KeystoneML: Optimizing Pipelines for Large-Scale Advanced Analytics

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Abstract
Modern advanced analytics applications make use of machine learning techniques and contain multiple steps of domain-specific and general-purpose processing with high resource requirements. We present KeystoneML, a system that captures and optimizes the end-to-end large-scale machine learning applications for high-throughput training in a distributed environment with a high-level API. This approach offers increased ease of use and higher performance over existing systems for large scale learning. We demonstrate the effectiveness of KeystoneML in achieving high quality statistical accuracy and scalable training using real world datasets in several domains. By optimizing execution KeystoneML achieves up to \(15 \times\) training throughput over unoptimized execution on a real image classification application.

1 Introduction
Today’s advanced analytics applications increasingly use machine learning (ML) as a core technique in areas ranging from business intelligence to recommendation to natural language processing \([39]\) and speech recognition \([29]\). Practitioners build complex, multi-stage pipelines involving feature extraction, dimensionality reduction, data transformations, and training supervised learning models to achieve high accuracy \([52]\). However, current systems provide little support for automating the construction and optimization of these pipelines.

To assemble such pipelines, developers typically piece together domain specific libraries\(^1\) for feature extraction and general purpose numerical optimization packages \([34] [44]\) for supervised learning. This is often a cumbersome and error-prone process \([53]\). Further, these pipelines need to be completely re-engineered when the training data or features grow by an order of magnitude—often the difference between an application that provides good statistical accuracy and one that does not \([23]\). As no broader system has purview of the end-to-end application, only narrow optimizations can be applied.

These challenges motivate the need for a system that

- Allows users to specify end-to-end ML applications in a single system using high level logical operators.
- Scales out dynamically as data volumes and problem complexity change.
- Automatically optimizes these applications given a library of ML operators and the user’s compute resources.

While existing efforts in the data management community \([27] [21] [44]\) and in the broader machine learning systems community \([34] [45] [3]\) have built systems to address some of these problems, each of them misses the mark on at least one of the points above.

We present KeystoneML, a framework for ML pipelines designed to satisfy the above requirements. Fundamental to the design of KeystoneML is the observation that model training is only one component of an ML application. While a significant body of recent work has focused on high performance algorithms \([61] [50],\)

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\(^1\) e.g. OpenCV for Images (http://opencv.org/), Kaldi for Speech (http://kaldi-asr.org/)
and scalable implementations [17] for model training, they do not capture the featurization process or the logical intent of the workflow. KeystoneML provides a high-level, type-safe API built around logical operators to capture end-to-end applications.

To optimize ML pipelines, database query optimization provides a natural motivation for the core design of such a system [32]. However, compared to relational database query optimization, ML applications present an additional set of concerns. First, ML operators are often iterative and may require multiple passes over their inputs, presenting opportunities for data reuse. Second, many ML operators provide only approximate answers to their inputs [50]. Third, numerical data properties such as sparsity and dimensionality are a necessary source of information when selecting optimal execution plans and conventional optimizers do not consider such measures. Finally, the system should be aware of the computation-vs-communication tradeoffs inherent in distributed processing of ML workloads [21] [34] and choose appropriate execution strategies in this regime.

To address these challenges we develop techniques to do both per-operator optimization and end-to-end pipeline optimization for ML pipelines. We use a cost-based optimizer that accounts for both computation and communication costs and our cost model can easily accommodate new operators and hardware configurations. To determine which intermediate states are materialized in memory during iterative execution, we formulate an optimization problem and present a greedy algorithm that works efficiently and accurately in practice.

We measure the importance of cost-based optimization and its associated overheads using real-world workloads from computer vision, speech and natural language processing. We find that end-to-end optimization can improve performance by $7 \times$ and that physical operator optimizations combined with end-to-end optimizations can improve performance by up to $15 \times$ versus unoptimized execution. We show that in our experiments, poor physical operator selection can result in up to a $260 \times$ slowdown. Using an image classification pipeline on over 1M images [52], we show that KeystoneML provides linear performance scalability across various cluster sizes, and statistical performance comparable to recent results [11] [52]. Additionally, KeystoneML can match the performance of a specialized phoneme classification system on a BlueGene supercomputer while using $8 \times$ fewer resources. In summary, we make the following contributions:

- We present KeystoneML, a system for describing ML applications using high level logical operators. KeystoneML enables end-to-end optimization of ML applications at both the operator and pipeline level.

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Figure 2: A text classification pipeline is specified using a small set of logical operators.

- We demonstrate the importance of physical operator selection in the context of input characteristics of three commonly used logical ML operators, and propose a cost model for making this selection.
- We present and evaluate an initial set of whole-pipeline optimizations, including a novel algorithm that automatically identifies a subset of intermediate data to materialize to speed up pipeline execution.
- We evaluate these optimizations in the context of real-world pipelines in a diverse set of domains: phoneme classification, image classification, and textual sentiment analysis, and demonstrate near-linear scalability over 100s of machines with strong statistical performance.
- We compare KeystoneML with several recent systems for large-scale learning and demonstrate superior runtime from our optimization techniques and scale-out strategy.

KeystoneML is open source software\footnote{http://www.keystone-ml.org/} and is being used in scientific applications in solar physics [50] and genomics [2].

## 2 Pipeline Construction and Core APIs

In this section we introduce the KeystoneML API that can be used to express end-to-end ML pipelines. Each pipeline is composed a number of operators that are chained together. For example, Figure 2 shows the KeystoneML source code for a complete text classification pipeline. We next describe the building blocks of our API.

