+1}) and the dimensionality of the TLB-preserving basis produced by iteration $i+1$ (k_{i+1}). Because DROP cannot directly measure r_{i+1} or k_{i+1} without performing iteration $i+1$, DROP instead *estimates* these quantities by performing online progress estimation.

DROP performs online parametric fitting via polynomial interpolation to compute future values based on prior iterates for r_i and k_i. By default, given a sample of size m_i in iteration i, DROP performs linear-interpolation-based estimation for k_{i+1}:

$$\hat{k}_{i+1} = k_i + \frac{k_i - k_{i-1}}{m_i - m_{i-1}}(m_{i+1} - m_i)$$

The estimate of r_{i+1} follows directly, as:

$$\hat{r}_{i+1} = r_i + \frac{r_i - r_{i-1}}{m_i - m_{i-1}}(m_{i+1} - m_i)$$

DROP can also substitute more sophisticated estimators and other progress estimation functions; however, in practice, we found this sufficient for accurate and efficient estimation.

3.5.2 Minimizing DROP's Objective. Given the ability to estimate the next iteration's runtime ($\hat{r}_{i+1}$) and resulting basis dimensionality ($\hat{k}_{i+1}$), DROP can estimate the optimal stopping point that minimizes the DROP objective function. Notably, we can prove that under mild assumptions, DROP's objective function is convex, implying that DROP should terminate if its objective function estimate for the next iteration is greater than its current objective function value. That is, if $obj_i < obj_j, i < j$, then there is no $k > i$ such that $obj_k < obj_i$, so DROP should terminate as soon as $obj_i < \widehat{obj}_{i+1}$, where $\widehat{obj}_{i+1}$ represents the estimated objective function for the next iteration. This gives us a simple, greedy stopping criterion used by CHECK-PROGRESS in Algorithm 2 line 8:

$$\begin{aligned} obj_i &< \widehat{obj}_{i+1} \\ C_m(k_i) + \sum_{j=0}^{i} r_j &< C_m(\hat{k}_{i+1}) + \sum_{j=0}^{i} r_j + \hat{r}_{i+1} \\ C_m(k_i) - C_m(\hat{k}_{i+1}) &< \hat{r}_{i+1} \end{aligned} \tag{2}$$

According to this criterion, DROP should terminate if the projected time to run an additional iteration of DROP exceeds the estimated benefit obtained in downstream tasks. This enables a simple policy for DROP's third step: estimate the next iteration's runtime and dimensionality per Section 3.5.1, and terminate by returning the current basis if the condition in Equation 2 is true.

We now proceed to show that under mild assumptions, DROP's objective is convex, and this local-minimum obtained from the next-iteration policy yields the optimal solution.

THEOREM 3.1. *Denote DROP's runtime after iteration i as R_i, and dimensionality of the TLB-preserving basis produced by DROP in iteration i as k_i. If $C_m(k)$ is convex and nondecreasing in k and k_i is a convex sequence in i, $obj_i = R_i + C_m(k_i)$ is convex in i.*

Theorem 3.1 states that given a convex, nondecreasing cost function, DROP's objective is convex. To examine this precondition, many cost functions, such as the runtime for analytics operators including k-NN ($O(m^2 d)$) are convex and nondecreasing in d. Further, we empirically find that larger samples result in smaller k_i, and this relationship between proportion of sampled points (and therefore iteration) decays roughly exponentially (convex).

We proceed to prove Theorem 3.1.

PROOF. The runtime of each iteration of DROP, r_i, is convex in i because each iteration of SVD-Halko requires time $O(mdk_i + k_i^2(m + d))$, which is convex in i. The sum of convex functions is also convex, so, given convexity of C_m, k_i, and R_i, we have that $R_i + C_m(k_i)$ is convex in i. □

3.6 Recap and Discussion

DROP combines database and machine learning techniques spanning online aggregation (§ 3.4.2), progress estimation (§ 3.5), progressive sampling (§§ 3.3, 3.4.2), and randomized PCA approximation (§ 3.4.1) for the first time that we are aware. DROP optimizes

the combination of runtime and dimensionality by repeating three steps: sampling, basis evaluation, and objective function estimation. As we demonstrate in our empirical evaluation (§4), this combination of sample-based query processing and randomized algorithms yields a substantially more scalable method for performing dimensionality reduction to accelerate end-to-end analytics pipelines.

4 EXPERIMENTS AND RESULTS

In this section we evaluate DROP's efficiency in dimensionality reduction along three dimensions: runtime, accuracy, and extensibility. We answer the following questions:

(1) How fast is DROP compared to alternative, non-sample-based PCA via SVD methods, and compared to an oracle? (§ 4.2)
(2) What is the effect of DROP's work reuse? (§ 4.2)
(3) Does DROP runtime scale with intrinsic dimensionality, and independently of data size? (§ 4.3)
(4) Can applying DROP as a pre-processor speed up end-to-end analytics pipelines including k-NN and clustering? (§ 4.4)
(5) Can DROP extend to data sets that are not time series? (§ 4.5)

Our results demonstrate that DROP obtains a *TLB*-preserving low-dimensional representation up to 50× faster than PCA via SVD and up to 15.5× faster than PCA via SVD-Halko (average: 4.8× and 2.9× faster, respectively). We illustrate that DROP is finds a low-dimensional representation in runtime proportional to dataset's intrinsic dimensionality and independent of the dataset's size. DROP enables faster end-to-end execution for k-NN (max: 33×, average: 2.70×) and DBSCAN [23] (max: 12.5×, average: 1.25×)—as well as effective dimensionality reduction for structured image datasets.

4.1 Experimental Setup

Implementation. We implement DROP on top of the open-source MacroBase system [5] as an in-memory, batch-oriented feature transformation dataflow operator. Our DROP implementation is in Java and utilizes the Matrix-Toolkits-Java (MTJ) library for compute-intensive linear algebra operations including matrix multiply and SVD. To provide an apples-to-apples comparison between operators, we disable multithreading in MTJ. All of our source code used in this evaluation is available at http://anonymized-for-review.

Environment. We run experiments on a server with four Intel Xeon E7-4850 v3 2.20GHz CPUs and restrict our DROP code to run on a single core. The server contains 1TB of RAM although all methods utilize far less memory than is available. We report DROP runtime in isolation, excluding data loading and parsing time, and report averages from multiple trials.

