DROP: Optimizing Stochastic Dimensionality Reduction via Workload-Aware Progressive Sampling

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ABSTRACT

Dimensionality reduction is a critical step in machine learning pipelines. Principal Component Analysis (PCA) is frequently the method of choice, yet is often prohibitively expensive. Theoretical means of accelerating PCA via sampling have been proposed, but typically treat PCA as a reusable statistical operator, independent of downstream analytics workflows. We show how accounting for downstream analytics operations during dimensionality reduction via PCA allows stochastic methods to efficiently operate over small (e.g., 1%) subsamples of input data, reducing computational overhead and end-to-end runtime. We propose a dimensionality reduction optimizer that enables speedups of up to 5× over Singular-Value-Decomposition-based PCA techniques, and achieves parity with or exceeds conventional approaches like FFT and PAA by up to 16× in end-to-end workloads.

1 INTRODUCTION

Continued, rapid growth in high-dimensional data from automated data sources [11, 38] poses a scalability challenge for machine learning (ML) pipelines. Dimensionality reduction (DR) techniques can alleviate this scalability challenge [15, 25, 39, 41]. In exchange for a runtime cost (R), DR methods transform an n-dimensional dataset to a lower k-dimensional representation while preserving salient dataset features, allowing downstream analytics routines to terminate in runtime proportional to $k > n$, while preserving accuracy on downstream tasks (see Figure 1).

Principal Component Analysis (PCA) is often the DR method of choice for practitioners with respect to transformation quality (k) for a target accuracy [37]. However, naïve implementations of PCA are data and workload-independent, and scale poorly with dimensionality, resulting in runtimes (R) that exceed the downstream runtime benefit of DR via PCA. Accordingly, practitioners often sacrifice quality for end-to-end runtime, and use alternative DR methods [22].

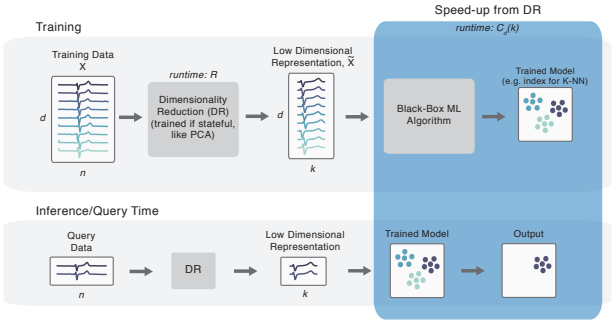

Figure 1: Sample machine learning pipeline with dimensionality reduction. Spending time on DR provides downstream runtime speed-ups.

Sample-based, stochastic PCA algorithms [19, 57] are a scalable alternative to classical PCA. However, the amount of sampling required is highly data-dependent. If we sample too many data points, then the runtime overhead of PCA in an end-to-end analytics workload could outweigh the statistical benefits. If we fail to sample enough data points, then PCA could fail to deliver a sufficiently high-quality reduction and compromise the runtime and/or accuracy of downstream analytics. This raises a critical question: can we develop a data and workload-dependent means of efficiently and accurately determining the sampling rate for stochastic PCA, such that we can obtain PCA's transformation quality while minimizing end-to-end workload runtime?

To this end, we develop DROP[1], a system that performs whole-workload runtime optimization by dynamically identifying the amount of sampling required for stochastic PCA. DROP takes a high-dimensional dataset,[2] property to preserve (e.g., pairwise Euclidean distance to 5%), and optional runtime model expressing downstream workload performance as a function of dimensionality (e.g., for k-Nearest Neighbors [k-NN], runtime is linear in dimensionality). DROP returns a low-dimensional transformation for the input using

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[1] https://github.com/stanford-futuredata/DROP

[2] Our primary focus for performance evaluation is a case study on time series similarity search, given the amount of study in the database community [22] and the resurgence of interest in time series analytics systems [10, 11, 53]. We provide a preliminary generalizability analysis in Section 5.

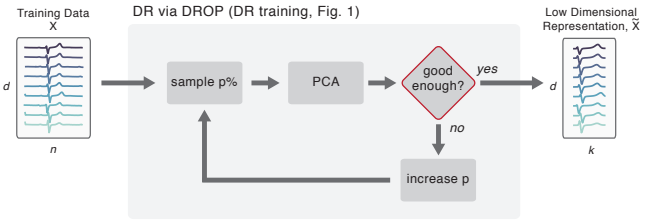

Figure 2: DROP is a workload-aware DR operator compatible with standard ML pipelines. The challenge DROP solves is when to stop training ("good enough?")

as few samples as needed to minimize the projected overall workload runtime while satisfying quality constraints.

To achieve this functionality, DROP addresses the question of how much to sample the input dataset via data-dependent progressive sampling and online progress estimation at runtime. DROP performs PCA on a small sample to obtain a candidate transformation, then progressively increases the number of samples until termination (see Figure 2). To identify the termination point that minimizes the overall runtime, DROP must overcome three challenges:

First, given the results of PCA on a data sample, DROP must *evaluate the quality* of the current candidate transformation. Popular analytics and data mining tasks often require approximate preservation of metrics such as average pairwise distances between data points [24, 33], which are costly to compute. Thus, DROP adapts confidence intervals for fast estimation of the input metric to preserve.

Second, DROP must *estimate the marginal benefit of sampling additional datapoints* for another iteration. When running PCA on a series of progressively larger samples, later samples will incur higher computational cost but may return lower-dimensional transformations. To navigate this trade-off between end-to-end runtime and transformation quality, DROP uses the results obtained from previous iterations to build a predictive performance model for future iterations.

Finally, given the current quality and expected marginal benefit of the next iteration, DROP must *optimize end-to-end runtime*. While an application-agnostic approach would iterate until successive iterations yield no benefit to quality, many analytics operators such as k-Nearest Neighbors are tolerant of error [25], so it is frequently advantageous to trade a slightly higher-dimensional basis for faster preprocessing (DR). To address this challenge, the system performs workload-specific optimization to minimize the expected runtime of the complete end-to-end analytics pipeline.