### 2.1 Logical ML Operators

Conventional analytics queries are typically composed using a small number of well studied relational database operators. This well-defined environment enables important optimizations. However, ML applications lack such an abstraction and practitioners typically piece together imperative libraries. Recent efforts have proposed...
using linear algebra operators such as matrix multiplication \cite{21}, convex optimization routines \cite{20} or multidimensional arrays as logical building blocks \cite{57}.

In contrast, with KeystoneML we propose a design where high-level ML operations (such as PCA, LinearSolver) are used as building blocks. Our approach has two major benefits: First, it simplifies building applications. Even complex pipelines can be built using just a handful of operators. Second, this higher level abstraction allows us to perform a wider range of optimizations. Our key insight here is that there are usually multiple well studied algorithms for a given ML operator, but that their performance and statistical characteristics vary based on the inputs and system configuration. We next describe the API for operators in KeystoneML.

Pipelines are composed of operators. Transformers and Estimators are two abstract types of operators in KeystoneML. An operator is a function which operates on zero or more inputs to produce some output. A logical operator satisfies some logical contract. For example, it takes an image and converts it to grayscale. Every logical operator must have at least one physical operator associated with it which implements its logic. Logical operators with multiple physical implementations are candidates for optimization. They are marked Optimizable and have a set of CostModels associated with them. Operators that are iterative with respect to their inputs are marked Iterative.

A Transformer is an operator that can be applied to individual data items (or to a collection of items) and produces a new data item (or a collection of data items)—it is a deterministic unary function without side-effects.

Figure 3: The KeystoneML API consists of two extendable operator types and interfaces for optimization.

\begin{figure}[h]
\centering
\begin{lstlisting}
trait Transformer[A, B] extends Pipeline[A, B] {
  def apply(in: Dataset[A]): Dataset[B] =
    in.map{apply}
  def apply(in: A): B
}
trait Estimator[A, B] {
  def fit(data: Dataset[A]): Transformer[A, B]
}
trait Optimizable[T, A, B] {
  val options: List[(CostModel, T[A,B])]
  def optimize(sample: Dataset[A], d: ResourceDesc): T[A,B]
}
class CostProfile{
  flops: Long, bytes: Long, network: Long
}
trait CostModel {
  def cost(sample: Dataset[A], workers: Int): CostProfile
}
trait Iterative {
  def weight: Int
}
\end{lstlisting}
\caption{Transformers and Estimators are chained using a syntax designed to allow developers to incrementally build pipelines.}
\end{figure}

Examples of Transformers in KeystoneML include basic data transformations, feature extractors and model application. The deterministic and side-effect free properties afford the ability to reorder and optimize the execution of the functions without changing the result.

An Estimator is applied to a distributed collection of data items and produces a Transformer—it is a function generating function. ML algorithms provided by KeystoneML are Estimators, while featurizers are Transformers. For example, LinearSolver is an Estimator that takes a data set and labels, finds the linear model which minimizes the square loss between the training data and labels, and produces a Transformer that can apply this model to new data.

\begin{figure}[h]
\centering
\begin{lstlisting}
trait Pipeline[A,B] {
  def andThen[C](next: Pipeline[B, C]): Pipeline[A, C]
  def andThen[C](est: Estimator[B, C],
  data: Dataset[A]): Pipeline[A, C]
  // Combine the outputs of branches
  // into a sequence
  def gather[A, B](branches: Seq[Pipeline[A, B]]): Pipeline[A, Seq[B]]
}
\end{lstlisting}
\caption{A pipeline DAG for image classification. Estimators are shaded.}
\end{figure}

2.2 Pipeline Construction

Transformers and Estimators are chained together into a Pipeline using a consistent set of rules. The chaining methods are summarized in Figure 4. In addition to linear chaining of nodes using andThen, KeystoneML’s API allows for pipeline branching. When a developer calls andThen a new Pipeline object is returned. By calling andThen multiple times on the same pipeline, users can create multiple pipelines that branch out. Developers join the output of multiple pipelines of using gather. Redundancy is eliminated via common subexpression optimization detailed in Section 5.1. We find these APIs are sufficient for a number of ML applications (Section 5.1), but expect to extend them over time.
### 2.3 Pipeline Execution

KeystoneML is designed to run with large, distributed datasets on commodity clusters. Our high level API and optimizers can be executed using any distributed data-flow engine. The execution flow of KeystoneML is shown in Figure 1. First, developers specify pipelines using the KeystoneML APIs described above. As calls to these APIs are made, KeystoneML incrementally builds an operator DAG for the pipeline. An example operator DAG for image classification is shown in Figure 2. Once a pipeline is applied to some data, this DAG is then optimized using a set of optimizations described below—we call this stage *optimization time*. Once the application has been optimized, the DAG is traversed depth-first and operators are executed one at a time, with nodes up until pipeline breakers (i.e., Estimators) packed into the same job—this stage is *runtime*. This lazy optimization procedure gives the optimizer full information about the application in question. We now consider the optimizations made by KeystoneML.

### 3 Operator-Level Optimization

In this section we describe the operator-level optimization procedure used in KeystoneML. Similar to database query optimizers, the goal of the operator-level optimizer is to choose the best physical implementation for every machine learning operator in the pipeline. This is challenging to do because operators in KeystoneML are distributed i.e. they involve computation and communication across the cluster. Operator performance may also depend on statistical properties like sparsity of input data and level of accuracy desired. Finally, as discussed in Section 2, KeystoneML consists of a set of high-level operators. The advantage of having high-level operators is that we can perform more wide-ranging optimizations. But this makes designing an optimizer more challenging because unlike relational operators or linear algebra, the set of operators in KeystoneML is not closed. We next discuss how we address these challenges.