Datasets. As a baseline for evaluation, we consider 80 time series from the UCR Time Series Classification Archive [13], considered the gold standard from the time series data mining community. We exclude datasets for which full SVD completes in shorter than 1 second, leaving 18 datasets remaining. In addition, we use the standard MNIST hand-written digits dataset [48] to demonstrate extensibility beyond time series data.

DROP Configuration. By default, we employ a cost function that models the running time of k-NN and clustering, scaling with

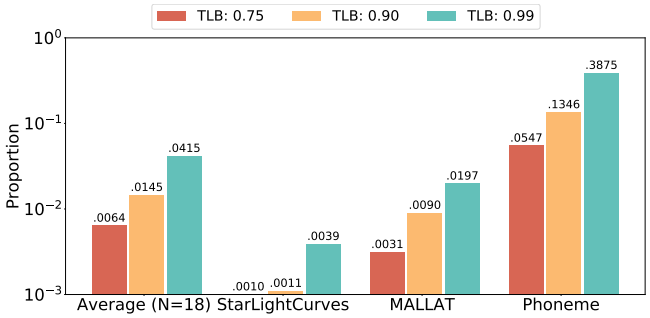

Figure 5: Proportion of data required for target *TLB*, when transforming to the PCA basis with output dimension (k) equal to input dimension (d).

$O(m^2d)$; in our end-to-end experiments below, we show this corresponds to minimizing the total time taken by both dimensionality reduction and k-NN/clustering, resulting in a target even split between reduction and analysis steps. We employ a default sampling schedule of [0.01, 0.02, 0.03, 0.04, 0.05, 0.10, 0.20, 0.30, 0.65, 1.00] for all time series; it is possible to optimize (and possibly overfit) this schedule for our target time series, but we sought to provide a conservative (and more general) schedule instead.

Baselines. We report runtime, accuracy, and reduced dimension compared to two methods utilizing non-sample-based PCA via SVD (via MTJ's built-in primitive) and SVD-Halko (implemented via MTJ), referred to as SVD and SVD-Halko, respectively. Each of these methods computes a transformation over the entire data, then performs binary search to identify the smallest dimensional basis that satisfies the target *TLB*. These methods complement those from our earlier study in Section 2.3 and represent a classic implementation of dimensionality reduction and an optimized implementation from the recent literature. In addition, we introduce an "oracle" baseline, which computes a transformation over the minimum proportion of data required to obtain a basis of the same size as binary searching with SVD (as above). This proportion is pre-computed offline for each dataset. We target a *TLB* of 0.98 by default and vary this in our sampling experiments in Section 4.2.

4.2 DROP Performance

Behavior under Sampling. In this section, we substantiate the use of sampling. We vary the target *TLB* while examining the minimum number of samples required to obtain a *TLB*-preserving basis with output dimension k equal to input dimension d. In this way, we isolate the effect of output basis size from data sampling. As Figure 5 illustrates, a small number of samples suffice to provide high-quality bases that preserve *TLB*. On average, across the 18 UCR time series datasets we consider, a sample of 0.64% of the input data is sufficient to obtain a *TLB* of 0.75, and a sample of size 4.15% is sufficient to attain a *TLB* of 0.99. Table 5 provides detailed results for all 80 datasets in the UCR time series archive.

The exact benefit of sampling is highly dataset-dependent. For example, the StarLightCurves dataset requires an extremely small number of samples to attain high *TLB*, while the Phoneme dataset

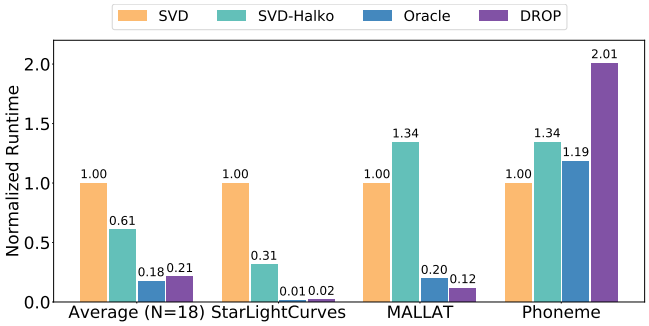

Figure 6: Dimensionality reduction time, normalized to SVD

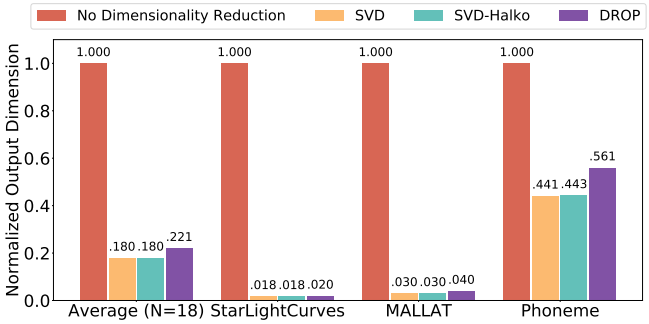

Figure 7: Output dimension, k, normalized to input dimension. DROP processes an average of 8.79% less data than oracle, resulting in slightly larger output dimension.

requires substantially more. In Table 5, we see that some smaller datasets, such as Earthquakes, require a sample of nearly 90%, but many of these datasets complete full SVD in less than 1 second. The overall trend demonstrates that for highly structured time series, sampling is a promising strategy for dimensionality reduction. However, as the minimum required sample size is not known a priori, DROP must perform adaptive sampling to determine when to stop sampling based on the input cost function, which we evaluate below.

Performance Comparison. Figure 6 illustrates that DROP is on average 4.76× faster than SVD with binary search, and 1.17× slower than the oracle approach where the necessary sample size is known a priori. Compared to the oracle strategy, DROP returns early, processing an average of 8.79% less data, but pays for this decreased use of data by returning a basis that is on average 1.23× larger than those found via SVD/Oracle (Figure 7). This slightly larger basis is due to DROP's default objective function, which seeks to equalize the time taken by dimensionality reduction and k-NN. Penalizing output dimension more would result in examining more of the data to provide smaller bases, at the cost of increased running time. DROP obtains speedups of up to 50× over SVD, as with StarLightCurves, but in the absolute worst-case, DROP is 2× slower than full SVD due to the choice of schedule, as with Phoneme. Further, as Figure 7 illustrates, Phoneme does not possess a low possess an intrinsic low dimensionality, resulting in poor performance from SVD-Halko-based implementations, affecting SVD-Halko, Oracle, and DROP in all experiments (noted in § 3.4.1).