We view DROP as a pragmatic combination of recent theoretical advances in dimensionality reduction and classic techniques from approximate query processing, and a useful system for performing end-to-end workflow optimization. We make the following contributions in this work:

- We show the data sample required to perform accuracy-achieving PCA is often small (as little as 1%), and data-dependent sampling can enable 91× speedup compared to PCA via singular value decomposition (SVD).
- We propose DROP, an online optimizer for DR that uses information about downstream analytics tasks to perform efficient stochastic PCA.
- We present techniques based on progressive sampling, approximate query processing, online progress estimation, and cost based optimization to enable up to 5× faster end-to-end execution over PCA via SVD.

2 BACKGROUND AND PROBLEM

We provide background on dimensionality reduction (DR), and define our problem of workload-aware DR.

2.1 Dimensionality Reduction

DR refers to finding a low-dimensional representation of a dataset that preserves properties of interest, such as data point similarity [18, 27]. Formally, consider a data matrix $X \in \mathbb{R}^{d \times n}$, where each row i corresponds to data point $x_i \in \mathbb{R}^n$, with $d > n$. DR computes a transformation function ($T : \mathbb{R}^n \rightarrow \mathbb{R}^k$) that maps each x_i to a new basis as $\tilde{x}_i \in \mathbb{R}^k$ where $k \leq n$, resulting in a new data matrix $T(X) = \tilde{X} \in \mathbb{R}^{d \times k}$.

Principal Component Analysis (PCA). PCA is a linear DR technique that identifies a new orthogonal basis for a dataset that captures its directions of highest variance. Of all linear transformations, this basis minimizes reconstruction error in a mean square sense. Classically implemented PCA uses a Singular Value Decomposition (SVD) routine [59].

2.2 DR for Repeated-Query Workloads

In workloads such as similarity search, clustering, or classification, ML models are periodically trained over historical data, and are *repeatedly queried* as incoming data arrives or new query needs arise (see Fig 1). Indexes built over this data can improve the efficiency of this repeated query workload in exchange for a preprocessing overhead. DR with a multidimensional index structure is a classic way of achieving this, and is the basis for popular similarity search procedures and extensions in the data mining and machine learning communities [7, 15, 33, 39, 41, 45, 54, 66]; a metric-preserving transformation reduces input dimensionality, and an index is built in this new space for subsequent queries.

DR in Similarity Search. Similarity search is a common repeated-query workload performed over a variety of data types including images, documents and time series [22, 28], which we use as a running case study given its popularity and

the large amount of research in the space. The Tightness of Lower Bounds (TLB) is typically the metric preserved by DR in this setting [22], as it measures how well a *contractive* DR transformation (i.e. distances in the transformed space are less than or equal to those in the original) preserves pairwise Euclidean distances. It can be used to identify the quality of a low dimensional transformation without performing the downstream similarity search task:

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

2.3 Problem: Workload-Aware DR

In workload-aware dimensionality reduction, we perform DR to minimize overall workload runtime. DR is a fixed cost (i.e., in index construction for similarity search), while each query (i.e., nearest neighbor query) over the dataset incurs a marginal cost that is dependent on DR quality: lower-dimensional data points result in faster queries.

As input, consider a set of data points, a desired level of metric preservation (B; e.g., $TLB \geq .99$) and, optional downstream runtime as a function of dimensionality ($C_d(n)$ for an $d \times n$ data matrix). We use this information to efficiently return a DR function that satisfies the metric constraint with a configurable degree of confidence. More formally, denoting DR runtime as R, we define the optimization problem:

Problem 2.1. *Given $X \in \mathbb{R}^{d \times n}$, TLB constraint $B \in (0, 1]$, confidence c, and workload runtime function $C_d : \mathbb{Z}_+ \rightarrow \mathbb{R}_+$, find k and transformation matrix $T_k \in \mathbb{R}^{n \times k}$ that minimizes $R + C_d(k)$ such that $TLB(XT_k) \geq B$ with confidence c.*

We assume the downstream runtime model $C_d(n)$ is monotonically increasing in n as the premise of DR for efficient analytics relies on downstream tasks running faster on lower dimensional data. Absent this, we default to execution until convergence (i.e, until k plateaus) as described in Section 3, and demonstrate the cost of doing so in Section 5.

The more time spent on DR (R), the smaller the transformation (k), thus the lower the workload runtime. To minimize $R + C_d(k)$, we must determine how much time to spend on DR to minimize end-to-end runtime.

3 SIMILARITY SEARCH CASE STUDY

To tackle workload-aware DR, we first perform a case study focusing on time series similarity search by revisiting a widely cited empirical comparison of DR techniques from VLDB 2008 [22]. We show that PCA can outperform classic techniques (return low k), but at a high computational cost (R). We then demonstrate how sample-based PCA methods can bridge this gap, but that the number of samples required varies per dataset. Finally, we show how progressively increasing the sampling rate can help dynamically identify how much to sample a given dataset, thus providing a foundation for workload-aware DR.

3.1 PCA Speed vs. Quality

While improved quality provides faster repeated query execution, the cost of DR via PCA dominates this speedup, encouraging the use of faster, lower-quality alternatives [22].

To briefly quantify this trade-off, we augment a widely-cited time series similarity search DR study from VLDB 2008 [22] by evaluating PCA—which the authors did not benchmark due to it being "untenable for large data sets." We compare PCA via SVD to baseline techniques based on runtime and DR performance with respect to TLB over the largest datasets from [22]. We use their two fastest methods as our baselines as they show the remainder exhibited "very little difference": Fast Fourier Transform (FFT) and Piecewise Aggregate Approximation (PAA).

