Learning Sparse Metrics via Linear Programming *

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ABSTRACT

Calculation of object similarity, for example through a distance function, is a common part of data mining and machine learning algorithms. This calculation is crucial for efficiency since it is often repeated a large number of times, the classical example being query-by-example (find objects that are similar to a given query object). Moreover, the performance of these algorithms depends critically on choosing a *good* distance function. However, it is often the case that (1) the correct distance is unknown or heuristically chosen, and (2) its calculation is computationally expensive (*e.g.,* such as for large dimensional objects). In this paper, we propose a method for constructing relative-distance preserving low-dimensional mappings (sparse mappings) to allow learning unknown distance functions or approximating known functions, with the additional property of reducing distance computation time. We present an algorithm that given examples of proximity comparisons among triples of objects (*e.g.,* object a is closer to b than to c), learns a distance function, in as few dimensions as possible, that preserves these distance relationships. The formulation is based on solving a Linear programming optimization problem that finds an optimal mapping for the given dataset and distance relationships. Unlike other popular embedding algorithms, the method can easily generalize to new points, does not have local minima, and explicitly models computational efficiency by finding a mapping that is sparse, i.e. that depends on a *small* subset of features or dimensions. Experimental evaluation shows that the method compares favorably with an state-of-the art method in several publicly available datasets.

Categories and Subject Descriptors

G.4 [**Mathematical Software**]; H.3 [**Information Storage and Retrieval**]: Information Search and Retrieval; H.4 [**Information Systems Applications**]: Miscellaneous

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General Terms

Algorithms, measurement, performance

Keywords

Metric learning, dimensionality reduction, linear programming, linear projections, convex optimization

1. INTRODUCTION AND RELATED WORK

The notion of a *distance* is essential in many machine learning and data mining concepts. From a practical point of view, the choice of a distance has a direct effect on the performance of many algorithms, both in terms of accuracy and efficiency. From an accuracy perspective, numerous algorithms rely on the user being able to provide a *good* distance function (*e.g.,* nearest neighbor, clustering methods, SVM, etc). Here, a *good distance function* is roughly one that is low for similar objects and high for dissimilar ones. Clearly, since objects can be similar or dissimilar in many respects, *similarity* is not absolute and depends on the task of interest; thus, different distance functions should in theory be chosen for different tasks. How to best choose an appropriate distance function remains an interesting problem. From an efficiency perspective, many widely used approaches for data mining, the classical example being query-by-example (find objects that are similar to a given query object), require evaluating a distance function between a large number of points [1]. These calculations often take an important part of the available CPU time and therefore, a relevant problem is how to automatically find accurate approximations to these distance functions but that are efficient to evaluate.

In this paper we present an approach, based on formulating and solving a simple linear programming problem, that allows for automatically building distance functions from examples (1) that are tailored to the problem at hand and (2) that have the additional property of being computationally efficient to evaluate. We are interested in solving the following problem. Let us represent the objects of interest [2] by points $\mathbf{x}_k$ in a D-dimensional space $\Re^D$, with $k = \{1, 2, ..., N\}$. The problem is how to change this representation to points $\hat{\mathbf{x}}_k$ such that distance relationships between points are appropriate for the task of interest according to *side information* provided by a user in the form of distance relationships (see Sec. 1.1) and in addition, the points

[1]Other examples include K-means and kernel-based methods in general

[2]Examples of objects of interest are: database records, user opinions, product characteristics, etc.

lie on lower dimensional space $\Re^d$. In order to achieve this, we are interested in finding a transformation $A : \Re^D \rightarrow \Re^d$ that relates any point in the original space to its low dimensional counterpart. When A is a linear transformation, this can be thought of as learning a Mahalanobis distance (*e.g.,* see [17, 12, 15]). Sec. 1.2 describes the connection and differences between the formulation introduced in this paper, the above, and other related methods.