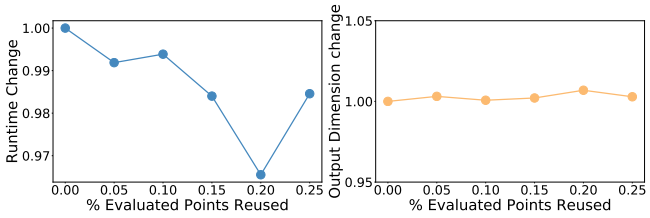

Figure 8: Effect of percentage of points used for work reuse on runtime and output dimension for DROP and SVD-Halko.

Work Reuse. To reuse work across iterations, DROP performs importance sampling based on the worst fit from previous iterations (§ 3.3.2). We quantify its benefit by varying the proportion of *TLB* evaluation points carried forward. Figure 8 illustrates the results. With its default of 10% reuse, DROP's runtime improves by approximately 1%. However, there is a trade-off: performing too much reuse increases runtime because more of the worst-fitting points are disproportionately likely to be sampled. Thus, on balance, we find that even a small amount of reuse can improve result speed.

4.3 Scalability

DROP processes only as much data as required to extract a basis that captures the intrinsic dimensionality of the dataset. For example, as we have discussed, data is generated by automated processes often grows much faster in size than intrinsic dimensionality; in extreme cases, a constant number of samples is required to fully characterize a dataset even as new time series are added.

To illustrate this phenomenon, we performed an experiment that increased dataset size while holding intrinsic dimensionality constant. We generate increasing data sizes by sampling linear combinations of sinusoids with random amplitude and phase shifts such that the intrinsic dimensionality remains fixed as 8 (i.e., data matrix is rank 8). Hence, the sample size an algorithm requires to uncover this dataset's intrinsic dimensionality is constant regardless of the full dataset size. As Figure 9 shows, using a fixed-size sampling schedule, DROP is able to find a 8-dimensional basis that preserves *TLB* to 0.98 within 102ms for dataset sizes up to 135K data points. Runtime is near constant, with small overhead due to sampling from larger datasets, and is 95× faster than binary search with SVD-Halko (9719ms), the faster of the two baseline algorithms. This near-constant runtime is due to DROP's ability to utilize random samples of the data (here, a sampling schedule that increases by 500 data points with each iteration). In contrast, PCA via SVD and SVD-Halko do not exploit the intrinsic dimensionality of the dataset and process all provided points, further illustrating the scalability and utility of sample-based dimensionality reduction.

4.4 End-to-End Analytics

In this section, we illustrate DROP's ability to optimize *end-to-end* analytics pipelines by trading off runtime and output dimensionality to decide when to stop sampling. We compare DROP's runtime and objective function to alternatives when running a k-NN single-neighbor retrieval task (referred to as the 2-NN retrieval task) and clustering using DBSCAN [23].

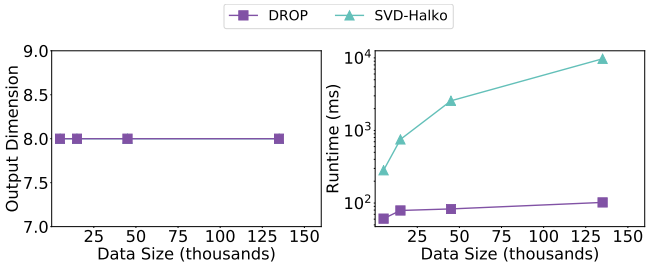

Figure 9: Effect of dataset size on time and output dimension (k), with constant intrinsic data dimensionality of 8

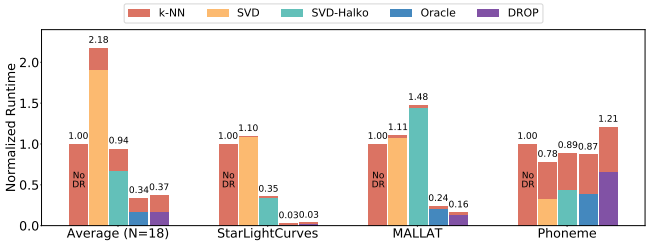

Figure 10: Average End-to-End k-NN Runtime, normalized to running on the raw data (i.e., no dimensionality reduction).

To validate DROP's utility in end-to-end analytics tasks, we evaluated the end-to-end runtime and accuracy of combining DROP with k-NN retrieval implemented in Cython as part of the scikit-learn package. We configured DROP to pre-process the k-NN inputs from the UCR Time Series datasets with a k-NN-specific cost function modeling k-NN runtime. We report combined DROP and 2-NN query runtime for the 18 largest UCR Time Series datasets in Table 3. Figure 10 illustrates the end-to-end runtime results, along with the proportion of time spent on k-NN versus dimensionality reduction. DROP enables end-to-end runtimes up to 33× faster than not running dimensionality reduction (2.7× on average), and are on average 5.9× faster than running the naïve SVD approach. As our cost function models the runtime of k-NN, we see that in each case, DROP attempts to equalize the amount of time taken in each stage.

To validate the quality of transformations returned by DROP, we compare points retrieved from the 2-NN retrieval task over the transformed data obtained via DROP and the baseline techniques, treating the results from running over the raw dataset as ground truth. As shown in Table 2 (complete results in Table 4), DROP is on average within 1% of our baselines (for *exact* classification, we could follow this retrieval with a verification step as in GEMINI [24] and follow-on work). Thus, by optimizing for the combination of pre-processing time with k-NN, DROP receives substantially faster but still accurate analytics results compared to simply running k-NN.

Sensitivity to Cost Function. A natural concern that arises from this evaluation is: how sensitive to specific cost function is DROP? To address this concern, we hold our cost function constant, and repeat our end-to-end experiments over another popular data analytics task—clustering with DBSCAN [23], also implemented in Cython as part of the scikit-learn package. Figure 12 illustrates the results.

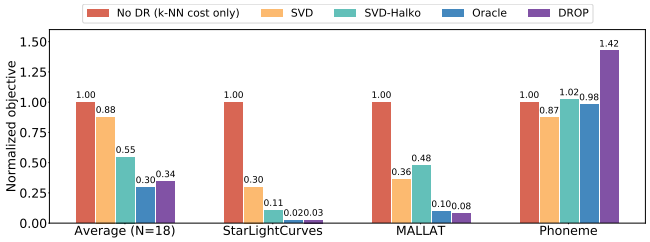

Figure 11: Objective value, normalized to no processing

	SVD	SVD-Halko	Oracle	DROP
Raw Average (n=18)	0.838	0.839	0.835	0.851
Relative Average (n=18)	1	1.002	0.998	1.016
StarLightCurves	1	1.052	1.061	1.059
MALLAT	1	1	1.056	1.075
Phoneme	1	1.005	0.802	0.799

Table 2: k-NN accuracy of reduced dimension data returned from each algorithm, treating k-NN over raw input data as ground truth. Relative values (bottom four rows) are normalized to the results of SVD+Binary Search.