TLB Performance Comparison We compute the minimum dimensionality achieved by each technique subject to a TLB constraint. On average, PCA provides bases that are 2.3× (up to 3.9×) and 3.7× (up to 26×) smaller than PAA and FFT for $TLB = 0.75$, and 2.9× (up to 8.3×) and 1.8× (up to 5.1×) smaller for $TLB = 0.99$. While the margin between PCA and alternatives is dataset-dependent, PCA almost always preserves TLB with a lower dimensional representation.

Runtime Performance Comparison PCA implemented via out-of-the-box SVD is on average over 26× (up to 56×) slower than PAA and over 4.6× (up to 9.7×) times slower than FFT when computing the smallest TLB-preserving basis.

3.2 Incremental, Progressive Sampling

To bridge this performance-runtime gap, we turn to data sampling. Many real-world datasets are intrinsically low-dimensional, as evidenced by their rapid falloff in their eigenvalue spectrum. A data sample thus captures much of the dataset's "interesting" behavior, so fitting models over data samples generalize well. We verify this by varying the target TLB and examining the minimum number of uniformly selected samples required to obtain a TLB-preserving transform with output dimension k equal to input dimension n.

On average, a sample of under 0.64% (up to 5.5%) of the input is sufficient for $TLB = 0.75$, and under 4.2% (up to 38.6%) is sufficient for $TLB = 0.99$. If this sample rate is known, we obtain up to 91× speedup compared to a naïve implementation of PCA via SVD—with no algorithmic improvement.

However, this benefit is dataset-dependent, and unknown a priori. We thus turn to progressive sampling (gradually increasing the sample size) to identify how large a sample suffices. Figure 3 shows how the dimensionality required to

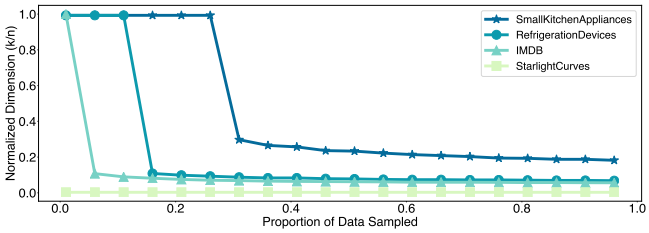

Figure 3: Improvement in representation size for $TLB = 0.80$ across three datasets. Higher sampling rates improve quality until reaching a state equivalent to running PCA over the full dataset ("convergence")

attain a given TLB changes when we vary dataset and proportion of data sampled. Increasing the number of samples provides lower dimensional transformations for the same quality. However, this decrease in dimension plateaus as the number of samples increases. Thus, while progressive sampling would allow us to tune the amount of time spent on DR, we must determine when the downstream value of decreased dimension is overpowered by the cost of additional DR—that is, whether to sample to convergence (evaluated in Section 5.3) or terminate early (e.g., at 0.3 proportion of data sampled for SmallKitchenAppliances).

4 DROP: WORKLOAD OPTIMIZATION

DROP answers a crucial question that stochastic PCA techniques have traditionally ignored: how long should these methods run?

4.1 DROP Architecture

DROP operates over a series of data samples, and determines when to terminate via a four-step procedure that is repeated for each iteration:

Step 1: Progressive Sampling (§4.2, Alg 1 L5, Fig 2A) DROP draws a data sample, performs PCA over it, and uses of a novel reuse mechanism across iterations (§4.7).

Step 2: Transform Evaluation (§4.3, Alg 1 L6, Fig 2B) DROP then evaluates the quality of the above by identifying the size of the smallest metric-preserving transformation that can be extracted.

Step 3: Progress Estimation (§4.4, Alg 1 L8, Fig 2C) Given the size of the metric-preserving transform and the time required to obtain this transform, DROP estimates the size and computation time of continued iteration.

Step 4: Cost-Based Optimization (§4.5, Alg 1 L9, Fig 2D) DROP optimizes over DR and downstream task runtime to determine if it should terminate.

Algorithm 1 DROP Algorithm

Input:
X: data matrix
B: target metric preservation level
C_d: cost of downstream operations; default tuned to k-NN

Output:
T_k: k-dimensional transformation matrix

```
1:  function DROP(X, B, C_d):
2:      Initialize: i = 0; k_0 = ∞   ▷ iteration and current basis size
3:      do
4:          i++, CLOCK.RESTART
5:          X_i = SAMPLE(X, SAMPLE-SCHEDULE(i))          ▷ § 4.2
6:          T_{k_i} = COMPUTE-TRANSFORM(X, X_i, B)       ▷ § 4.3
7:          r_i = CLOCK.ELAPSED                          ▷ R = ∑_i r_i
8:          k̂_{i+1}, r̂_{i+1} = ESTIMATE(k_i, r_i)        ▷ § 4.4
9:      while OPTIMIZE(C_d, k_i, r_i, k̂_{i+1}, r̂_{i+1})  ▷ § 4.5
10: return T_{k_i}
```

4.2 Progressive Sampling

DROP repeatedly chooses a subset of data and computes PCA on the subsample (via one of the methods in § 4.6). We consider a simple uniform sampling strategy: each iteration, DROP samples a fixed percentage of the data.

4.3 Evaluating Transformations

Given a transformation obtained by running PCA over a sample, DROP must accurately and efficiently evaluate the performance of this transformation with respect to a metric of interest over the entire dataset, not just the data sample.

We define the performance of a transformation computed over a sample as the size of the lowest dimensional TLB-preserving transform (k) that can be extracted. There are two challenges in evaluating this performance. First, the k that achieves the TLB constraint is rarely known a priori. Second, brute-force TLB computation would dominate the runtime of computing PCA over a sample.

4.3.1 *Computing the Lowest Dimensional Transformation.*

DROP first computes a full, n-dimensional basis via PCA over the data sample. To reduce dimensionality, DROP must determine if a smaller dimensional TLB-preserving transformation can be computed over this sample, and return the smallest such transform. Ideally, the smallest k would be known a priori, but in practice, this is not true. Thus, DROP uses the TLB constraint and two properties of PCA to automatically identify the size of the returned transformation.

