Distributed Information-Theoretic Metric Learning in Apache Spark

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Abstract—Distance metric learning (DML) is an effective similarity learning tool to learn a distance function from examples to enhance the model performance in applications of classification, regression, and ranking, etc. Most DML algorithms need to learn a Mahalanobis matrix, a positive semidefinite matrix that scales quadratically with the number of dimensions of input data. This brings huge computational cost in the learning procedure, and makes all proposed algorithms infeasible for extremely high-dimensional data even with the low-rank approximation. Differently, in this paper, we take advantage of the power of parallel computation and propose a novel distributed distance metric learning algorithm based on a state-of-the-art DML algorithm, Information-Theoretic Metric Learning (ITML). More specifically, we utilize the property that each positive semidefinite matrix can be decomposed into a combination of rank-one and trace-one matrices and convert the original sequential training procedure into a parallel one. In most cases, the communication demands of the proposed method are also reduced from $O(d^2)$ to $O(cd)$, where $d$ is the number of dimensions of the data and $c$ is the number of constraints in DML and can be smaller than $d$ by appropriate selection. Moreover importantly, we present a rigorous theoretical analysis to upper bound the Bregman divergence between the sequential algorithm and the parallel algorithm, which guarantees the correctness and performance of the proposed algorithm. Our experiments on datasets with $O(10^3)$ features demonstrate the competitive scalability and the performance compared with the original ITML algorithm.

INTRODUCTION

Learning an appropriate distance metric is an important topic in both machine learning and data mining. Distance metric learning has been widely applied in many problems, such as image retrieval [1], face recognition [1], bioinformatics analysis [2], software error detection [3], [4]. Earlier publications formulate the learning problem as an convex optimization problem by maximizing the sum of difference between the dissimilar instances while restricting the distance between the similar instances to be small [5]. However, solving such problem by semidefinite programming (SDP) solver or eigenvalue decomposition is time-consuming and poorly scalable to medium and high dimensional data. Recent developments such as Large Margin Nearest Neighbors (LMNN) [6], [7], BoostMetric [8] and Information-Theoretic Metric Learning (ITML) [3] try to speedup DML by the special structure of Mahalanobis matrix, partial eigenvalue decomposition or low-rank approximation.

However, Most of existing algorithms are incapable of handling high-dimensional data. LMNN is very easy to overfit for high-dimensional data. BoostMetric employing the max eigenvalue decomposition needs a huge number of iterations to converge for high-dimensional data. ITML conducts heavy matrix multiplications which is very time-consuming for high-dimensional data.

For other earlier work, is a popular solution for DML problem but it is very easy to overfit especially for high-dimensional data. [9] relies on the special structure of Mahalanobis matrix. [8] is an efficient DML solution only related with the max eigenvalue decomposition, however, it needs a huge number of iterations to converge for high-dimensional data.

In the high dimensional setting, most existing work mainly exploit the low-rank structure of the learned matrix or the sparsity of the covariance matrix. Instead of learning the full rank matrix A, [10] factorizes the matrix A as $RR^T$ and learned a low rank approximation of the Mahalanobis matrix. [11] imposes a different prior on learning the Mahalanobis distance based on the sparsity of sample concentration matrix $\Sigma^{-1}$, where $\Sigma$ is the covariance matrix of samples. [12] proposed the low dimensional projection to extract a compact feature representation for originally high dimensional data. However, all the above properties may not hold for highly complex data in real-life applications. Although each of these algorithm was shown to yield excellent performance in classification and clustering tasks, they do not generalize learning an arbitrary metric, parameterized by an arbitrary matrix. To the best of our knowledge, it is still nontrivial to learn the approximated distance between two instances with high dimensionality if the low-rank property is not satisfied. Hence, how to learn the metric without highly depending on the low-rank assumption still requires sophisticated designs and experimental explorations.