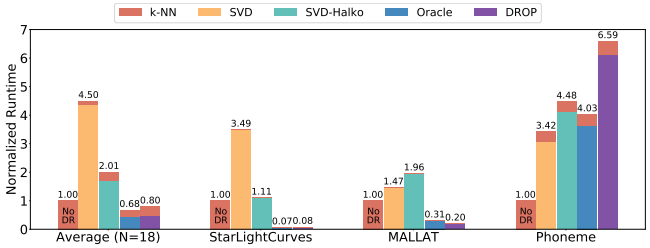

Figure 12: Average End-to-End DBSCAN Runtime, normalized to running on the raw data (i.e., no dimensionality reduction).

DROP provides a less significant improvement, just 1.25× on average (max: 12.5×) compared to not running dimensionality reduction. However, the trends seen in the previous plots hold, and DROP still outperforms other baseline techniques—on average, 5.63× SVD and 2.5× SVD-Halko with binary search.

4.5 Beyond Time Series

We examined a representative workload from image classification as a preliminary study of DROP's applicability beyond time series data. We repeat the sampling and k-NN retrieval experiments from Section 4.4 using the MNIST hand-written digit image dataset containing 70,000 images of dimension 784 (obtained by flattening each 28×28-dimensional image into a single vector [48], combining both the provided training and testing datasets).

The oracle strategy requires only 3.19% of the data, providing a 14.3× speedup over SVD-Halko (29143 versus 2042ms). As in the case of time series data, DROP examines 1.4% of the data, returning a basis 1.25× larger than the baseline techniques, but 28.2× faster

than SVD-Halko, and 1.98× faster than the oracle approach. Further, as in the previous workloads, the representation provided by DROP maintains the same accuracy on the 2-NN retrieval task when compared to the representations provided by the baseline strategies. These results provide compelling evidence that the sampling-based dimensionality reduction provided by DROP can be effective for other regularly structured, high-volume datasets as well.

5 RELATED WORK

Dimensionality Reduction. Dimensionality reduction is a classic operation in analytics [16, 26, 49, 66] and is well studied in the database [3, 9, 43, 61], data mining [42, 44, 45, 50], statistics and machine learning [18, 63], and theoretical computer science [32, 38] communities, with techniques for use in pre-processing [28, 34, 72], indexing [24, 41, 47, 75], and visualizing [51, 62, 68] datasets.

In this paper, inspired by [19], we study the problem of reducing the dimensionality of increasingly prevalent high-volume time series data [22]. We extend the study of [19] by considering Principal Component Analysis (PCA), the gold standard for linear dimensionality reduction in the statistics literature, which [19] previously been eschewed due to its expense at scale.

Recent breakthroughs in the theoretical statistics community provided new algorithms for PCA that promise substantial scalability improvements without compromising result quality [17, 18, 20, 33, 38, 52, 67]. Foremost among these algorithms are techniques for randomized SVD [33], which avoid computing SVD over the full data matrix and instead compute SVD over a projection of the data matrix; we adopt this technique as DROP's SVD operator. However, to the best of our knowledge, these techniques have not been empirically compared head-to-head with conventional dimensionality reduction approaches such as Piecewise Approximate Averaging [42], especially on real datasets. In addition, DROP *combines* these techniques with row-level sampling to provide additional benefit, performing SVD-Halko over an aggressively truncated input matrix.

Approximate Query Processing. A core problem in DROP is determining the appropriate sample size for both basis computation and basis evaluation. To address this challenge, we turned to the approximate query processing literature.

Inspired by approximate query processing engines [57] as in online aggregation [35], DROP performs progressive sampling, drawing only as many samples as required to attain a *TLB* threshold. Similar to prior work including [27], this threshold-based pruning strategy [37] provides runtime that is *data-dependent* as opposed to data-agnostic. In contrast with more general data dimensionality estimation methods [8], DROP optimizes for *TLB*. As we illustrated in Section 4, this strategy confers substantial runtime improvements.

DROP also leverages importance sampling to reuse work across iterations. The literature contains a wealth of techniques for this kind of biased sampling [4, 10], including sampling strategies that are aware of query histories [29] and storage hierarchies [59]. DROP leverages the pairs sampled in the course of its basis evaluation as the foundation for its importance sampling routine. More sophisticated importance sampling routines including coreset extraction are extremely promising here but their runtime cost must be weighed against their potential benefit.

Finally, DROP performs online progress estimation to minimize the end-to-end analytics cost function. This is analogous to query progress estimation [11, 12, 54] and performance prediction [21, 56] in database and data warehouse settings and has been exploited in approximate query processing engines such as BlinkDB [2, 73]. DROP adopts a relatively simple derivative-based estimator but could benefit from more sophisticated techniques from the literature.

Scalable Complex Analytics. As a framework for dimensionality reduction, DROP is designed as an analytics operator within larger analytics dataflow pipelines. Thus, DROP can be viewed as a natural extension of recent results on integrating complex analytics function including signal processing [15, 31, 40, 58], model training [25, 39, 46], and data exploration [53, 65, 70, 71, 74] operators into scalable analytics engines. In the DROP implementation in this paper's evaluation, we evaluate DROP as a custom feature transformation dataflow operator in the MacroBase engine, combining it with a downstream k-NN classification operator.

6 CONCLUSION

Dimensionality reduction techniques offer a powerful means of efficiently processing increasingly high-volume and high-dimensional time series by improving the runtime of downstream analytics operators without compromising accuracy. In this work, we revisit canonical operators for time series dimensionality reduction and the measurement study of [19] and show that PCA is more effective than popular alternatives in the data mining literature often by a margin of over 2× on average on gold-standard time series benchmark data sets with respect to output data dimension. More surprisingly, we empirically demonstrate that a small number of samples are sufficient to accurately characterize directions of maximum variance and obtain a high-quality low-dimensional basis.