**Approach:** The approach we take in KeystoneML is to develop a cost-based optimizer that splits the cost model into two parts: an operator-specific part and a cluster-specific part. The operator-specific part models the computation and communication time given statistics of the input data and number of workers and the cluster specific part is used to weigh their relative importance. More formally, the cost estimate for each physical operator, $f$ can be expressed as:

$$c(f, A_s, R) = R_{exec}c_{exec}(f, A_s, R_w) + R_{coord}c_{coord}(f, A_s, R_w)$$

**Table 1:** Resource requirements for linear solvers. $w$ is the number of workers in the cluster, $i$ the number of passes over the dataset. For the sparse solvers $s$ is the the average number of non-zero features per example, and $b$ is the block size for the block solver. Compute and Memory requirements are per-node, while network requirements are in terms of the data sent over the most loaded link.

Where $f$ is the operator in question, $A_s$ contains statistics of a dataset to be used as its input, and $R$, the *cluster resource descriptor* represents the cluster computing, memory, and networking resources available. The cluster resource descriptor is collected via configuration data and microbenchmarks. Statistics captured include per-node CPU throughput (in GFLOP/s), disk and memory bandwidth (GB/s), and network speed (GB/s), as well as information about the number of nodes available. $A_s$ is determined through a process we will discuss in Section 4. $R_w$ is the number of cluster nodes available.

The functions, $c_{exec}$, and $c_{coord}$ are developer-defined operator-specific functions (defined as part of the operator *CostModel*) that describe execution and coordination costs in terms of the longest critical path in the execution graph of the individual operators [59], e.g. the most FLOPS used by a node in the cluster or the amount of data transferred over the most loaded link. Such functions are also used in the analysis of parallel algorithms [6] and are well known for common linear algebra based operators. $R_{exec}$ and $R_{coord}$ are determined by the optimizer from the cluster resource descriptor ($R$) and capture the relative speed of local and network resources on the cluster.

Splitting the cost model in this fashion allows the the optimizer to easily adapt to new hardware (e.g., GPUs or Infiniband networks) and also for it to work with both existing and future operators. Operator developers only need to implement a *CostModel* and the system accounts for hardware properties. Finally we note that the cost model we use here is approximate and that the cost $c$ need not be equal to the actual running time of the operator. Rather, as in conventional query optimizers, the goal of the cost model is to avoid bad decisions, which a roughly accurate model will do. At the boundary of two nearly equivalent operators, either should be acceptable in terms of runtime. We next illustrate the cost functions for three central operators in KeystoneML and the performance trade-offs that arise from varying input properties.
Linear Solvers are supervised Estimators that learn a linear map $X$ between an input dataset $A \in \mathbb{R}^{n \times d}$ to a labels dataset $B \in \mathbb{R}^{n \times k}$ by finding the $X$ which minimizes the value $||AX - B||_F$. In a multi-class classification setting, $n$ is the number of examples or data points, $d$ the number of features and $k$ the number of classes. In the KeystoneML Standard Library we have several implementations of linear solvers, distributed and local, including

- Exact solvers [18] that compute closed form solutions to the least squares loss and return an $X$ to extremely high precision.
- Block solvers that partition the features into a set of blocks and use second-order Jacobi or Gauss-Seidel [9] updates to converge to the right solution.
- Gradient based methods like SGD [50] or L-BFGS [14] which perform iterative updates using the gradient and converge to a globally optimal solution.

Table 1 summarizes the cost model for each method. Constants are omitted for readability but are necessary in practice.

To illustrate these cost tradeoffs empirically, we vary the number of features generated by the featurization stage of two different pipelines and measure the training time and the training loss. We compare the methods on a 16 node cluster.

On an Amazon Reviews dataset (see Table 3) with a text classification pipeline, as we increase the number of features from 1k to 16k we see in Figure 6 that L-BFGS performs 5-20× faster than the exact solver and 26-260× faster than the block-wise solver. Additionally the exact solver crashes for greater than 4k features as the memory requirements are too high. The reason for this speedup is that the features generated in text classification problems are sparse and the L-BFGS solver exploits the sparse inputs to calculate gradients cheaply.

The optimal solver choice does not always stay the same as we increase the problem size or as sparsity changes. For the TIMIT dataset, which has dense features, we see that the exact solver is 3-9× faster than L-BFGS for smaller number of features. However when the number of features goes beyond 8k we see that the exact solver becomes slower than the block-wise solver which is also 2-3× faster than L-BFGS.

Principal Component Analysis (PCA) is an Estimator used for tasks ranging from dimensionality reduction to whitening to visualization. PCA takes an input dataset $A \in \mathbb{R}^{n \times d}$, and a value $k$ and produces a Transformer which can apply a matrix $P \in \mathbb{R}^{d \times k}$, where $P$ consists of the first $k$ eigenvectors of the covariance matrix of $A$. The $P$ matrix can be found using several techniques including the SVD or via an approximate algorithm, Truncated SVD [24]. In our cost model, SVD has runtime $O(nd^2)$ and offers an exact answer, while TSVD runs in $O(nk^2)$. Both methods may parallelized over a cluster.