1.1 Specifying distance information as side information

In this paper, only distance relationships among a number of points are needed to capture the structure of the space, no absolute distances are necessary. These relationships may be provided by a user; thus, it would be beneficial to make the information required from the user (1) simple to obtain and (2) easy to provide. We believe that relationships of the form *object i is closer to j than to k* are both simple to specify and sufficiently informative to capture the properties of the task of interest. In case that an appropriate metric or an algorithm for determining relative similarity were available (but cannot always be used because *e.g.,* it is expensive to evaluate), this information can be obtained more automatically. In choosing this type of relative relationships, we were inspired by the work in [1]; however, distance relationships of this type were also employed in [12]. Note that we are not interested in preserving absolute distances, which are in general much more difficult to obtain[3].

Another interesting property of this type of distance relationships is that they do not require the concept of class labels (*e.g.,* [15]) or the specification of examples of similar objects vs. dissimilar ones (*e.g.,* [17]). The concepts of similar vs. dissimilar are limited by the fact that a user would need knowledge of at least some (and preferably all) of the rest of the objects in order to determine whether two objects are similar or dissimilar (a reference frame is needed).

1.2 Metric learning with dimensionality reduction

The framework presented in this paper is related to different sets of approaches. A first set can be represented by unsupervised methods that have approached the problem of finding low dimensional representations of the data. Some approaches attempt to capture the variance of the data such as Principal Components Analysis [9], while others build low-dimensional embeddings, that is, by transforming a set of data points into a lower dimensional one such that (some or all) distances are preserved. Examples of these approaches include algorithms such as Multidimensional Scaling (MDS) [5], Locally Linear Embeddings (LLE) [11], ISOMAP [13], and low-dimensional embeddings via SDP [16]. These methods can implicitly reduce the amount of computation regarding distance calculations; however due to their purely unsupervised nature, they rely on a distance function to be given and cannot build a function such that the accuracy of certain (*e.g.,* classification) algorithms is improved. In other words, they are not designed to capture the concept of an appropriate distance.

[3]Absolute distances imply relative distances, but the converse is not true.

Another set of approaches that are related to ours in a different manner are those that attempt to learn an appropriate distance function from examples. The most closely related approaches are [17, 12, 1]. The first two require some form of supervision and are designed just to learn good distance functions, without explicitly attempting to improve the efficiency of distance calculations. BoostMap [1] is the most related to our approach in terms of the goals targeted, that is, finding a distance function that is both accurate for the task and efficient to evaluate. Like our method, both [1] and [12] attempt to preserve distance relationships. However, BoostMAP, based on using AdaBoost to combine multiple 1D embeddings to preserve the proximity structure of the data, has the disadvantage that it leads to an iterative, greedy algorithm to optimize the embedding and thus does not have strong optimality guarantees. In contrast, the method in [12] proposes a convex optimization problem based on SVMs. Its disadvantages include the facts that the problem requires quadratic programming and is only designed to find appropriate weights for the different coordinates of the data; thus a very small subset of linear transformations is explored to obtain a solution. Comparing the properties of the solution space, [17] is the most related approach. It is based on finding a square matrix that defines a Mahalanobis distance. The distance is optimized to respect distance constraints represented by two sets, one of similar and one of dissimilar points. The formulation leads to a convex optimization problem.

As we will show, while the general problem formulated in this paper does not appear to accept efficient algorithms, a proposed comparable problem can be solved using just linear programming.

Table 1 shows a collection of approaches that share some of the goals or motivations of the approach presented in this paper. It also highlights several important distinguishing attributes. In particular we have considered (1) computational efficiency: whether the method attempts to find low dimensional representations for efficient distance evaluation, (2) generalization to new points: whether the method can easily generalized to new unseen points, (3) distance learning capability: whether it can learn a distance function from user examples, and (4) power of learning algorithm: whether the learning algorithm finds local-free optima (such as it is the case for convex formulations).

1.3 Notation and background

In the following, vectors will be assumed to be column vectors unless transposed to a row vector by a superscript $\top$. The scalar (inner) product of two vectors $\mathbf{x}$ and $\mathbf{y}$ in the d-dimensional real space $\Re^d$ will be denoted by $\mathbf{x}^\top \mathbf{y}$. The 2-norm and 1-norm of $\mathbf{x}$ will be denoted by $|||\mathbf{x}|||_2$ and $|||\mathbf{x}|||_1$ respectively. For a matrix $A \in \Re^{m \times n}, A_i \in \Re^n$ denotes a row vector formed by the elements of the i-th row of A . Similarly $A_{.j} \in \Re^m$ denotes a column vector formed by the elements of the j-th column of A. A column vector of ones of arbitrary dimension will be denoted by $\vec{e}$, and one of zeros will be denoted by $\vec{0}$. The identity matrix of arbitrary dimension will be denoted by I.