First, PCA via SVD produces an orthogonal linear transformation where the principal components are returned in order of decreasing dataset variance explained. Once DROP has computed the transformation matrix for dimension n,

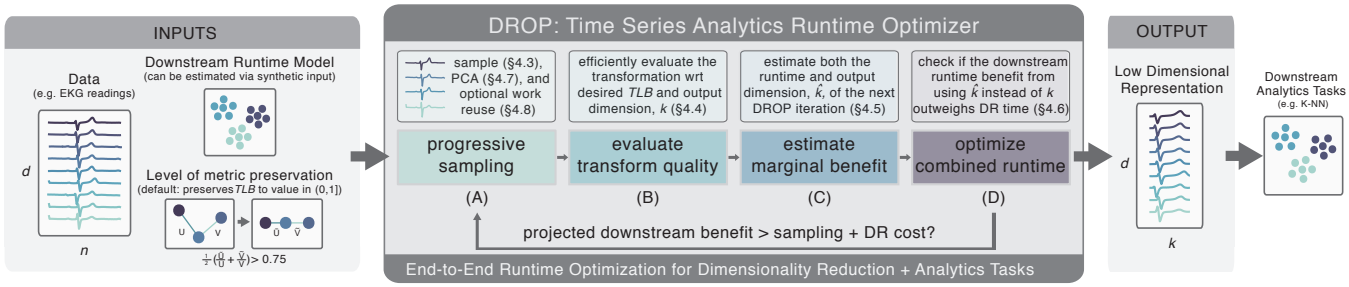

Figure 4: High-level DROP architecture depicting DROP's inputs, outputs, and core components.

DROP obtains the transformations for all dimensions k less than n truncating the matrix to $n \times k$, as .

Second, with respect to TLB preservation, the more principal components that are retained, the better the lower-dimensional representation in terms of TLB. This is because orthogonal transformations such as PCA preserve inner products. Therefore, a n-dimensional PCA perfectly preserves $\mathcal{L}_2$-distance between data points. As the $\mathcal{L}_2$-distance is a sum of squared (positive) terms, the more principal components that are retained, the better the representation preserves $\mathcal{L}_2$-distance.

Using the first property, DROP obtains all low-dimensional transformations for the sample from the n-dimensional basis. Using the second property, DROP runs binary search over these transformations to return the lowest-dimensional basis that attains B (i.e., COMPUTE-TRANSFORM, line 1 of Algorithm 2). If a target B cannot be realized with this sample, DROP omits all further optimization steps in this iteration and continues the next iteration by drawing a larger sample.

Computing the full n-dimensional basis at every step may be wasteful. Thus, if DROP has previously found a candidate TLB-preserving basis of size $n' < n$ in prior iterations, then DROP only computes n' components at the start of the next iteration. This allows for more efficient PCA computation for future iterations, as advanced PCA routines can exploit the n'-th eigengap to converge faster (§6).

4.3.2 TLB Computation. Given a transformation, DROP must efficiently determine if the basis preserves the desired TLB. Computing pairwise TLB for all data points requires $O(d^2 n)$ time, which dominates the runtime of computing PCA on a sample. However, as the TLB is an average of random variables bounded from 0 to 1, DROP can use statistical sampling and confidence intervals to compute the TLB to arbitrary confidences.

Given a transformation, DROP iteratively refines an estimate of its TLB (function EVALUATE-TLB in Algorithm 2, line 11) by incrementally sampling an increasing number of pairs from the input data (Algorithm 2, line 15), transforming each pair into the new basis, then measuring the distortion of $\mathcal{L}_2$ distance between the pairs, providing a TLB estimate to confidence level c (Algorithm 2, line 19). If the confidence interval's lower bound is greater than the target TLB, the basis is a sufficiently good fit; if its the upper bound is less than the target TLB, the basis is not a sufficiently good fit. If the confidence interval contains the target TLB, DROP cannot determine if the target TLB is achieved. Thus, DROP automatically samples additional pairs to refine its estimate.

To estimate the TLB to confidence c, DROP uses the Central Limit Theorem (similar to online aggregation [34]): computing the standard deviation of a set of sampled pairs' TLB measures and applying a confidence interval to the sample according to the c. For data with low variance, DROP evaluates a candidate basis with few samples from the dataset as the confidence intervals shrink rapidly.

The techniques in this section are presented in the context of TLB, but can be applied to any downstream task and metric for which we can compute confidence intervals and are monotonic in number of principal components retained.

4.4 Progress Estimation

Given a low dimensional TLB-achieving transformation from the evaluation step, DROP must identify the quality (dimensionality) and cost (runtime) of the transformation that would be obtained from an additional DROP iteration.

Recall that DROP seeks to minimize objective function $R + C_d(k)$ such that $TLB(XT_k) \geq B$, with R denoting DROP's total runtime, T_k the k-dimensional TLB-preserving transformation of data X returned by DROP, and $C_d(k)$ the workload cost function. Therefore, given a k_i-dimensional transformation T_{k_i} returned by the evaluation step of DROP's i^{th} iteration, DROP can compute 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 transformation, DROP must be able to estimate the objective function value of future iterations.