To better illustrate how the choice of a PCA implementation affects the run time, we construct a microbenchmark that varies problem size along $n$, $d$, and $k$, and execute both local and distributed implementations of the approximate and exact algorithm on a 16-node cluster. In Table 2 we can see that as data volumes increase in $n$ and $d$ it makes sense to run PCA in a distributed fashion, while for relatively small values of $k$, it can make sense to use the approximate method.

**Convolution** is a critical building block of Signal, Speech, and Image Processing pipelines. In image processing, the Transformer takes in an Image of size $n \times n \times d$ and applies a bank of $b$ filters (each of size $k \times k$, where $k < n$) to the Image and returns the $b$ resulting convolved images of size $m \times m$, where $m = n - k + 1$. There are three main ways to implement convolutions: via
Figure 7: Time to perform 50 convolutions on a 256x256 3-channel image. As convolution size increases, the optimal method changes.

a matrix-vector product scheme when convolutions are separable, using BLAS matrix-matrix multiplication [5], or via a Fast Fourier Transform (FFT) [41].

The cost model for the matrix-vector product scheme takes $O(dbk(n - k + 1)^2 + bk^3)$ time, but only works when filters are linearly separable. Meanwhile, the matrix-matrix multiplication scheme has a cost of $O(dbk^2(n - k + 1)^2)$. Finally, the FFT based scheme takes $O(6dbn^2\log n + 4dhn^2)$, and the time taken does not depend on $k$.

To illustrate the tradeoffs between these methods, in Figure 7 we vary the size of the convolution filter, $k$, and use representative input images and batch sizes. For small values of $k$, we see that BLAS the is fastest operator. However, as $k$ grows, the algorithm’s dependence on $k^2$ makes this approach inappropriate. If the filters are separable, it is faster to use the matrix-vector algorithm. The FFT algorithm does not depend on $k$ and thus performs the same regardless of $k$.

**Cost Model Evaluation:** To evaluate how well our cost model works, we compared the physical operator chosen by our optimizer against the best choice from empirically measured values for linear solvers (Figure 6) and PCA (Table 2). We found that our optimizer made the right choice 90% of the time for linear solvers and 84% of the time for PCA. In both cases we found that the wrong choices were made when the running time of two operators were close to each other and thus the approximate cost model did not severely impact overall performance. For example, for the linear solver with 4096 dense features, the optimizer chooses the BlockSolver but empirically the Exact solver is about 30% faster.

As seen from the three examples above, the choice of optimal physical execution depends on hardware properties and on properties of the input data. Thus, choices made in support of operator-level optimization depend on upstream processing and cheaply estimating data properties at various points in the pipeline is an important problem. We next discuss how operator chaining semantics can help in achieving this.

### 4 Whole-Pipeline Optimization

#### 4.1 Execution Subsampling

Operator optimization in KeystoneML requires the collection of statistics about input data at each pipeline stage. For example, a text featurization operator might map a string into a 10,000-dimensional sparse feature vector. Without statistics about the input (e.g., vector sparsity) after featurization, a downstream operator will be unable to make its optimization decision. As such, dataset statistics ($A_s$) are determined by first estimating the size of the initial input dataset (in records), and optimizing the first operator in the pipeline with statistics derived from a sample of the input data. The optimized operator is then executed on the sample, and subsequent operators are optimized. This procedure continues until all nodes have been optimized. Along the way, we form a pipeline profile, which includes not just the information needed to form $A_s$ at each step, but also information about operator execution time and memory consumption of each operator’s execution on the sample. We use the pipeline profile to inform the Automatic Materialization optimization described below. We also evaluate the overheads from profiling in Section 5.3.

#### 4.2 Common Sub-expression Elimination

One of the whole-pipeline rewrites done by KeystoneML is a form of common sub-expression elimination. It is common for training data or the output of featurization stages to be used in several stages of a pipeline. As a concrete example, in a text classification pipeline we might first tokenize the training data then determine the 100,000 most common bigrams in a text corpus, featurize the data to a binary vector indicating the presence of each bigram, and then train a classifier on the same training data. Thus, we need the bigrams of each document both in the most common features calculation as well as when training the classifier. KeystoneML identifies and merges such common sub-expressions to enable computation reuse.

#### 4.3 Automatic Materialization

Cache management and automatic selection of materialized views are important optimizations used by database management systems [15] and they have been studied in the context of analytical query systems [63, 25], and feature selection [60]. For ML workloads, materialization of intermediate data is very important for performance because the iterative nature of these workloads means that recomputation costs are multiplied across iterations. By capturing the iterative nature of the pipelines in the DAG,
ing whether a node is cached or not, and

\[ \chi \]

where \( \kappa \) is the cache set that minimizes total execution time.

ory budget, we want to find the set of nodes to include in

estRuntime is a procedure that computes

\[ \text{estRuntime} \]

maximize time saved subject to memory constraints.

The caching algorithm in KeystoneML builds a cache set by finding the node that will maximize time saved subject to memory constraints. estRuntime is a procedure that computes \( T(v) \) for a given DAG, cache set, and node.