Meanwhile, with large volumes of data available in many real life applications, the problem of scalability becomes the key concern in designing many machine learning algorithms. Most of the existing work in scalable machine learning relies on approximation methods and parallel computing schemes. Specifically, in term of the algorithm aspect, most existing work mainly focus on stochastic gradient descent method...
for convex optimization problem [13], [14], [15] or proximal descent method for non-convex problem [16], [17], [18]. Few effort has been done on solving the semi-definite programming problem for matrices in a distributed cluster, especially for DML problem. Very recently, [19] proposed a distributed approach to speedup the computation of DML problem. Unfortunately, both of its methodology and proofs heavily rely on the low-rank property of Mahalanobis matrix. Forcing low-rank assumption without understanding the data may destroy the completeness of the data and yield suboptimal performance.

To address the above two challenges, taking advantage of powerful multi-thread cluster, we will explore to design a general parallel approach to solve DML problem for high-dimensional data without low-rank assumption about the Mahalanobis matrix. In this paper, we will design a scalable solution to speedup the training of ITML, which repeats Bregman projection [20]. By decomposing the Mahalanobis matrix into a linear combination of rank-one matrices, and dispatching them into different machines like a divide-and-conquer scheme, our implementation performs Bregman projection on these rank-one matrices without low-rank assumption about the Mahalanobis matrix. Finally, after iterations, the Mahalanobis matrix can be reconstructed from these rank-one matrices to calculate the pair-wise distances.

In summary, the proposed work contributes on the following aspects:

- By making a trade-off between accuracy and running time, we first propose a scalable approach to learn metrics from high-dimensional data without low-rank assumption.
- We compare the proposed method with the original ITML method from a theoretical perspective and give an upper error bound brought by our parallel update.
- The experiments conducted on the data with different scales demonstrate the correctness and the scalability of the our method.

**Related Work**

Since Xing et al. [5] formulate the distance metric learning problem as an optimization problem and solve it by semi-definite programming, there are many DML algorithms in the literature, which are developed for different objectives, such as learning global metric [8], local metric [21] or any special structured metric [22]. Completed surveys from different perspectives can be found in [4], [23]. Some algorithms focus on pairs-wise constraints [24], [25], some solves the optimization problem with relative constraints [6]. Due to the high complexity of computation, the majority of DML algorithms target low-dimensional or intermediate dimensional data up to hundreds of dimensions.

Several algorithms [11], [26] attempt to meet the challenge of high-dimensional metric learning. [27] assumes the Mahalanobis matrix as low-rank matrix and represented as $RR^T$. Meanwhile, [11] takes another form of low-rank assumption that the Mahalanobis matrix is sparse. [28] reduces the computational complexity during the eigendecomposition by picking up the largest eigenvalue and the corresponding eigenvector in a variant Frank-Wolfe algorithm [29], [30] targets to the similar objective by taking the top-$k$ eigenvalues and those corresponding eigenvectors. [26] simplifies the high-dimensional metric learning with multiple stages. [31] reformulates the high-dimensional Mahalanobis matrix as a combination of low-rank matrices, which are computed from gradient boosting as weak learners. In this paper, we also employ the similar formulation but with different approach to update the low-rank matrices.

**Formulation**

The distance metric learning task could be formulated as learning a Mahalanobis distance from a set of similar and dissimilar pairs of sample data. The Mahalanobis distance is defined as follows:

$$d(x,y) = \sqrt{(x-y)^TA(x-y)} \quad \forall x, y \in \mathbb{R}^n$$

where $A \in \mathbb{S}_+$. In most cases, we only take care about the squared Mahalanobis distance, which is denoted as $d_A$ in the following context. Now the problem is translated to learn the positive semi-definite matrix $A$ through the input data point. The input data are two sets representing pairs of similar data points and pairs of dissimilar data points respectively.

Given $n$ instances $\{x_1, x_2, \ldots, x_n\}$ in $\mathbb{R}^d$, we aims at learning the matrix $A$ which is involved in the Mahalanobis distance function $d_A(x_i, x_j) = (x_i - x_j)^TA(x_i - x_j)$.