In Section 4.5 we show that DROP requires obj_{i+1} to minimize this objective function. To estimate obj_{i+1}, DROP must

Algorithm 2 Basis Evaluation and Search

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

function COMPUTE-TRANSFORM($X, X_i B$):
  PCA.FIT(X_i) ▷ fit PCA on the sample
  Initialize: high = k_{i-1}; low = 0; $k_i = \frac{1}{2}$(low + high); $B_i = 0$
  while (low ! = high) **do**
    T_{k_i}, B_i = EVALUATE-TLB(X, B, k_i)
    if $B_i \leq B$ **then** low = $k_i + 1$
    else high = k_i
    $k_i = \frac{1}{2}$(low + high)
  T_{k_i} = cached k_i-dimensional PCA transform
return T_{k_i}

function EVALUATE-TLB(X, B, k):
  numPairs = $\frac{1}{2}d(d-1)$
  $p = 100$ ▷ number of pairs to check metric preservation
  while ($p <$ numPairs) **do**
    B_i, B_{lo}, B_{hi} = TLB(X, p, k)
    if ($B_{lo} > B$ or $B_{hi} < B$) **then break**
    else pairs ×= 2
return B_i

function TLB(X, p, k):
  return mean and 95%-CI of the TLB after transforming p d-dimensional pairs of points from X to dimension k. The highest transformation computed thus far is cached to avoid recomputation of the transformation matrix.

estimate the runtime required for iteration $i+1$ (which we denote as r_{i+1}, where $R = \sum_i r_i$ after i iterations) and the dimensionality of the TLB-preserving transformation 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 performs online progress estimation to estimate these quantities. Specifically, DROP performs online parametric fitting to compute future values based on prior values for r_i and k_i in line 8 of Algorithm 1. By default, given a sample of size m_i in iteration i, DROP performs linear extrapolation to estimate k_{i+1} and r_{i+1}. The estimate of r_{i+1}, for instance, is:

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

4.5 Cost-Based Optimization

Given the results of the progress estimation step, DROP must determine if continued PCA on additional samples will be beneficial to overall runtime, or if it is better to terminate.

Given predictions of the next iteration's runtime ($\hat{r}_{i+1}$) and dimensionality ($\hat{k}_{i+1}$), DROP uses a greedy heuristic in estimating the optimal objective-minimizing stopping point. Concretely, if the objective function estimate for the next iteration is greater than its current objective function value ($obj_i < \widehat{obj}_{i+1}$), then DROP will terminate. If DROP's runtime is convex in the number of iterations, it is straightforward to prove that this condition is in fact the optimal stopping criterion (i.e., via convexity of composition of convex functions). This stopping criterion leads to a simple check at each DROP iteration that is used by OPTIMIZE in Algorithm 1 line 9:

$$obj_i < \widehat{obj}_{i+1}$$
$$C_d(k_i) + \sum_{j=0}^{i} r_j < C_d(\hat{k}_{i+1}) + \sum_{j=0}^{i} r_j + \hat{r}_{i+1}$$
$$C_d(k_i) - C_d(\hat{k}_{i+1}) < \hat{r}_{i+1} \quad (2)$$

DROP terminates when the projected time of the next iteration exceeds the estimated downstream runtime benefit.

4.6 Choice of PCA Subroutine

At each iteration, DROP uses PCA as its means of DR. The most straightforward means of implementing this PCA step is to compute a full SVD over the data (§2.1). However, this approach is computationally inefficient compared to other DR techniques (§2).

In our DROP implementation, we compute PCA via a randomized SVD algorithm from [31] (SVD-Halko). While additional advanced methods for efficient PCA exist (§6), we found that not only is SVD-Halko asymptotically of the same running time as techniques used in practice, it is straightforward to implement, can take advantage of optimized linear algebra libraries, and does not require tuning for hyperparameters such as batch size, learning rate, or convergence criteria. While SVD-Halko is not as efficient as other techniques with respect to communication complexity as in [23], or convergence rate as in [19], these techniques can be easily substituted for SVD-Halko in DROP's architecture.

4.7 Work Reuse

A natural question arises due to DROP's iterative architecture: can we combine the information from each sample's transformation without computing PCA over the union of the sampled data points? While stochastic methods for PCA enable such work reuse across samples as they iteratively refine a single transformation matrix, other methods do not. We propose an algorithm that allows reuse of previous work when utilizing arbitrary PCA routines with DROP.

DROP uses two key insights in order to enable this work reuse. First, given two transformation matrices produced via PCA, T_1 and T_2, the horizontal concatenation of these matrices $H = [T_1|T_2]$ is a transformation into the union of their range spaces. Second, for datasets that have rapid drop off in spectrum, the principal components returned from running PCA on repeated data samples will generally

concentrate to the true top principal components. Thus, work reuse proceeds via two step concatenate-distill approach: DROP first maintains a transformation history consisting of the horizontal concatenation of all PCA transformations to this point, and then computes the SVD of this history matrix and returns the first k columns as the transformation matrix.

Although this routine requires an SVD computation, computational overhead is not dependent on the raw dataset size, but on the size of the history matrix, H. This size is proportional to the original dimensionality n and size of lower dimensional transformations, which are in turn proportional to the data's intrinsic dimensionality and the TLB constraint. As preserving *all history* can be expensive in practice, DROP periodically shrinks the history matrix using DR via PCA. We validate the benefit of using work reuse—up to 15% on real-world data—in Section 5.

5 EXPERIMENTAL EVALUATION

We evaluate DROP's efficiency along three dimensions: runtime, accuracy, and extensibility. We demonstrate that (1) DROP outperforms PAA and FFT in end-to-end, repetitive-query workloads, (2) DROP's optimizations each contribute to performance, and (3) DROP extends beyond time series.

5.1 Experimental Setup

Implementation We implement DROP as an in-memory, batch-oriented feature transformation dataflow operator in Java using the multi-threaded Matrix-Toolkits-Java (MTJ) library [32] and netlib-java [4] linked against Intel MKL [5] for compute-intensive linear algebra operations. We use multi-threaded JTransforms [2] for FFT, and implement multi-threaded PAA from scratch. We use the Statistical Machine Intelligence and Learning Engine (SMILE) library [1] for k-NN with different index structures, and k-means.

Datasets We first consider the UCR Time Series Classification Archive [17] for indexing experiments and lesion studies. We exclude datasets with fewer than 1 million entries, and fewer datapoints than dimensionality, leaving 14 datasets.