These observations motivate the design of DROP, a new dimensionality reduction optimizer. DROP combines progressive sampling, progress estimation, and online aggregation to identify a high quality low dimensional bases without processing the entire dataset, by balancing runtime and achieved dimensionality. Our empirical results illustrate that progressive sampling can improve the runtime of conventional, non-sampling approaches to PCA by several orders of magnitude. In addition, DROP improves the end-to-end runtime of full analytics pipelines; a small amount of pre-processing can deliver substantially faster downstream analytics. By adapting classic techniques from approximate query engines and recent developments in randomized linear algebra, DROP bridges the gap between quality and efficiency in time series dimensionality reduction.

ACKNOWLEDGEMENTS

We thank the members of the Stanford InfoLab as well as Aaron Sidford, Mary Wootters, and Moses Charikar for valuable feedback on this work. This research was supported in part by affiliate members and other supporters of the Stanford DAWN project—Intel, Microsoft, Teradata, and VMware—and industrial gifts and support from Toyota Research Institute, Juniper Networks, Visa, Keysight Technologies, Hitachi, Facebook, Northrop Grumman, NetApp, and the NSF Graduate Research Fellowship, grant DGE-1656518

REFERENCES

[1] D. Achlioptas. Database-friendly random projections. In *PODS*, 2001.

[2] S. Agarwal, B. Mozafari, A. Panda, H. Milner, S. Madden, and I. Stoica. Blinkdb: queries with bounded errors and bounded response times on very large data. In *Proceedings of the 8th ACM European Conference on Computer Systems*, pages 29–42. ACM, 2013.

[3] C. C. Aggarwal. On the effects of dimensionality reduction on high dimensional similarity search. In *PODS*, 2001.

[4] B. Babcock, S. Chaudhuri, and G. Das. Dynamic sample selection for approximate query processing. In *Proceedings of the 2003 ACM SIGMOD international conference on Management of data*, pages 539–550. ACM, 2003.

[5] P. Bailis, E. Gan, S. Madden, D. Narayanan, K. Rong, and S. Suri. Macrobase: Prioritizing attention in fast data. In *SIGMOD*. ACM, 2017.

[6] P. Bailis, E. Gan, K. Rong, and S. Suri. Prioritizing attention in fast data: Principles and promise. 2017.

[7] C. M. Bishop. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006.

[8] F. Camastra. Data dimensionality estimation methods: a survey. *Pattern recognition*, 36(12):2945–2954, 2003.

[9] K. Chakrabarti and S. Mehrotra. Local dimensionality reduction: A new approach to indexing high dimensional spaces. In *VLDB*, 2000.

[10] S. Chaudhuri, G. Das, and V. Narasayya. Optimized stratified sampling for approximate query processing. *ACM Transactions on Database Systems (TODS)*, 32(2):9, 2007.

[11] S. Chaudhuri and V. Narasayya. Self-tuning database systems: a decade of progress. In *VLDB*. VLDB Endowment, 2007.

[12] S. Chaudhuri, V. Narasayya, and R. Ramamurthy. Estimating progress of execution for sql queries. In *SIGMOD*, 2004.

[13] Y. Chen, E. Keogh, B. Hu, N. Begum, A. Bagnall, A. Mueen, and G. Batista. The ucr time series classification archive, July 2015. www.cs.ucr.edu/~eamonn/time_series_data/.

[14] K. L. Clarkson. Coresets, sparse greedy approximation, and the frank-wolfe algorithm. *ACM Transactions on Algorithms (TALG)*, 6(4):63, 2010.

[15] C. Cranor, T. Johnson, O. Spataschek, and V. Shkapenyuk. Gigascope: a stream database for network applications. In *SIGMOD*, 2003.

[16] J. P. Cunningham and Z. Ghahramani. Linear dimensionality reduction: survey, insights, and generalizations. *Journal of Machine Learning Research*, 16(1):2859–2900, 2015.

[17] B. De Sa, Christopher an He, I. Mitliagkas, C. Re, and P. Xu. Accelerated stochastic power iteration. *arXiv:1707.02670*, 2017.

[18] C. De Sa, K. Olukotun, and C. Ré. Global convergence of stochastic gradient descent for some non-convex matrix problems. In *ICML*, 2015.

[19] H. Ding, G. Trajcevski, P. Scheuermann, X. Wang, and E. Keogh. Querying and mining of time series data: experimental comparison of representations and distance measures. In *VLDB*, 2008.

[20] P. Drineas and M. W. Mahoney. RandNLA: randomized numerical linear algebra. *Communications of the ACM*, 59(6):80–90, 2016.

[21] J. Duggan, U. Cetintemel, O. Papaemmanouil, and E. Upfal. Performance prediction for concurrent database workloads. In *SIGMOD*, 2011.

[22] P. Esling and C. Agon. Time-series data mining. *ACM Computing Surveys (CSUR)*, 45(1):12, 2012.

[23] M. Ester, H.-P. Kriegel, J. Sander, X. Xu, et al. A density-based algorithm for discovering clusters in large spatial databases with noise. In *KDD*, 1996.

[24] C. Faloutsos, M. Ranganathan, and Y. Manolopoulos. *Fast subsequence matching in time-series databases*. 1994.

[25] X. Feng, A. Kumar, B. Recht, and C. Ré. Towards a unified architecture for in-rdbms analytics. In *SIGMOD*, 2012.

[26] I. K. Fodor. A survey of dimension reduction techniques. Technical report, Lawrence Livermore National Lab., CA (US), 2002.

[27] E. Gan and P. Bailis. Scalable kernel density classification via threshold-based pruning. In *SIGMOD*, 2017.

[28] A. Gersho and R. M. Gray. *Vector quantization and signal compression*, volume 159. Springer Science & Business Media, 2012.

[29] P. B. Gibbons and Y. Matias. New sampling-based summary statistics for improving approximate query answers. In *SIGMOD*, 1998.

[30] A. Gionis, P. Indyk, R. Motwani, et al. Similarity search in high dimensions via hashing. In *VLDB*, volume 99, pages 518–529, 1999.

[31] L. Girod et al. Wavescope: a signal-oriented data stream management system. In *ICDE*, 2006.

[32] N. Goyal, S. Vempala, and Y. Xiao. Fourier pca and robust tensor decomposition. In *STOC*, 2014.

[33] N. Halko, P.-G. Martinsson, and J. A. Tropp. Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. *SIAM review*, 53(2):217–288, 2011.