We can state the problem of minimizing pipeline execution time formally as an optimization problem with linear constraints as follows:

\[ \min_{\kappa} T(sink(G)) \]

s.t. \( \sum_{v \in V} size(v) \kappa_v \leq \text{memSize} \)

Where \( sink(G) \) is the pipeline terminus, \( size(v) \) the size of \( v \)'s output, and \( \text{memSize} \) the memory constraint. This problem can also be thought of as problem of finding an optimal cache schedule. It is tempting to reach for classical results [7, 48] in the optimal paging literature to identify an optimal or near-optimal schedule for this problem. However, neither of these results matches our problem setting fully. In particular, Belady’s algorithm is only optimal when each item has a fixed cost to bring into cache (as is common in reads from a two-level memory hierarchy), while in our problem these costs are variable and depend heavily on the computation time to materialize them—in many cases recomputing may be two orders of magnitude faster than reading from disk but

Algorithm 1: The caching algorithm in KeystoneML builds a cache set by finding the node that will maximize time saved subject to memory constraints. estRuntime is a procedure that computes \( T(v) \) for a given DAG, cache set, and node.

Algorithm 1: GreedyOptimizer:

input : G, t, size, memSize
output: cache

1: procedure GreedyOptimizer:
2: input : G, t, size, memSize
3: output: cache
4: cache ← ∅;
5: memLeft ← memSize;
6: next ← pickNext (G, cache, size, memLeft, t);
7: while nextNode ≠ ∅ do
8:     cache ← cache ∪ next;
9:     memLeft ← memLeft - size(next);
10:    next ← pickNext (G, cache, size, memLeft, t);
11: return cache;
12: end

1: Algorithm GreedyOptimizer:
2: input : G, t, size, memSize
3: output: cache
4: cache ← ∅;
5: memLeft ← memSize;
6: next ← pickNext (G, cache, size, memLeft, t);
7: while nextNode ≠ ∅ do
8:     cache ← cache ∪ next;
9:     memLeft ← memLeft - size(next);
10:    next ← pickNext (G, cache, size, memLeft, t);
11: return cache;
12: end

1: Procedure pickNext:
2: input : G, cache, size, memLeft, t
3: output: next
4: minTime ← ∞;
5: next ← ∅;
6: for v ∈ nodes(G) do
7:     runtime ← estRuntime (G, cache ∪ v, t);
8:     if runtime < minTime & size(v) < memLeft then
9:         next ← v;
10:        minTime ← runtime;
11: end
12: return next;
13: end
an order of magnitude slower than reading from memory, and each operator will have a different computational profile. Second, algorithms for the weighted paging problem don’t take into account weights that are dependent on the current state of the cache. e.g. it may be much faster to compute image features if images are already in cluster memory than if they need to be retrieved from disk.

However, it is possible to rewrite the optimization problem above as a mixed-integer linear program (ILP), but in our experiments the cost of solving these problems for reasonably complex pipelines with high end ILP solvers was prohibitive for practical use [22] at optimization time. Instead, we implement the greedy Algorithm [1]. Given an unoptimized pipeline DAG, the algorithm chooses to cache the node which will lead to the largest savings in terms of execution time but whose output fits in available memory. This process proceeds iteratively until either no benefit to additional caching is possible or all available memory has been used.

5 Evaluation

To evaluate the effectiveness of KeystoneML, we explore its ability to efficiently support large scale ML applications in three domains. We also compare KeystoneML with other systems for large scale ML and show how our high-level operators and optimizations can improve performance. Following that we break down the end-to-end benefits of the previously discussed optimizations. Finally, we assess the system’s ability to scale and show that KeystoneML scales well by enabling the development of scalable, composable components.

Implementation: We implement KeystoneML on top of Apache Spark, a cluster computing engine that has been shown to have good scalability and performance for many iterative ML algorithms [44]. In KeystoneML we added an additional cache-management layer that is aware of the multiple Spark jobs that comprise a pipeline, and implemented ML operators in the KeystoneML Standard Library that are absent from Spark MLLib. While the current implementation of the system is Spark-specific, Spark is merely a distributed execution environment and our system can be ported to other backends.

Experiments are run on Amazon EC2 r3.4xlarge instances. Each machine has 8 physical cores, 122 GB of memory, and a 320 GB SSD, and was running Apache Spark 1.3.1, Scala 2.10, and HDFS from the CDH4 distribution of Hadoop. We have also run KeystoneML on Apache Spark 1.5.1, 1.6 and not encountered any performance regressions. We use OpenBLAS for numerical operations and Vowpal Wabbit [34] v8.0 and SystemML [21] v0.9 in our comparisons. If not otherwise specified, we run on a 16-node cluster.

5.1 End-to-End ML Applications

To demonstrate the flexibility and generality of the KeystoneML API, we implemented end-to-end machine learning pipelines in several domains including text classification, image classification and speech recognition. We next describe these pipelines and compare statistical accuracy and performance results obtained using KeystoneML to previously published results. We took every effort to recreate these pipelines as they were described by their authors, and made sure that our pipelines achieved comparable or better statistical results than those reported by each benchmark’s respective authors.

The operators used to implement these applications are outlined in Table 4 and the datasets used to train them are described in Table 3. In each case, the datasets significantly increase in size as part of the featurization process, so at model fitting time the size is substantially larger than the raw data, as shown in the last two columns of the table. The Solve Size is the size of the dataset that is input to a Linear Solver. This may be too large for available cluster memory, as is the case for TIMIT. Accuracy results on each dataset achieved with KeystoneML as well as those achieved with the original authors code or (where code was unavailable) as reported in their respective works, are reported in Table 5.