2. LEARNING METRICS

Table 1: Summary of Approaches for Dimensionality Reduction or Metric Learning

Approach	Low dim effic. eval.	Generaliz. to new data	Learns from examp.	Local-min. free (convex)
Athitsos et al. [1]	Y	Y	Y	N
FastMap [6]	Y	Y	N	N
MDS [5]	Y	N	N	N
Schultz-Joachims[12]	N	Y	Y	Y (QP)
Wagstaff et al. [10]	N	Y	Y	N
Weinberger et al. [15]	N	Y	Y	Y (SDP)
Xing et al. [17]	N	Y	Y	Y (IterProj)
This paper	Y	Y	Y	Y (LP)

Table 2: QP=Quadratic Programming, SDP= Semidefinite Programming, IterProj= Iterative Projections + gradient descent, LP= Linear Programming.

Let us say we are given a set of points $\mathbf{x}_k \in \Re^D$ with $k = \{1, ..., N\}$ for which an appropriate distance metric is unknown or expensive to compute. In addition we are given information about a few relative distance comparisons. Formally, we are given a set $\mathcal{T} = \{(i, j, k) | f(\mathbf{x}_i, \mathbf{x}_j) < f(\mathbf{x}_i, \mathbf{x}_k)\}$ for some *distance* function f. As indicated above, f may not be known explicitly, instead a user may only be able to provide this distance relationships sparsely or by example. We are interested in finding a linear transformation $A : \Re^D \rightarrow \Re^d$ such that:

$$\forall (i, j, k) \in \mathcal{T}, ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||_2^2 < ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_k||_2^2 \quad (1)$$

where $\hat{\mathbf{x}}_k = A\mathbf{x}_k$. Additionally, since we would like to enforce efficiency, we would prefer to find matrices A that produce a projection to a lower-dimensional space $\Re^d$.

That is, we would like to find a new representation of the original space in a lower dimension where the L_2 norm respects the desired distance relationships.

It is easy to show that if $A_k = \vec{0}$ (the k-th column of A is equal to the zero vector), then the k-th original dimension (in $\Re^D$) can be ignored to calculate the projection.

3. BASE FORMULATION

Putting the above ideas together, the projection matrix A can be formally defined as the optimal solution to the following optimization problem:

$$\max_{A:\Re^D \rightarrow \Re^d} \sum_{m=1}^{D} \mathbf{1}(A_m = \vec{0}) \quad s.t. \quad \forall (i, j, k) \in \mathcal{T}, ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||_2^2 < ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_k||_2^2, \quad (2)$$

where t indexes the set $\mathcal{T}$ and $\mathbf{1}(\mathcal{E})$ is the indicator function which return the value 1 if the logical expression $\mathcal{E}$ evaluates to true and zero otherwise. The above definition of A is useful at formalizing the desired concept of an optimal projection. However, as formulated, it is not amenable to practical calculation since it is unclear whether there exist an efficient algorithm for finding A given the set $\mathcal{T}$. We now concentrate on formulating similar problems that can be more efficiently approached.

Note that the feasible set for the above problem could be empty. In that case, there is no matrix A that can solve the problem and A is undefined. Since in practice we may still be interested in finding a *good* A even if it does not satisfy all of the constraints, in the following we also address a redefinition of A for the cases where not all constraints can be satisfied.

4. CONVEX FORMULATIONS

Here we concentrate on convex approximations to the problem in Sec.3.