[34] J. Han, J. Pei, and M. Kamber. *Data mining: concepts and techniques*. Elsevier, 2011.

[35] J. M. Hellerstein, P. J. Haas, and H. J. Wang. Online aggregation. In *SIGMOD*, 1997.

[36] IDC. The digital universe of opportunities: Rich data and the increasing value of the internet of things, 2014. http://www.emc.com/leadership/digital-universe/.

[37] I. F. Ilyas, G. Beskales, and M. A. Soliman. A survey of top-k query processing techniques in relational database systems. *ACM Computing Surveys (CSUR)*, 40(4):11, 2008.

[38] P. Jain, C. Jin, S. M. Kakade, P. Netrapalli, and A. Sidford. Streaming pca: Matching matrix bernstein and near-optimal finite sample guarantees for oja's algorithm. In *COLT*, 2016.

[39] R. Jampani, F. Xu, M. Wu, L. L. Perez, C. Jermaine, and P. J. Haas. MCDB: a Monte Carlo approach to managing uncertain data. In *SIGMOD*, 2008.

[40] Y. Katsis, Y. Freund, and Y. Papakonstantinou. Combining databases and signal processing in plato. In *CIDR*, 2015.

[41] E. Keogh. A decade of progress in indexing and mining large time series databases. In *VLDB*, 2006.

[42] E. Keogh, K. Chakrabarti, M. Pazzani, and S. Mehrotra. Dimensionality reduction for fast similarity search in large time series databases. *Knowledge and information Systems*, 3(3):263–286, 2001.

[43] E. Keogh, K. Chakrabarti, M. Pazzani, and S. Mehrotra. Locally adaptive dimensionality reduction for indexing large time series databases. *ACM Sigmod Record*, 30(2):151–162, 2001.

[44] E. Keogh, J. Lin, and A. Fu. Hot sax: Efficiently finding the most unusual time series subsequence. In *ICDM*, 2005.

[45] E. Keogh and M. Pazzani. A simple dimensionality reduction technique for fast similarity search in large time series databases. *Knowledge Discovery and Data Mining. Current Issues and New Applications*, pages 122–133, 2000.

[46] T. Kraska, A. Talwalkar, J. C. Duchi, R. Griffith, M. J. Franklin, and M. I. Jordan. Mlbase: A distributed machine-learning system. In *CIDR*, 2013.

[47] H.-P. Kriegel, P. Kröger, and M. Renz. Techniques for efficiently searching in spatial, temporal, spatio-temporal, and multimedia databases. In *ICDE*. IEEE, 2010.

[48] Y. LeCun. The MNIST database of handwritten digits. *http://yann. lecun. com/exdb/mnist/*, 1998.

[49] J. A. Lee and M. Verleysen. *Nonlinear dimensionality reduction*. Springer Science & Business Media, 2007.

[50] J. Lin, E. Keogh, W. Li, and S. Lonardi. Experiencing sax: a novel symbolic representation of time series. *Data Mining and knowledge discovery*, 15(2):107, 2007.

[51] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. *Journal of Machine Learning Research*, 9(Nov):2579–2605, 2008.

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

[53] A. Meliou, S. Roy, and D. Suciu. Causality and explanations in databases. In *VLDB*, 2014.

[54] C. Mishra and N. Koudas. A lightweight online framework for query progress indicators. In *ICDE*, 2007.

[55] M. Mitzenmacher and E. Upfal. *Probability and Computing: Randomization and Probabilistic Techniques in Algorithms and Data Analysis*. Cambridge university press, 2017.

[56] K. Morton, A. Friesen, M. Balazinska, and D. Grossman. Estimating the progress of mapreduce pipelines. In *ICDE*, 2010.

[57] B. Mozafari. Approximate query engines: Commercial challenges and research opportunities. In *SIGMOD*, 2017.

[58] M. Nikolic, B. Chandramouli, and J. Goldstein. Enabling signal processing over data streams. In *SIGMOD*. ACM, 2017.

[59] F. Olken and D. Rotem. Random sampling from databases: a survey. *Statistics and Computing*, 5(1):25–42, 1995.

[60] A. B. Owen. *Monte Carlo theory, methods and examples*. 2013.

[61] K. Ravi Kanth, D. Agrawal, and A. Singh. Dimensionality reduction for similarity searching in dynamic databases. In *SIGMOD*, 1998.

[62] S. T. Roweis and L. K. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.

[63] O. Shamir. A stochastic pca and svd algorithm with an exponential convergence rate. In *ICML*, pages 144–152, 2015.

[64] A. Shrivastava, A. Gupta, and R. Girshick. Training region-based object detectors with online hard example mining. In *CVPR*, 2016.

[65] T. Siddiqui, A. Kim, J. Lee, K. Karahalios, and A. Parameswaran. Effortless data exploration with zenvisage: an expressive and interactive visual analytics system. In *VLDB*, 2016.

[66] L. N. Trefethen and D. Bau III. *Numerical linear algebra*, volume 50. Siam, 1997.

[67] M. Udell, C. Horn, R. Zadeh, S. Boyd, et al. Generalized low rank models. *Foundations and Trends® in Machine Learning*, 9(1):1–118, 2016.

[68] M. Vlachos, C. Domeniconi, D. Gunopulos, G. Kollios, and N. Koudas. Nonlinear dimensionality reduction techniques for classification and visualization. In *KDD*, 2002.

[69] M. Wand and M. Jones. *Kernel Smoothing*. Chapman & Hall/CRC Monographs on Statistics & Applied Probability. Taylor & Francis, 1994.

[70] A. Wasay, X. Wei, N. Dayan, and S. Idreos. Data canopy: Accelerating exploratory statistical analysis. In *SIGMOD*, 2017.
[71] E. Wu and S. Madden. Scorpion: Explaining away outliers in aggregate queries. In *VLDB*, 2013.
[72] J. Ye. Generalized low rank approximations of matrices. In *ICML*, 2004.
[73] K. Zeng, S. Gao, B. Mozafari, and C. Zaniolo. The analytical bootstrap: a new method for fast error estimation in approximate query processing. In *SIGMOD*, 2014.
[74] E. Zgraggen, A. Galakatos, A. Crotty, J. D. Fekete, and T. Kraska. How progressive visualizations affect exploratory analysis. *IEEE Transactions on Visualization and Computer Graphics*, 2016.
[75] Y. Zhu and D. Shasha. Warping indexes with envelope transforms for query by humming. In *SIGMOD*, 2003.