Table 4: Operators used in constructing pipelines for datasets in Table 3

| Task          | Type   | Operators Used                                      |
|---------------|--------|-----------------------------------------------------|
| Amazon Reviews Classification | Text   | LowerCase, Tokenize NGrams, TermFrequency LogisticRegression |
| TIMIT Kernel SVM Classification | Speech | RandomFeatures, Pipeline.gather LinearSolver |
| ImageNet Classification | Image  | GrayScale, SIFT, PCA, GMM FisherVector, LinearSolver |
| VOC Classification | Image  | GrayScale, SIFT, PCA, GMM FisherVector, LinearSolver |
| CIFAR-10 Classification | Image  | Windower, PatchExtractor ZCAWhitener, Convolver, LinearSolver SymmetricRectifier, Pooler |

Text Analytics: KeystoneML makes it simple for developers to scale their text pipelines to large datasets. Combined with libraries like CoreNLP [40], KeystoneML allows for scalable implementations of many text classification pipelines such as the one shown in Figure 2. We evaluated a text classification pipeline based on [39] on the Amazon Reviews dataset of 65m product reviews [42] with 100k sparse features. We find that KeystoneML matches the statistical performance of a Vowpal Wabbit [34] pipeline when run on identical resources.
Table 3: Dataset Characteristics. While raw input sizes may be modest, intermediate state may grow by orders of magnitude before being input to a solver.

| Dataset  | Train Size (GB) | Num Train | Test Size (GB) | Num Test | Classes | Type          | Solve Features | Solve Size (GB) |
|----------|-----------------|-----------|----------------|----------|---------|---------------|----------------|-----------------|
| Amazon   | 13.97           | 65000000  | 3.88           | 18091702 | 2       | text          | 100000         | 89.1            |
| TIMIT    | 7.5             | 2251569   | 0.39           | 115934   | 147     | 440-dim vector| 528000         | 8857            |
| ImageNet | 74              | 1281167   | 3.3            | 500000   | 1000    | 10k pixels image | 262144         | 2502            |
| VOC      | 0.428           | 5000      | 0.420          | 5000     | 20      | 260k pixels image | 409600         | 1.52            |
| CIFAR-10 | 0.500           | 500000    | 0.001          | 10000    | 10      | 1024 pixels image | 135168         | 62.9            |
| Youtube8m| 22.07           | 5786881   | 6.3            | 1652167  | 4800    | 1024-dim vector | 1024           | 44.15           |

Table 5: Time to Accuracy with KeystoneML obtained on ML pipelines described in the relevant publication. Accuracy for VOC is mean average precision. Accuracy for ImageNet is Top-5 error.

| Dataset         | KeystoneML Accuracy | Time (m) | Reported Accuracy | Time (m) |
|-----------------|----------------------|----------|-------------------|----------|
| Amazon          | 91.6%                | 3.3      | -                 | -        |
| TIMIT           | 66.06%               | 138      | 66.33%            | 120      |
| ImageNet        | 367.43%              | 270      | 66.58%            | 5760     |
| VOC 2007        | 57.2%                | 7        | 59.2%             | 87       |
| CIFAR-10        | 84.0%                | 28.7     | 84.0%             | 50.0     |

5.2 KeystoneML vs. Other Systems

We compare runtimes for the KeystoneML solver with both a specialized system, **Vowpal Wabbit** [34], built to estimate linear models, and **SystemML** [21], a general purpose ML system, which optimizes the implementation of linear algebra operators used in specific algorithms (e.g., Conjugate Gradient Method), but does not choose among logically equivalent algorithms. We compare solver performance across different feature sizes for two binary classification problems: Amazon and a binary version of TIMIT. The systems were run with identical inputs and objective functions, and we report end-to-end solve time. For this comparison, we solve binary problems because SystemML does not include a multiclass linear solver.

The results are shown in Figure 8. The optimized
The reasons for these performance differences are twofold: first, since KeystoneML raises the level of abstraction to the logical level, the system can automatically select, for example, a sparse solver for sparse data or an exact algorithm when the number of features is low, or a block solver when the features are high. In the middle, particularly for KeystoneML vs. SystemML on the Binary TIMIT dataset, the algorithms are similar in terms of complexity and access patterns. In this case KeystoneML is faster because feature extraction is pipelined with the solver, while SystemML requires a conversion process for data to be fed into a format suitable for the solver. If we only consider the solve step of the pipeline, KeystoneML is roughly 1.5× faster than SystemML for this problem.

TensorFlow is a newly open-sourced ML system developed by Google [3]. Developed concurrently to KeystoneML, TensorFlow also represents pipelines as graph of dataflow operators. However, the design goals of the two systems are fundamentally different. KeystoneML is designed to support horizontally scalable workloads to offer good scale out performance for conventional machine learning applications consisting of featurization and model estimation, while TensorFlow is designed to support neural network models trained via minibatch Stochastic Gradient Descent (SGD) with back-propagation. We compare against TensorFlow v0.8 and adapt a multi-GPU example [1] to a distributed setting in a procedure similar to [13].

To illustrate the differences, we compare the systems’ performance on CIFAR-10 top-1 classification performance. While the learning tasks are identical (i.e., make good predictions on a test dataset, given a training dataset), the workloads are not identical. Specifically, TensorFlow implements a model similar to the one presented in [33], while in KeystoneML we implement a version of the model similar to [16]. TensorFlow was run with default parameters and we experimented with strong scaling (fixed 128 image batch size) and weak scaling (batch size of 128 × Machines).