Due to the relatively small size of these time series datasets, we consider three additional datasets to showcase tangible wall-clock runtime improvements with DROP. We use the standard MNIST hand-written digits dataset [46], the FMA featurized music dataset [21], and a labeled sentiment analysis IMBD dataset [8], which also demonstrates extensibility beyond time series data.

DROP Configuration We use a runtime cost function for k-NN obtained via linear interpolation on data of varying dimension (implemented via cover trees [12], K-D trees [56],or brute force search in SMILE). To evaluate the sensitivity to cost model, we also report on the effect of operating without a cost model (i.e., sample until convergence) in Section 5.3. We set TLB constraints such that the accuracy of K-NN tasks remain unchanged before and after indexing via DR, corresponding to $B = 0.99$ for the UCR datasets. Unless otherwise specified, we use a default sampling schedule that begins with and increases by 1% of the input. It is possible to optimize (and possibly overfit) this schedule for our target time series, but we provide a conservative, more general schedule.

Baselines We report runtime, accuracy, and reduced dimension compared to FFT, PAA, PCA via SVD-Halko, and PCA via SVD. Each computes a transformation over the entire data, then performs binary search to identify the smallest dimensional basis that satisfies the target TLB.

Similarity Search/k-NN Setup While many methods for similarity search exist, as in [22], we consider k-NN in our evaluation as it is classically used and interoperates with new use cases including one-shot learning and deep metric learning [49, 55, 62]. To evaluate DR performance when used with downstream indexes, we vary k-NN's multidimensional index structure: cover trees, K-D trees, or no index.

End-to-end performance depends on the number of queries in the workload, and DROP is optimized for the repeated-query use case. Due to the small size of the UCR datasets, we choose a 1:50 ratio of data indexed to number of query points, and vary this index-query ratio in later microbenchmarks and experiments. We also provide a cost model for assessing the break-even point that balances the cost of a given DR technique against it's indexing benefits to each query point.

5.2 DROP Performance

We evaluate DROP's performance compared to PAA and FFT using the time series case study.

k-NN Performance We summarize DROP's results on an end-to-end 1-Nearest Neighbor classification in Figure 5. We display the end-to-end runtime of DROP, PAA, and FFT for each of the considered index structures: no index, K-D trees, cover trees. We display the size of the returned dimension for the no indexing scenario, as the other two scenarios return near identical values. This occurs as many of the datasets used in this experiment are small and possess low intrinsic dimensionality; DROP's cost model thus determines to quickly identify this dimensionality prior to termination. We do not display k-NN accuracy as all techniques meet the TLB constraint, and achieve the same accuracy within 1%.

On average, DROP returns transformations that are 2.3× and 1.4× smaller than PAA and FFT, translating to significantly smaller k-NN query time. End-to-end runtime with DROP is on average 2.2× and 1.4× (up to 10× and 3.9×) faster than PAA and FFT, respectively, when using brute force linear search, 2.3× and 1.2× (up to 16× and 3.6×) faster when

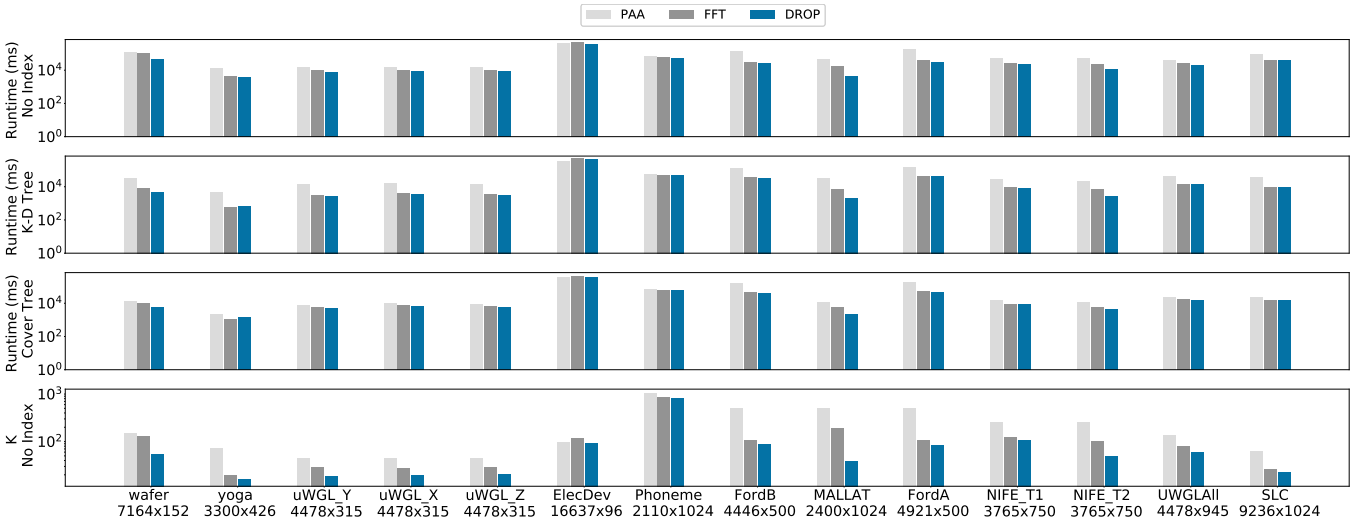

Figure 5: End-to-End DR and k-NN runtime (top three) and returned lower dimension (bottom) over the largest UCR datasets for three different indexing routines. DROP consistently returns lower dimensional bases than conventional alternatives (FFT, PAA), and is on average faster than PAA and FFT.

using K-D trees, and 1.9× and 1.2× (up to 5.8× and 2.6×) faster when using cover trees. When evaluating Figure 5, it becomes clear that DROP's runtime improvement is data dependent for both smaller datasets, and for datasets that do not possess a low intrinsic dimension (such as Phoneme, elaborated on in Section 5.3) Determining if DROP is a good fit for a dataset is an exciting area for future work (§7).