APPENDIX

A AUGMENTED RESULTS

In this section, we provide additional information to augment results provided in the measurement study and evaluation. Table 3 provides complete end-to-end runtime results for data processing and the k-NN retrieval task, while Table 4 displays the corresponding accuracies with respect to running the retrieval task on the raw data. Table 5 displays the proportion of data required to attain a given TLB when using a PCA transformation where output dimension is equal to input dimension. Table 6 illustrates the output dimension required for each algorithm (PAA, FFT, and PCA) to attain a target TLB.

Table 3: End-to-End runtime comparison of DROP and baseline techniques with k-NN retrieval task, in ms

Dataset	No DR	SVD	SVD-Halko	Oracle	DROP
ChlorineConcentration	458	4054	424	207	178
CinC	1809	3068	5738	884	894
ECG5000	1855	5689	561	362	482
ElectricDevices	38222	83302	28433	27260	30701
FordA	21906	10546	5300	4270	4286
FordB	18271	8984	4917	3773	3792
HandOutlines	5160	5620	9479	2832	2678
InlineSkate	579	1420	2081	548	704
InsectWingbeatSound	805	977	425	200	212
MALLAT	2593	2895	3870	643	450
NonInvasiveFatalECG	5157	5229	3235	944	1043
Phoneme	8490	6710	7687	7534	10446
StarLightCurves	32024	35129	11429	1079	1238
Two	5728	8916	2849	2860	3335
UWaveGestureLibraryAll	25825	8147	5509	1298	1355
uWaveGestureLibrary	4734	5669	1067	402	310
wafer	1536	12911	749	403	403
yoga	1199	2943	1029	174	153

Table 4: Raw accuracy in k-NN retrieval task

Dataset	SVD	SVD-Halko	Oracle	DROP
ChlorineConcentration	0.893	0.886	0.906	0.903
CinC	0.894	0.892	0.899	0.929
ECG5000	0.855	0.855	0.856	0.874
ElectricDevices	0.877	0.875	0.866	0.888
FordA	0.892	0.878	0.884	0.9
FordB	0.875	0.875	0.871	0.874
HandOutlines	0.908	0.901	0.907	0.92
InlineSkate	0.832	0.818	0.803	0.805
InsectWingbeatSound	0.815	0.815	0.811	0.848
MALLAT	0.83	0.83	0.876	0.892
NonInvasiveFatalECG	0.82	0.822	0.836	0.827
Phoneme	0.848	0.852	0.68	0.678
StarLightCurves	0.615	0.648	0.653	0.651
Two	0.899	0.903	0.901	0.902
UWaveGestureLibraryAll	0.846	0.853	0.856	0.883
uWaveGestureLibrary	0.797	0.797	0.808	0.838
wafer	0.808	0.818	0.833	0.888
yoga	0.791	0.791	0.797	0.818

Table 5: Proportion of data required to obtain a TLB-preserving transformation with full PCA (i.e., output dimension = input dimension)

	TLB		
Dataset	**0.75**	**0.90**	**0.99**
50words	0.0106	0.0185	0.0391
Adiac	0.0077	0.0145	0.0484
ArrowHead	0.0285	0.0626	0.2907
Beef	0.0494	0.0898	0.19
BeetleFly	0.3073	0.4449	0.7979
BirdChicken	0.156	0.2357	0.5437
Car	0.0428	0.0979	0.3719
CBF	0.0273	0.0775	0.1407
ChlorineConcentration	0.001	0.0029	0.014
CinC	0.007	0.0157	0.0391
Coffee	0.1224	0.2715	0.8632
Computers	0.0596	0.1889	0.6818
Cricket	0.0198	0.0574	0.2488
DiatomSizeReduction	0.015	0.0282	0.176
DistalPhalanxOutlineAgeGroup	0.0094	0.0241	0.0987
DistalPhalanxOutlineCorrect	0.006	0.0168	0.0642
DistalPhalanxTW	0.0097	0.0236	0.098
Earthquakes	0.3733	0.6052	0.8988
ECG200	0.0288	0.0942	0.3287
ECG5000	0.001	0.0025	0.0132
ECGFiveDays	0.0073	0.0114	0.0275
ElectricDevices	0.0026	0.0043	0.0088
FaceAll	0.0078	0.0171	0.0355
FaceFour	0.1143	0.2727	0.7708
FacesUCR	0.0077	0.0169	0.0355
FISH	0.0181	0.0433	0.1587
FordA	0.0054	0.0114	0.0198
FordB	0.008	0.0146	0.0248
Gun	0.0282	0.0477	0.134
Ham	0.0811	0.1558	0.4486
HandOutlines	0.0045	0.0091	0.0372
Haptics	0.017	0.0394	0.1234
Herring	0.0599	0.1447	0.4878
InlineSkate	0.0085	0.0162	0.0388
InsectWingbeatSound	0.0048	0.0119	0.0255
ItalyPowerDemand	0.0068	0.01	0.0198
LargeKitchenAppliances	0.0987	0.2373	0.6068
Lighting2	0.186	0.4505	0.9132
Lighting7	0.1439	0.3534	0.9022
MALLAT	0.0031	0.009	0.0197
Meat	0.0398	0.0528	0.3494
MedicalImages	0.007	0.0103	0.0256
MiddlePhalanxOutlineAgeGroup	0.0096	0.0191	0.0939
MiddlePhalanxOutlineCorrect	0.0065	0.0127	0.0548
MiddlePhalanxTW	0.0089	0.0206	0.0916
MoteStrain	0.0148	0.0323	0.0838
NonInvasiveFatalECG	0.0021	0.0043	0.0375
OliveOil	0.0936	0.1727	0.6366
OSULeaf	0.0258	0.0435	0.1104
PhalangesOutlinesCorrect	0.0023	0.0046	0.0187
Phoneme	0.0547	0.1346	0.3875
Plane	0.0285	0.0683	0.2068
ProximalPhalanxOutlineAgeGroup	0.0068	0.0171	0.0825
ProximalPhalanxOutlineCorrect	0.0046	0.0134	0.0512
ProximalPhalanxTW	0.0052	0.0153	0.0831
RefrigerationDevices	0.1414	0.2777	0.6696
ScreenType	0.0324	0.1087	0.5341
ShapeletSim	0.497	0.7498	0.969
ShapesAll	0.0048	0.0137	0.0278
SmallKitchenAppliances	0.2489	0.422	0.7194
SonyAIBORobotSurface	0.0211	0.0442	0.0969
SonyAIBORobotSurfaceII	0.0143	0.0272	0.0708
StarLightCurves	0.001	0.0011	0.0039
Strawberry	0.005	0.0086	0.0225
SwedishLeaf	0.0083	0.0178	0.0727
Symbols	0.0071	0.0096	0.0246
synthetic	0.0281	0.0642	0.0964
ToeSegmentation1	0.0548	0.0992	0.2988
ToeSegmentation2	0.0718	0.144	0.3784
Trace	0.0222	0.0555	0.3752
TwoLeadECG	0.0045	0.0081	0.0259
Two	0.0038	0.0097	0.0259
UWaveGestureLibraryAll	0.0025	0.0056	0.024
uWaveGestureLibrary	0.0017	0.0024	0.0081
wafer	0.001	0.0032	0.0097
Wine	0.031	0.0477	0.1745
WordsSynonyms	0.0094	0.0196	0.0389
Worms	0.0661	0.109	0.3177
WormsTwoClass	0.0575	0.1193	0.3289
yoga	0.0017	0.0028	0.0096