For this workload, TensorFlow achieves its best performance on 4-node cluster with 32 total CPU cores, running in 57 minutes. Meanwhile, KeystoneML surpasses its performance at 8 nodes and continues to improve in total runtime out to 32 nodes, achieving a minimum runtime of 29 minutes, or a 1.97× speedup. These results are summarized in Table 6. We ran TensorFlow on CPUs for the sake of comparability. Prior benchmarks [1] have shown that the speed of a single multi-core CPU is comparable to a single GPU; thus the same pipeline finishes in 50 minutes on a 4 GPU machine.

TensorFlow’s lack of scalability on this task is fundamental to the chosen model and the algorithm being used to fit it. Minimizing a non-convex loss function via minibatch Stochastic Gradient Descent (SGD) requires coordination of the model parameters after a small number of examples are seen. In this case, the coordination requirements surpass the savings from parallelism at a small number of nodes. While TensorFlow has better scalability on some model architectures [58], it is not scalable for other architectures. By contrast, by using a communication-avoiding solver we are able to scale out KeystoneML’s performance on this task significantly further.

Table 6: Time, in minutes, to 84% accuracy on the CIFAR-10 dataset with KeystoneML and TensorFlow configured for both strong and weak scaling. In large weak scaling regimes TensorFlow failed to converge to a good model.

Finally, a recent benchmark dataset from YouTube [4] describes learning pipelines involving featurization with a neural network [58] followed by a logistic regression model or SVM. The authors claim that “models train to convergence in less than a day on a single machine using the publicly-available TensorFlow framework.” We performed a best-effort replication of this pipeline us-

Figure 8: KeystoneML’s optimizing linear solver outperforms both Vowpal Wabbit and SystemML because it selects an appropriate algorithm to solve the logical problem, as opposed to relying on a one-size fits all operator. At 1024 features for the Binary TIMIT problem, KeystoneML chooses to run an exact solve, while from 2048 to 32768 features it chooses a Dense L-BFGS implementation. At 65536 features (not pictured), KeystoneML finishes in 17 minutes, while SystemML takes 1 hour and 40 minutes to converge to worse training loss over 10 iterations, a speedup of 5.5×.

The reasons for these performance differences are twofold: first, since KeystoneML raises the level of abstraction to the logical level, the system can automatically select, for example, a sparse solver for sparse data or an exact algorithm when the number of features is low, or a block solver when the features are high. In the middle, particularly for KeystoneML vs. SystemML on the Binary TIMIT dataset, the algorithms are similar in terms of complexity and access patterns. In this case KeystoneML is faster because feature extraction is pipelined with the solver, while SystemML requires a conversion process for data to be fed into a format suitable for the solver. If we only consider the solve step of the pipeline, KeystoneML is roughly 1.5× faster than SystemML for this problem.

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We are unable to replicate the author’s claimed accuracy—our pipeline achieves 21% mAP while they report 28% mAP. KeystoneML trains a linear classifier on this dataset in 3 minutes, and a converged logistic regression model with worse accuracy in 90 minutes (31 batch gradient evaluations) on a 32-node cluster. The ability to choose an appropriate solver and readily scale out are the key enablers of KeystoneML’s performance.

We now study the impact of KeystoneML’s optimizations.

### 5.3 Optimization Levels

The end-to-end results reported earlier in this section are achieved by taking advantage of the complete set of optimizations available in KeystoneML. To understand how important the per-operator and whole-pipeline optimizations described in Sections 3 and 4 are, we compare three different levels of optimization: a default unoptimized configuration (`None`), a configuration where only whole-pipeline optimizations are used (`Pipe Only`) and a configuration with operator-level and whole-pipeline optimizations (`KeystoneML`).

Results comparing these levels, with a breakdown of stage-level timings on the VOC, Amazon and TIMIT pipelines are shown in Figure 9. For the Amazon pipeline the whole-pipeline optimizations improve performance by 7×, but the operator optimizations do not help further, because the Amazon pipeline uses CoreNLP featurizers which do not have statistical optimizations associated with them, and the default L-BFGS solver turns out to be optimal. The performance gains come from caching intermediate features just before the L-BFGS solve. For the TIMIT pipeline, run with 16k features, we see that the end-to-end optimizations only give a 1.3× speedup but that selecting the appropriate solver results in a 8× speedup over the baseline. Finally in the VOC pipeline the whole pipeline optimization gives around 3× speedup. Operator-level optimization chooses good PCA, GMM and solver operators resulting in a 12× improvement over the baseline, or 15× if we amortize the optimization costs across many runs of a similar pipeline. Optimization overheads are insignificant except for the VOC pipeline. This dataset has relatively few examples, so the sampling strategy takes more time relative to the other datasets.

### 5.4 Automatic Materialization Strategies

As discussed in Section 4, one key optimization enabled by KeystoneML’s ability to capture the complete application DAG to dynamically determine where to materialize reused intermediate objects, particularly in the presence of memory constraints. In Figure 10 we demonstrate the effectiveness of the greedy caching algorithm proposed in Section 4. Since the algorithm needs local profiles of each node’s performance, we measured each node’s running time on two samples of 512 and 1024 examples. We extrapolate the node’s memory usage and runtime to

![Figure 10: The KeystoneML caching strategy outperforms a rule-based and LRU caching strategy at many levels of memory constraints and responds well to memory pressure.](image)

![Figure 11: On the VOC workload, the KeystoneML caching strategy selects the colored nodes for caching when allotted 80 GB of cache per machine. As memory resources become scarce, the strategy automatically picks less memory intensive nodes to cache. At smaller scales, only the nodes in dark gray are cached.](image)
full scale using linear regression. We found that memory estimates from this process are highly accurate and runtime estimates were within 15% of actual runtimes. If estimates are inaccurate, we fall back to an LRU replacement policy for the cache set determined by this procedure. While this measurement process is imperfect, it is adequate at identifying relative running times and thus is sufficient for our purpose of resource management.