Varying Index-Query Ratio

DROP is optimized for highly structured data and a low index-query ratio, as in many streaming and/or high-volume data use cases. If there are many more data points queried than used for training/constructing an index, DROP will outperform alternatives. A natural question that arises is in which scenarios is it beneficial to use DROP, and in which would a lower quality but faster reduction suffice. Domain experts are typically aware of the scale of their query workloads. However, we also provide a heuristic to answer this question given rough runtime and cardinality estimates of the downstream task at hand and the choice of alternative DR technique.

Let x_d and x_a be the per-query runtime of running a downstream task with the output of DROP and a given alternative method, respectively. Let r_d and r_a denote the amortized per-datapoint runtime of DROP and the alternative method, respectively. Let n_i and n_q the number of indexed and queried points. DROP is faster when $n_q x_d + n_i r_d < n_q x_a + n_i r_a$.

To verify, we obtained estimates of the above and compared DROP against FFT and PAA in lower-query-volume scenarios when running k-NN using cover trees, and display

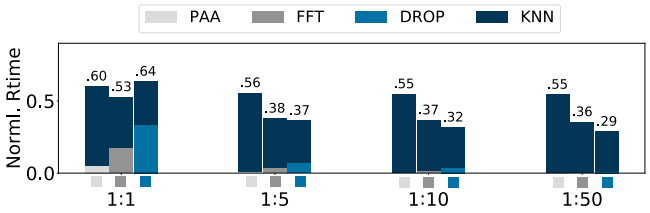

Figure 6: Effect of decreasing the index-query ratio. As an index is queried more frequently, DROP's relative runtime benefit increases.

the results in Figure 6. We first found that in the 1:1 index-query ratio setting, DROP should be slower than PAA and FFT, as observed. However, as we decrease the ratio, DROP becomes faster, with a break-even point of slightly lower than 1:3. We show that DROP does indeed outperform PAA and FFT in the 1:5 index-query ratio case, where it is is on average 1.51× faster than PAA and 1.03× faster than FFT. As the ratio decreases to 1:50, DROP is 1.24× faster than FFT and 1.9× faster than PAA.

Time Series Similarity Search Extensions Given the breadth of research in time series indexing, a natural question to ask is how DROP, a general operator for PCA, compares to state-of-the-art time series indexes. As a preliminary evaluation, we consider iSAX2+ [14], a state-of-the-art indexing tool in a 1:1 index-query ratio setting, using a publicly available Java implementation [3]. While these indexing techniques also optimize for the low index-query ratio setting, we find index construction to be a large bottleneck in these

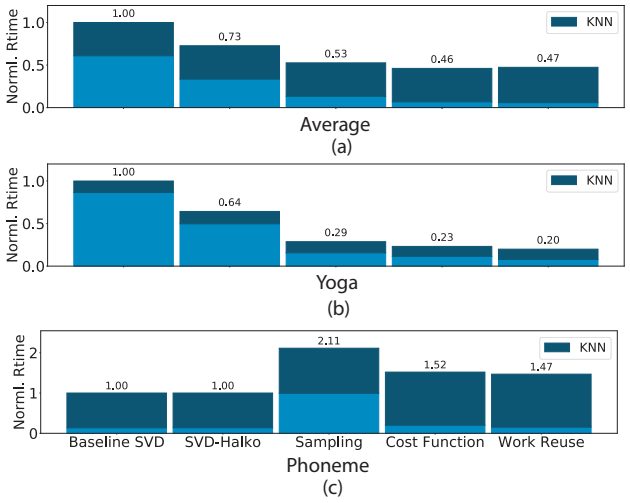

Figure 7: Lesion studies over the UCR datasets.

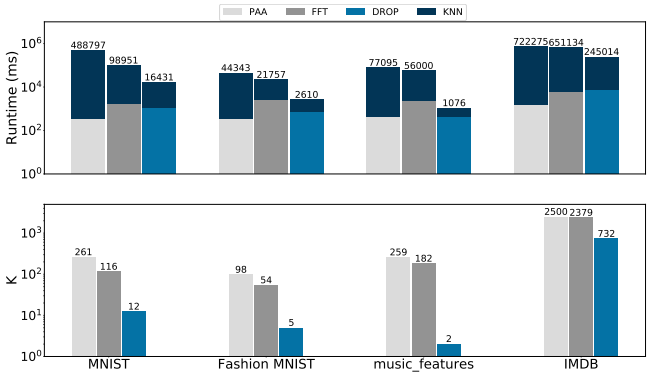

Figure 8: End-to-End k-NN runtime (top) and returned dimension k (bottom) over the entire MNIST dataset and the FMA featurized music dataset.

workloads. For iSax2+, index construction is on average 143× (up to 389×) slower than DR via DROP, but is on average only 11.3× faster than k-NN on the reduced space. However, given high enough query workload, these specialized techniques will surpass DROP.

We also verify that DROP is able to perform well when using downstream similarity search tasks relying on alternative distance metrics, namely, Dynamic Time Warping (DTW)—a commonly used distance measure in the literature [58]. As proof-of-concept, we implement a 1-NN task using DTW with a 1:1 index-query ratio, and find that even with this high ratio, DROP provides on average 1.2× and 1.3× runtime improvement over PAA and FFT, respectively.

5.3 Lesion Study

We perform a factor analysis of the incremental runtime and dimensionality contributions of each of DROP's components compared to baseline SVD methods. We only display the results of k-NN with cover trees; the results hold for the other indexes. We use a 1:1 index-query ratio with data inflated by 5× to better highlight the effects of each contribution to the DR routine, and display average results over the UCR datasets in Figure 7, excluding Phoneme.

Figure 7 first demonstrates the boost from using SVD-Halko over a naïve implementation of PCA via SVD, which comes from not computing the full transformation a priori, incrementally binary searching as needed. It then shows the runtime boost obtained from running on samples until convergence, where DROP samples and terminates after the returned lower dimension from each iteration plateaus. This represents the naïve sampling-until-convergence approach that DROP defaults to sans user-specified cost model. We finally introduce cost based optimization and work reuse. Each of these optimizations improves runtime, with the exception of work reuse, which has a negligible impact on average but disproportionately impacts certain datasets.