Suppose that we have the similar and dissimilar pairs of instances $(x_i, x_j)$ in the set $S$ and $D$ respectively. We would like to keep the distance of the similar pairs small, i.e. $d_A(x_i, x_j) \leq u$ when $(x_i, x_j) \in S$, while separate the dissimilar pairs as possible, i.e. $d_A(x_i, x_j) \geq l$ when $(x_i, x_j) \in D$, where $u$ and $l$ are constant.

$$S = \{(x_i, x_j) : d_A(x_i, x_j) \leq u\}$$

$$D = \{(x_i, x_j) : d_A(x_i, x_j) \geq l\}$$

**Information-Theoretic Metric Learning (ITML)**

ITML is one of the start-of-art algorithm for distance metric learning. It brings an assumption that the data come from multivariate Gaussian distribution, which is very common in most applications. Under this assumption, the Mahalanobis distance matrix $A$ can be expressed as the inverse of the covariance matrix of the multivariate Gaussian distribution. Because the probability density function of multivariate Gaussian can be reformulated as $p(x; \mu) = \frac{1}{(2\pi)^{n/2}\det(A)}\exp(-\frac{1}{2}(x-\mu)^TA(x-\mu))$. Hence, the original DML problem is expressed as finding a proper multivariate Gaussian by minimizing difference relative entropy with the initial Mahalanobis distance function. The objective function is reformulated as:
\[
\begin{align*}
\min & \quad KL(p(x; \mu_0)||p(x; \mu)) \\
\text{s.t.} & \quad d_A(x_i, x_j) \leq u, \quad (i, j) \in S \\
& \quad d_A(x_i, x_j) \geq l, \quad (i, j) \in D
\end{align*}
\]

where,

\[
KL(p(x|\mu_0, A_0)||p(x|\mu, A)) = \int p(x|\mu_0, A_0) \log \frac{p(x|\mu_0, A_0)}{p(x|\mu, A)} dx
\]

\(A_0\) is usually assigned to the identity matrix.

More specifically, the KL divergence in Eq.(2) can be expressed as a convex combination between a Mahalanobis distance between means and the Bregman divergence with respect to function \(\phi(A) = -\log \det(A)\) between covariance matrices [32]:

\[
KL(p(x|\mu_0, A_0)||p(x|\mu, A)) = \frac{1}{2} D_\phi(A, A_0) + \frac{1}{2} d_{\Sigma^{-1}}(\mu_0, \mu)
\]

where the Bregman divergence is defined as:

\[
D_\phi(A, A_0) = \phi(A) - \phi(A_0) - \text{tr}(\nabla \phi(A_0)^T(A - A_0))
\]

With the assumption that the mean vectors of two Gaussian distribution are the same, ITML formulates the DML problem as:

\[
\begin{align*}
\min & \quad D_\phi(A, A_0) \\
\text{s.t.} & \quad \text{tr}(A(x_i - x_j)(x_i - x_j)^T) \leq u, \quad (x_i, x_j) \in S \\
& \quad \text{tr}(A(x_i - x_j)(x_i - x_j)^T) \geq l, \quad (x_i, x_j) \in D
\end{align*}
\]

This problem is then cast into a particular Bregman Matrix Divergence problem [33], which contains global optimal solution and can be solved efficiently by Eq.(6) without eigenvalue computations or semi-definite programming.

\[
A_{t+1} = A_t + \beta A_t (x_i - x_j)(x_i - x_j)^T A_t
\]

where \(\beta\) is a scalar for the learning rate. The actual distance between a pair of data sample \((x_i, x_j)\) in each iteration is computed from:

\[
p(t) = (x_i - x_j)^T A_t (x_i - x_j)
\]

**Parallel Distance Metric Learning**

The algorithm (see details in [3]) repeats the Bregman projection in Eq.(6) with different constraints sequentially. For each projection, it involves the computation on \(A_t \in \mathbb{R}^{d \times d}\), where \(d\) is the number of dimensions of the input data. When \(d\) is large enough, the running time of the Bregman projection in single PC is not acceptable. That why the previous work with sequential update is only capable of handling the data with \(O(10^2)\)-dimension.