We compare this strategy with two alternatives—the first is a simple rule-based approach which only caches the results of Estimators. This is a sensible rule to follow, as the result of an Estimator (a Transformer or model) is computationally expensive to acquire and typically holds a small memory footprint. However, this is not sufficient for most practical pipelines because if a pipeline contains more than one Estimator, often the input to the first Estimator will be used downstream, thus presenting an opportunity for reuse. The second approach is a Least Recently Used (LRU) policy: in a regime where memory is unconstrained, LRU matches the ideal strategy and further, LRU is the default memory management strategy used by Apache Spark. However, LRU does not take into account that datasets from other jobs (even ones in the same pipeline) are vying for presence in cluster memory.

From Figure 10 we notice several important trends. First, the KeystoneML strategy is nearly always better than either of the other strategies. In the unconstrained case, the algorithm is going to remember all reused items as late in their journey through the pipeline as possible. In the constrained case, it will do as least as well as remembering the (small) estimators which are by definition reused later in the pipeline. Additionally, the strategy degrades effectively, mixing between the best performance of the limited-memory rule-based strategy and the LRU based “cache everything” strategy which works well in unconstrained settings. Curiously, as we increased the memory available to caching per-node, the LRU strategy performed worse for the Amazon pipeline. Upon further investigation, this is because Spark has an implicit admission control policy which only allows objects under some proportion of the cache size to be admitted to the cache at runtime. As the cache size gets bigger in the LRU case, massive objects which are not then reused are admitted to the cache and evict smaller objects which are reused and thus need to be recomputed.

To give a concrete example of the optimizer in action, consider the VOC pipeline (Figure 11). When memory is not unconstrained (80 GB per node), the outputs from the SIFT, ReduceDimensions, Normalize and TrainingLabels are cached. When memory is restricted (5 GB per node) only the output from Normalize and TrainingLabels are cached. These results show that both per-operator and whole-pipeline optimizations are important for end-to-end performance improvements. We next study the scalability of the system on three workloads.

5.5 Scalability

As discussed in previous sections, KeystoneML’s API design encourages the construction of scalable operators. However, some estimators like linear solvers need coordination among workers to compute correct results. In Figure 12 we demonstrate the scaling properties from 8 to 128 nodes of the text, image, and Kernel SVM pipelines on the Amazon, ImageNet (with 16k features) and TIMIT datasets (with 65k features) respectively. The ImageNet pipeline exhibits near-perfect horizontal scalability up to 128 nodes, while the Amazon and TIMIT pipeline scale well up to 64 nodes.

To understand why the Amazon and TIMIT pipeline do not scale linearly to 128 nodes, we further analyze the breakdown of time by stage. We see that each pipeline is dominated by a different part of its computation. The TIMIT pipeline is dominated by its solve stage, while featurization dominates the Amazon and ImageNet pipelines. Scaling linear solvers is known to require coordination, which leads directly to sub-linear scalability of the whole pipeline. Similarly, in the Amazon pipeline, one of the featurization steps uses an aggregation tree which does not scale linearly.

6 Related Work

ML Frameworks: ML researchers have traditionally used MATLAB or R packages to develop ML routines. The importance of feature engineering has led to tools like scikit-learn and KNIME adding support for featurization for small datasets. Further, existing libraries for large scale ML like Vowpal Wabbit, GraphLab, MLlib, RIOT, DimmWitted focus on efficient implementations of learning algorithms like regression, classification and linear alge-
Query Optimization, Modular Design, Caching: There are several similarities between the optimizations made by KeystoneML and traditional relational query optimizers. Even the earliest relational query optimizers used multiple physical implementations of equivalent logical operators, and like many relational optimizers, the KeystoneML optimizer is cost-based. However, KeystoneML supports much richer set of data types than a traditional relational query system, and our operators lack some relational algebra semantics, such as commutativity, limiting the system’s ability to perform certain optimizations. Further, KeystoneML switches among operators that provide exact answers vs approximate ones to save time due to the workload setting. Data characteristics such as sparsity are not traditionally considered by optimizers.

The caching strategy employed by KeystoneML can be viewed as a form of view selection for materialized view maintenance over queries with expensive user-defined functions. We focus on materialization for intra-query optimization, as opposed to inter-query optimization. While much of the related work focuses on the challenging problem of view maintenance in the presence of updates, KeystoneML exploits the iterative nature and immutable properties of this state.

7 Future Work and Conclusion

KeystoneML represents a significant first step towards easy-to-use, robust, and efficient end-to-end ML at massive scale. We plan to investigate pipeline optimizations like node reordering to reduce data transfers and also look at how hyperparameter tuning can be integrated into the system. The existing KeystoneML operator APIs are synchronous and our existing pipelines are acyclic. In the future we plan to study how algorithms like asynchronous SGD or back-propagation can be integrated with the robustness and scalability that KeystoneML provides.

We have presented the design of KeystoneML, a system that enables the development end-to-end ML pipelines. By capturing the end-to-end application, KeystoneML can automatically optimize execution at both the operator and whole-pipeline levels, enabling solutions that automatically adapt to changes in data, hardware, and other environmental characteristics.

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