Table 6: Output dimension required for target TLB across dimensionality reduction technique.

	TLB: 0.75			TLB: 0.90			TLB: 0.99		
Dataset	*PAA*	*FFT*	*PCA*	*PAA*	*FFT*	*PCA*	*PAA*	*FFT*	*PCA*
50words	9	9	7	18	14	10	62	28	25
Adiac	7	8	4	15	13	6	69	34	20
ArrowHead	9	9	4	16	13	8	73	33	26
Beef	7	15	2	20	18	3	89	48	7
BeetleFly	16	16	6	28	21	12	99	34	22
BirdChicken	8	14	3	14	17	6	48	20	15
Car	7	16	2	15	19	6	70	37	24
CBF	15	13	7	61	57	45	114	114	107
ChlorineConcentration	46	34	2	93	81	5	153	153	30
CinC	29	44	26	58	53	40	241	107	48
Coffee	14	17	3	46	37	6	225	158	38
Computers	21	24	16	94	66	44	636	614	192
Cricket	14	14	9	47	35	21	248	202	113
DiatomSizeReduction	7	11	7	11	13	10	87	55	21
DPOAgeGroup	12	12	2	27	17	6	66	60	36
DPOCorrect	12	12	2	26	16	7	66	57	32
DistalPhalanxTW	12	12	2	27	16	6	66	60	34
Earthquakes	276	269	103	410	400	190	491	490	340
ECG200	8	7	3	29	22	6	72	56	41
ECG5000	14	14	3	30	24	7	115	88	31
ECGFiveDays	31	28	2	53	40	5	111	65	13
ElectricDevices	36	36	27	62	57	49	78	79	74
FaceAll	28	24	8	50	35	20	110	81	48
FaceFour	36	31	5	67	43	12	277	228	61
FacesUCR	28	24	9	48	34	22	109	53	49
FISH	10	15	5	20	18	11	91	37	28
FordA	63	47	16	98	61	35	297	106	82
FordB	69	49	19	102	65	39	318	107	85
Gun	5	6	3	11	9	5	56	24	14
Ham	34	32	7	73	58	18	261	114	61
HandOutlines	11	70	10	25	83	32	93	91	46
Haptics	10	29	6	19	35	14	173	81	32
Herring	10	15	3	25	18	8	111	63	39
InlineSkate	7	49	7	15	58	17	55	63	22
InsectWingbeatSound	15	14	7	28	22	13	100	42	33
ItalyPowerDemand	6	6	2	11	10	5	19	17	15
LargeKitchenAppliances	59	49	36	165	125	89	624	545	284
Lighting2	41	34	9	152	149	28	557	490	82
Lighting7	31	27	9	126	118	26	280	269	81
MALLAT	19	30	10	46	36	26	297	182	36
Meat	13	14	2	32	24	4	218	213	23
MedicalImages	12	10	3	20	17	7	66	34	17
MPOAgeGroup	12	12	2	27	16	4	66	60	31
MPOCorrect	12	12	2	27	16	5	66	58	30
MiddlePhalanxTW	12	12	2	27	16	5	66	60	32
MoteStrain	12	11	7	39	37	26	76	75	63
NonInvasiveFatalECG	16	22	3	42	31	18	201	121	82
OliveOil	33	25	2	61	51	5	375	213	23
OSULeaf	11	13	9	20	16	14	73	30	29
PhalangesOutlinesCorrect	11	12	2	26	16	5	65	56	28
Phoneme	87	70	59	268	201	160	920	858	535
Plane	12	11	3	22	14	6	76	39	21
PPOAgeGroup	12	12	2	26	18	4	65	58	28
PPOCorrect	12	12	2	27	18	5	66	58	28
ProximalPhalanxTW	12	12	2	26	18	5	65	59	28
RefrigerationDevices	94	76	60	222	154	121	645	586	316
ScreenType	18	24	20	70	55	40	614	614	207
ShapeletSim	275	272	62	410	402	111	491	490	180
ShapesAll	7	14	7	14	17	14	49	25	20
SmallKitchenAppliances	259	235	104	497	423	204	698	678	398
SonyAIBORobotSurface	15	14	5	28	21	13	56	43	38
SonyAIBORobotSurfaceII	18	18	6	30	24	13	57	45	39
StarLightCurves	5	27	2	14	33	21	51	36	35
Strawberry	10	11	2	24	21	6	98	41	13
SwedishLeaf	9	9	5	19	14	10	71	37	32
Symbols	7	11	6	12	13	11	46	26	14
synthetic	14	14	7	37	38	28	58	59	54
ToeSegmentation1	12	10	8	24	19	16	116	49	43
ToeSegmentation2	10	13	6	21	20	13	101	49	34
Trace	6	9	2	18	17	7	120	69	31
TwoLeadECG	12	9	2	25	19	4	70	51	14
Two	13	11	7	34	24	20	108	102	98
UWGLAll	15	27	18	35	32	28	151	82	59
uWaveGestureLibrary	4	10	5	10	11	10	43	27	20
wafer	12	10	4	37	29	11	125	112	49
Wine	10	9	2	27	20	3	104	58	9
WordsSynonyms	9	9	7	17	14	10	62	31	25
Worms	9	26	8	26	30	17	123	62	41
WormsTwoClass	10	26	8	25	30	17	124	61	42
yoga	6	13	3	11	15	11	44	21	16