In this paper, we try to conduct the Bregman projection with the power of parallel computation. The key step in Eq.(6) is to update the Mahalanobis matrix which is a \(d \times d\) positive semi-definite matrix. Typically, there are two roads to parallel this update: 1) compute the matrix multiplication in Eq.(6) directly in distributed way. For example, the matrix is decomposed into blocks which are dispatched into different machines. When the local computation with respect to blocks finishes, the intermediate results are collected to form a complete matrix update. The drawback of this kind of approaches is obvious that there are heavy communications demand for carrying out the data in blocks; 2) design a Hogwild! [34]-like approach to update the Mahalanobis matrix based on partial information simultaneously. Unfortunately, the positive semi-definite property of Mahalanobis matrix is difficult to hold from multiple partial updates.

In order to hold the positive semi-definite property, we borrow the idea from [8] that any positive semi-definite matrix can be decomposed into a linear combination of rank-one matrices. Therefore, we have proposed a novel parallel solution for DML problem by reformulating the Mahalanobis matrix \(A\) as \(A = I + \sum c_i z_i z_i^T\) where \(z_i \in \mathbb{R}^d\). By observing the update in Eq.(6), it is easy to find that \(A_t (x_i - x_j)\) is a vector with \(d\) dimension and \(A_t (x_i - x_j)(x_i - x_j)^T A_t^T\) is a rank-one matrix. Hence, we can concretely the formula of \(A\) by summing over the Bregman projection through all pairs of constraints in Eq.(8)

\[
A_{t+1} = I + \sum_{i=1}^C \beta_i(t) z_i(t) z_i(t)^T
\]

where, \(I\) is the unit matrix with the size of \(d \times d\), \(C\) is the number of pairs of constraints, \(\beta_i\) is the step from Bregman projection in Eq.(6) and \(z_i(t)(x_i, x_j)\) for the \(i\)-th pair of constraint \((x_j, x_k)\). Actually, in the proposed framework, we only store \(z\) rather than \(A_t\) because \(A_t\) is a huge matrix when \(d\) becomes large. Consequently, the update of \(z\) is changed to Eq.(9)

\[
z_{k}(t + 1) = A_{t+1} c_k = \left( I + \sum_{i=1}^C \beta_i(t) z_i(t) z_i(t)^T \right) c_k
\]

Based on the original algorithm in [3], \(\beta_i(t)\) is a function of \(p_i(t)\) in Eq. (7) and the upper bound or lower bound of constraints (see the details in Algorithm 1). The key step of updating \(\beta_k(t)\) is to compute the actual distance \(p_k(t)\). Combined with Eq.(8), the actual distance for the \(k\)-th constraint \(c_k\) can be expressed in Eq.(10)

\[
p_k(t) = c_k^T A_t c_k = c_k^T \left( I + \sum_{i=1}^C \beta_i(t) z_i(t) z_i(t)^T \right) c_k
\]

Due to the separable property of the Mahalanobis matrix \(A\) in Eq. (8), we can dispatch the tasks for updating \(z\) in Eq.(9)
Algorithm 1 Parallel Distance Metric Learning

Input: $S$: set of similar pairs; $D$: set of dissimilar pairs; $u, l$: distance thresholds; $\gamma$: slack parameter