Work reuse typically only slightly affects end-to-end runtime as it is useful primarily when a large number of DROP iterations are required. We also observe this behavior on certain small datasets with moderate intrinsic dimensionality, such as the yoga dataset in Figure 7b. Work reuse provides a 15% improvement in addition to cost based optimization.

DROP's sampling operates on the premise that the dataset has data-point-level redundancy. However, datasets without this structure are more difficult to reduce the dimensionality of. Phoneme is an example of one such dataset (Figure 7c). In this setting, DROP incrementally examines a large proportion of data before enabling cost-based optimization, resulting in a performance penalty.

5.4 Beyond the Time Series Case Study

We consider generalizability beyond our initial case study along two axes: data domain and downstream workload. These preliminary results show promise in extension to additional domains and target tasks.

Data Domain. We examine classification/similarity search workloads across image classification, music analysis, and natural language processing. To better show the trade-off in DR and downstream workload, we repeat the k-NN retrieval experiments with a 1:1 index-query ratio. We use 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 [46], combining both the provided training and testing datasets); FMA's featurized music dataset, providing 518 features across 106,574 music

tracks; a bag-of-words representation of an IMDB sentiment analysis dataset across 25,000 movies with 5000 features [8]; Fashion MNIST's 70,000 images of dimension 784 [64]. We present our results in Figure 8. As the given datasets are larger than the ones presented in [17], DROP's ability to find a *TLB*-preserving low dimensional basis is more valuable as this more directly translates to significant reduction in end-to-end runtime—up to a 7.6 minute wall-clock improvement in MNIST, 42 second improvement in Fashion MNIST, 1.2 minute improvement in music features, and 8 minute improvement in IMDB compared to PAA. These wall-clock runtime effects will only be amplified as the index-query ratio decreases, to be more typical of the repeated-query setting. For instance, when we decrease the ratio to 1:5 on the music features dataset, DROP provides a 6.1 and 4.5 minute improvement compared to PAA and FFT, respectively.

Downstream Workload. To demonstrate the generalizability of both DROP's pipeline as well as black-box runtime cost-model estimation routines, we extend our pipeline to perform a k-means task over the MNIST digits dataset. We fit a new downstream workload runtime model as we did with k-NN, and operate under a 1:1 index-query ratio. In this workload, DROP terminates in 1488ms, which is 16.5× faster than PAA and 6.5× faster than FFT.

6 RELATED WORK

Dimensionality Reduction DR is a classic operation [18, 27, 47, 59] that is well studied in the database [7, 15, 41, 54], data mining [40, 48], statistics and machine learning [20, 57], and theoretical CS [29, 35] communities.

Recent breakthroughs in the theoretical statistics community provided new algorithms for PCA that promise substantial scalability improvements without compromising result quality [19, 20, 31]. Foremost among these techniques are advanced stochastic methods [19, 57], and techniques for randomized SVD [31]. While we default to the latter for use by DROP's PCA operator, DROP's modular architecture makes it simple to use any method in its place, including recent systems advances in scalable PCA [23]. To the best of our knowledge, advanced methods for PCA have not been empirically compared head-to-head with conventional dimensionality reduction approaches such as Piecewise Approximate Averaging [40], especially on real datasets. In addition, DROP *combines* these methods with row-level sampling to provide benefits similar to using stochastic methods for PCA, regardless of the chosen PCA subroutine.

Approximate Query Processing Inspired by approximate query processing engines [52] as in online aggregation [34], DROP performs progressive sampling. In contrast with more general data dimensionality estimation methods [13], DROP optimizes for *TLB*. As we illustrated in Section 5, this strategy confers substantial runtime improvements. While DROP performs simple uniform sampling, the literature contains a wealth of techniques for various biased sampling techniques [9, 16]. Finally, DROP performs online progress estimation to minimize the end-to-end analytics cost function. This is analogous to query progress estimation [50] and performance prediction [51] in database and data warehouse settings and has been exploited in approximate query processing engines such as BlinkDB [6].

Scalable Workload-Aware, Complex Analytics DROP is an operator for analytics dataflow pipelines. Thus, DROP is as an extension of recent results on integrating complex analytics function including model training [26, 36, 44] and data exploration [61, 63, 65] operators into analytics engines.

7 FUTURE WORK AND CONCLUSIONS

DROP provides a first step in bridging the gap between quality and efficiency in DR for downstream analytics. However, there are several avenues to explore for future work, such as sophisticated sampling methods and streaming execution.

7.1 Data-Aware Sampling

DROP's efficiency is determined by the dataset's spectrum; MALLAT, with the sharpest drop-off, performs extremely well, and Phoneme, with a near uniform distribution, does not. Datasets such as Phoneme perform poorly under the default configuration as we enable cost-based optimization after reaching a feasible point. Thus, DROP spends a disproportionate time sampling (Fig. **??**). Extending DROP to more efficiently determine if a dataset is amenable to aggressive sampling is an exciting area of future work. For instance, recent theoretical results that use sampling to estimate spectrum, even when the number of samples are small in comparison to the input dimensionality [43], can be run alongside DROP with minimal alteration.

7.2 Streaming Execution

Given a stationary input distribution, users can extract fixed-length sliding windows from the source and apply DROP's transformation over these segments as they arrive. Should the data distribution not be stationary over time, DROP can be be periodically retrained in one of two ways. First, DROP can use of the wide body of work in changepoint or feature drift detection [30, 42] to determine when to retrain. Alternatively, DROP can maintain a reservoir sample of incoming data [60], tuned to the specific application, and retrain if the metric of interest no longer satisfies user-specified constraints. Due to DROP's default termination condition, cost-based optimization must be disabled until the metric constraint is achieved to prevent early termination.

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