4.1 Optimizing for A

In order to address the discrete nature of the base cost function, we transform the problem into a continuous problem. Additionally, to address the case where the feasible set is empty, we relax the constraints by introducing slack variables ϵ_t. The problem is now as follows:

$$\begin{aligned} \min_{A:\Re^D \rightarrow \Re^d} \textstyle\sum_t \epsilon_t &+ \alpha \textstyle\sum_{m=1}^{D} ||A_m||_1 \\ s.t. & \\ \forall (i, j, k) \in \mathcal{T}, ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||_2^2 &< ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_k||_2^2 + \epsilon_t \\ \forall t, \epsilon_t &> 0 \end{aligned} \quad (3)$$

where t indexes the set $\mathcal{T}$, $\alpha \in \Re$ is a scalar that balances the trade off between the sparsity of A and compliance with the inequalities generated by the triples in $\mathcal{T}$, and $\epsilon_t \in \Re$ represents a slack variable. The 1-norm tends to suppress terms and to produce sparse solutions, this fact has been empirically validated in the SVM framework [4, 7]. Hence, the expression $\sum_{m=1}^{D} ||A_m||_1$ in equation (3) is a reasonably *good* approximation to the ideal expression $\sum_{m=1}^{D} \mathbf{1}(A_m = \vec{0})$ that will lead to a 0-1 Mixed Integer Programming (MIP) problem which is known to be NP-hard.

Note that, each distance constraint can be written as:

$$\begin{aligned} (Ax_i)^\top (Ax_i) - 2(Ax_i)^\top (Ax_j) + (Ax_j)^\top (Ax_j) & \\ -(Ax_i)^\top (Ax_i) + 2(Ax_i)^\top (Ax_k) - (Ax_k)^\top (Ax_k) &< \epsilon_t \end{aligned} \quad (4)$$

and by defining $B = A^\top A \in \Re^D \times \Re^D$, Eq. 4 can be further simplified to:

$$\begin{aligned} (x_j^\top B x_j) - (x_k^\top B x_k) + 2[(x_i^\top B x_k) - (x_i^\top B x_j)] &< \epsilon_t \\ B &\succ 0 \\ B &= B^\top \end{aligned} \quad (5)$$

The main advantage of the new equation is that it produces linear constraints in the new variable B, instead of quadratic constraints in A. However, in order for the equivalence to hold, we must have B symmetric and positive semidefinite. Assuming the cost function remains convex in B, this problem is still convex in B. However it becomes a semidefinite programming problem (SDP). Next, we will show how the much more efficient linear programming method (LP) can be employed instead to solve different instances of this formulation.

4.2 Optimizing for $B = A^\top A$

We first focus on finding a cost function equivalent to Eq. 3. For this we note that for $B = A^\top A$:

$$A_k = \vec{0} \Rightarrow B_k = \vec{0}, (B^\top)_k = \vec{0}, \quad (6)$$

Also note that since:

$$||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||_2^2 = ||A(x_i - x_j)||_2^2 = (\mathbf{x}_i - \mathbf{x}_j)^\top B(\mathbf{x}_i - \mathbf{x}_j)$$

we have that:

$$B_k = \vec{0} \Rightarrow ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||_2^2 \text{ does not depend on dimension } k.$$

Thus, we now focus on the following problem:

$$\begin{aligned} &\min_{\epsilon,B} \textstyle\sum_t \epsilon_t + \lambda \sum_{m=1\ldots D} ||B_m||_1 \\ &\qquad s.t. \\ &\forall (i,j,k) \in \mathcal{T}, -2(\mathbf{x}_i^\top B \mathbf{x}_j) + (\mathbf{x}_j^\top B \mathbf{x}_j) \\ &\qquad -2(\mathbf{x}_j^\top B \mathbf{x}_k) + (\mathbf{x}_k^\top B \mathbf{x}_k) \;<\; \epsilon_t \\ &\qquad \forall t, \epsilon_t \;>\; 0 \\ &\qquad B \;=\; B^\top \\ &\qquad B \;\succ\; 0 \end{aligned} \quad (7)$$

This is also a semi-definite programming (SDP) problem which is convex and can be solved using specialized SDP solvers like SeDuMi [14]. However, we will further simplify the formulation presented above by restricting our solution space to a subfamily of the SDP matrices: the diagonal dominant matrices. In order to provide a better understanding of the motivation for our next formulation we present the following theorem as stated in [8]:

THEOREM 4.1. **Diagonal Dominance Theorem** *Suppose that M is symmetric and that for each $i = 1, \ldots, n$, we have:*

$$M_{ii} \geq \sum_{j \neq i} |M_{ij}|$$

Then M is positive semi-definite (PSD). Furthermore, if the inequalities above are all strict, then M is positive definite.