Output: $A$: Mahalanobis matrix

1. $A = I, C = |S| + |D|
2. for constraint $(x_p, x_q)_k, k \in \{1, 2, \ldots, C\}$ do
   3. $\lambda_k \leftarrow 0$
   4. $d_k \leftarrow u$ for $(x_p, x_q)_k \in S$ otherwise $d_k \leftarrow l$
   5. $c_k \leftarrow (x_p - x_q)_k, z_k \leftarrow c_k$
   6. end for
7. while $\beta$ does not converge do
   8. for all worker $k \in \{1, 2, \ldots, C\}$ do in parallel
      9. $z_k = c_k + \sum_{i=1}^{C} \beta_i z_i z_i^T c_k$
     10. $p \leftarrow c_k^T z_k$
     11. if $(x_p, x_q)_k \in S$ then
         12. $\alpha \leftarrow \min \left(\lambda_k, \frac{1}{\gamma} \left(\frac{1}{p} - \frac{1}{d_k}\right)\right)$
         13. $\beta \leftarrow \frac{\alpha}{1 + \alpha p d_k}$
         14. $d_k \leftarrow \frac{\gamma d_k - \alpha}{\gamma + \alpha p d_k}$
     15. else
         16. $\alpha \leftarrow \min \left(\lambda_k, \frac{1}{\gamma} \left(\frac{1}{d_k} - \frac{1}{p}\right)\right)$
         17. $\beta \leftarrow \frac{\alpha}{1 + \alpha p d_k}$
         18. $d_k \leftarrow \frac{\gamma d_k - \alpha}{\gamma + \alpha p d_k}$
     19. end if
   20. $\lambda_k \leftarrow \lambda_k - \alpha$
   21. $z_k \leftarrow \left(I + \sum_{i=1}^{C} \beta_i z_i z_i^T\right) c_k$
   22. send $z_k$ to other workers.
   23. end for
7. end while
24. $A = I + \sum_{i=1}^{C} \beta_i z_i z_i^T$

and $p$ in Eq.(10) into $C$ workers which is an abstract concept representing the parallel executors, such as process in a single machine or different machines.

In our framework, worker $k$ needs to receive all the update of $z$ from other workers at the previous iteration first, then computes the update for the next iteration.

Overall, each work only sends a vector $z$ rather than the matrix $\beta A(x_i - x_j)(x_i - x_j)^T A$ and receive $(C - 1)$ times $z$ rather than the whole Mahalanobis matrix in the original sequential algorithm. Hence, the communications demand for each work reduces from $O(d^2)$ to $O(cd)$. When the number of dimensions exceeds the number of constraints, which is a very commonly happened situation for high-dimensional metric learning tasks, the demand of communications reduces significantly compared with the original ITML algorithm.

Furthermore, when the number of constraints keep relative small, our work is equivalent to a ITML-based method with low-rank assumption about the Mahalanobis matrix. If the number of constraints becomes large, even larger than the number of dimensions, our method still works although the cost for communications will increase inevitably. Therefore, our method is a general parallel approach no matter the Mahalanobis matrix is low-rank or not.

IMPLEMENTATION

We implement our method on Apache Spark [35], which is a general propose, high-efficient, distributed in-memory computing platform. It provides a flexible data structure called Resilient Distributed Dataset (RDD) to support parallel computing on RDDs. The data or parameters in RDDs are cached in memory instead of loading from disk at each iteration like Hadoop 1. Usually, the content of RDD is distributed in different machines and will be re-dispatched automatically without manual operation. Therefore, Spark is suitable for developers who only need to provide high-level logic to parallel the algorithm instead of caring about many details in cluster.

In our implementation, the list of $z$ and the corresponding $\beta$ are stored in a RDD. For each element of this RDD, we assign a “mapper” function to compute the update of $z$ in Eq.(9) and the partial distance in Eq.(10). All these “mapper” function will generate a new RDD to store the new $z$ for next iteration. We also declare a constant “Broadcast” variable which is shared for all workers to store constraints $c$, because the computation of new $z$ in each worker needs its corresponding $c$ and the computation of partial distance iterates all constraints. In most cases, the “Broadcast” variable is cached in memory and can be fetched efficiently. Finally, another special component in Spark, called “Accumulator” will be created to collect the partial distance from each workers.

With the help of the global “Broadcast” and “Accumulator”, the whole distributed algorithm is conducted in bulk synchronous parallel (BSP) [36], which guarantees that all parameters will be updated within the same iteration. More specifically, the employment of “Broadcast” and “Accumulator” in our implementation illustrated in Fig. 1 significantly reduce the redundant computation of the distance between each pairs of data sample under the learned metric space. Because the procedure of computing distance is divided into blocks which are shared among all workers.

THEORETICAL ANALYSIS

In this section, we will analyze the difference and give the upper bound of the proposed algorithm compared with the sequential algorithm in [3]. Because the result of the parallel computation of $z$ in our algorithm may be different with the sequential version of the original algorithm.