4.2.1 Imposing diagonal dominance on B

We can now propose the following formulation:

$$\begin{aligned} &\min_{\epsilon,B} \quad \textstyle\sum_t \epsilon_t + \lambda \sum_{m=1\ldots D} |B_{mm}|_1 \\ &\qquad s.t. \\ &\forall (i,j,k) \in \mathcal{T}, -2(x_i^\top B \mathbf{x}_j) + (\mathbf{x}_j^\top B \mathbf{x}_j) \\ &\qquad -2(x_j^\top B \mathbf{x}_k) + (\mathbf{x}_k^\top B \mathbf{x}_k) \;<\; \epsilon_t \\ &\qquad \forall t, \epsilon_t \;>\; 0 \\ &\qquad B \;=\; B^\top \\ &\qquad \forall (m) B_{mm} \;\geq\; \textstyle\sum_n |B_{mn}|, \end{aligned} \quad (8)$$

where the last constraint is equivalent to diagonal dominance which implies positive semidefiniteness according to theorem 4.1. As it was explained before, the sum of 1-norms in the cost function cause preference for sparse solutions (when combined with the last constraint). The projection matrix A can be recovered by an inexpensive Cholesky factorization of the symmetric matrix B [8] or by an eigenvalue decomposition.

The constraint involving $\mathbf{x}$ and B can be rewritten as follows. For any $\mathbf{x}_i, \mathbf{x}_j \in \Re^D$, define $\tilde{X}_{ij} = \text{vect}(\mathbf{x}_i \mathbf{x}_j^\top)$, where vect() means (column-wise) alignment of all of the matrix elements in a column vector. Define $b = \text{vect}(B)$. The constraint can now be written:

$$\forall (i,j,k) \in \mathcal{T} [\tilde{X}_{jj} + \tilde{X}_{kk} - 2(\tilde{X}_{ij} + \tilde{X}_{jk})] b < \epsilon_t$$

Finally, using equations (9) formulation (8) can be rewritten as a Linear Program in the following way:

$$\begin{aligned} &\min_{\epsilon,B,S} \quad \textstyle\sum_t \epsilon_t + \lambda \sum_{m=1\ldots D} B_{mm} \\ &\qquad s.t. \\ &\forall (i,j,k) \in \mathcal{T} [\tilde{X}_{jj} + \tilde{X}_{kk} - 2(\tilde{X}_{ij} + \tilde{X}_{jk})] b \;<\; \epsilon_t - 1 \\ &\qquad \forall t, \epsilon_t \;>\; 0 \\ &\qquad B \;=\; B^\top \\ &\qquad \forall (m,n,m \neq n) - S_{mn} \;\leq\; B_{mn} \leq S_{mn} \\ &\qquad B_{mm} \;>=\; \textstyle\sum_{\substack{n=1 \\ m \neq n}}^{D} S_{mn} \end{aligned} \quad (9)$$

Since the matrix B is symmetric, the number of components of B to be found can be reduced to $D(D+1)/2$ instead of D^2, furthermore by doing this, the constraints $B = B^\top$ can be discarded. The right hand side of the first set of inequalities has been changed from ϵ_t to $\epsilon_t - 1$ in order to enforce numerical stability and to avoid obtaining the trivial solution $B = \vec{0}$. In order to better understand the motivation for formulation (9) it is important to note that:

(*i*) minimizing $\sum_{m=1\ldots D} B_{mm}$ implies minimizing $\sum_{\substack{n=1 \\ m \neq n}}^{D} S_{mn}$ since $B_{mm} >= \sum_{\substack{n=1 \\ m \neq n}}^{D} S_{mn}$.