First, we will compare the difference between the sequential version and the parallel version. In sequential order, the algorithm conducts $C$ times Bregman projection to cover all pairs of constraints. After $C$ iterations since iteration $t$, the Mahalanobis matrix $A_{t+C}$ can be expressed as:

$$A_{t+C} = A_t + \sum_{i=1}^{C} \beta_i A_{t+i-1} c_i c_i^T A_{t+i-1}^T$$

(11)

For parallel version algorithm, if we rearrange the order of computation like a series of sequential updates, one iteration in

1https://hadoop.apache.org/
The parallel version algorithm is equal to $C$ iterations in sequential algorithm but with the same $A_t$ rather than $A_{t+i-1}$. The formula of parallel algorithm is expressed in Eq. (12):

$$
\hat{A}_{t+C} = A_t + \sum_{i=1}^{C} \beta_i A_t c_i^T A_t^T
$$

By observing the difference between Eq.(11) and Eq.(12), we can find that the Bregman projection related with the $i$-th constraint in parallel algorithm is applied on a $i$-delayed Mahalanobis matrix. Figure 2 illustrates the difference between the normal update and the delayed update.

For convenience, we use the sequential version with delayed update to represent the parallel algorithm.

**Theorem 1. Delayed Update under Bregman Divergence**

Assume the difference of matrices is measured by the Bregman divergence with respect to LogDet divergence $\phi(X) = -\log \det(X)$. The minimizer of $D_\phi(A_0, A)$ after $T$ iterations is $A^*$. The length of convergence path is denoted as $\Omega$. The upper error bound of Algorithm 1 is

$$
R[A] := \sum_{t=1}^{T} D_\phi(A_t, A^*) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

where $||\cdot||_*$ is the Fenchel-Legendre dual norm [38].

Sum up these inequality in Eq.(13) as:

$$
\sum_{t=1}^{T} D_\phi(A_t, A^*) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

**Proof.** From the definition of Bregman divergence and the convexity of function $\phi(A)$ we know:

$$
\phi(A_t) - \phi(A^*) \leq \nabla \phi(A^*)^T (A_t - A^*)
$$

$$
\nabla \phi(A^*)^T (A_t - A^*) \leq \frac{1}{2} ||\lambda_{t-\tau}||^2_2
$$

$$
\sum_{t=1}^{T} D_\phi(A_t, A^*) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

From Lemma 10 in [37], we have easily derived the matrix version as:

$$
\text{tr} \left( \lambda_{t-\tau}^T (A_t - A^*) \right) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

$$
\text{tr} \left( \lambda_{t-\tau}^T (A_t - A^*) \right) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

$$
\sum_{t=1}^{T} D_\phi(A_t, A^*) \leq \frac{1}{\beta_{t-\tau}} (D_\phi(A^*, A_t) - D_\phi(A^*, A_{t+1})) + \frac{1}{2} \beta_{t-\tau} ||\lambda_{t-\tau}||^2_2
$$

Figure 1. Framework of Parallel Distance Metric Learning on Apache Spark

Figure 2. Delayed vs Normal Versions of Projection
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without changing the metric, the proposed method enhances the accuracy of $k$-NN classification from 0.682 to 0.83 on ImageNet dataset.

The comparison between ITML and the proposed method displayed in Fig. 5 shows both of the algorithms will converge with the similar number of iterations. In these experiments, the slack variable $\gamma$ is assigned to 100. Table I also demonstrates the proposed method is able to improve the performance of $k$-NN classification and the accuracy gap between these two algorithms is relative small.

**CONCLUSION**

In this paper, based on the observation that the positive semi-definite Mahalanobis matrix can be decomposed into a series of rank-one matrices, we have developed a parallel distance metric learning algorithm called DITML in order to learn the proper metric from high-dimensional data without low-rank approximation, which is infeasible for previous DML algorithms. Furthermore, the performance gap between the proposed method and the original ITML method is bounded from the theoretical perspective and can be ignored in actual experiments.

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