(*ii*) Since we are implicitly minimizing $\sum_{\substack{n=1 \\ m \neq n}}^{D} S_{mn}$, at the optimal solution $\{B^*, S^*, \epsilon^*\}$ to problem (9), we have that:

$$0 \geq S_{mn}^* = |B_{mn}^*|, \forall (m,n,m \neq n)$$

(*iii*) Combining (*i*) and (*ii*) we obtain:

$$\forall (m) B_{mm}^* \geq \sum_n S_{mn}^* = \sum_n |B_{mn}^*|$$

which implies that B^* is diagonal dominant and hence positive semidefinite.

This last formulation works quite effectively as indicated by the numerical examples presented in the next section.

5. EXPERIMENTAL EVALUATION

This section presents numerical results obtained by applying the above formulation to the problem of learning metrics.

5.1 Experimental Setting

We tested our approach in a collection of nine publicly available datasets. These datasets are part of the UCI repository [4]. The overall properties of the datasets are shown in Table 3. These datasets are commonly used in machine learning tasks as benchmark for performance evaluation. In particular, a related, competing approach [17] (Xing et al.) was

[4]http://www.ics.uci.edu/∼mlearn/MLRepository.html

evaluated using these datasets. We have chosen to compare our formulation against this method. In addition to being a state-of-the art method, several other reasons motivated this choice: the code has been made public [5] and, like our approach, it attempts to find a linear transformation of the original space and it is supervised (learns from user input). In addition this method compared well against K-means by finding a distance function that produced *good* clusterings.

The datasets employed in this comparison are generally used for classification since class labels are available for every point. Our method does not require class labels, but instead only relative distance comparison among a subset of points (clearly class labels provide more information). We use the available class labels to generate a set of triples with distance comparisons that respect the classes. More explicitly, given a randomly chosen set of three points (from the training set), if two of these belong to the same class and a third belongs to a different class, then we place this triple in our set $\mathcal{T}$ (*i.e.,* i and j are the points in the same class, k is the remaining point). In other words, in order to make use of the available class labels, we decided to make points in the same class have smaller pairwise distance among themselves than with points in any of the other classes (after projected by A). In [17], the supervision is in the form of two sets, one called a *similar* set and the other a *dissimilar* set. Again we use the class labels, now to build a similar set of pairs (likewise for a dissimilar set of pairs). Given this supervision, this method should also attempt to make points in the same class closer after an optimal Malahanobis distance matrix is found.

For every triple $(i, j, k) \in \mathcal{T}$ used in our approach for learning, we use $(i, j) \in \mathcal{S}$ and $(i, k) \in \mathcal{D}$ for learning in [17]; where $\mathcal{S}$ and $\mathcal{D}$ are the similar and dissimilar sets required. We believe this provides a fair level of supervision for both algorithms since roughly the same information is provided. It is possible to obtain a superset of $\mathcal{T}$ from $\mathcal{S}$ and $\mathcal{D}$, and by construction $\mathcal{S}$ and $\mathcal{D}$ can be obtained from $\mathcal{T}$.

In order to evaluate performance, we use a 0.85/0.15 split of the data into training and testing. From the training portion, we generate 5000 triples,as explained above, for actual training. This information is provided, in the appropriate representation, to both algorithms. For testing, we randomly choose three points, and if their class labels imply that any two points are closer to each other than to a third (*i.e.,* again if two points have the same class and a third has a different class label), then we check that the correct relationships are satisfied. That is, whether the two points in the same class are closer to each other than any of these points (chosen at random) to the third point. This same measure is used for both algorithms. Thus, we define the *percentage correct* simply as the proportion of points from the test set (sampled at random) that respect the class-implied distance relationship. Both methods compared are attempting to improve this performance measure given the training data and thus we believe this is a valid measure.

[5]Data for all experiments and code for [17] was downloaded from http://www.cs.cmu.edu/∼epxing/papers/. The class for dataset 1 was obtained by thresholding the median value attribute to 25K

5.2 Discussion

Since our method requires setting the balancing parameter λ, we chose it using cross validation (on the training set) by letting λ take values in $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1, 10, 10^{2}\}$. This indirectly influences d, the optimal number of dimensions the data should be projected to, since a small λ favors low-dimensionality (*i.e.,* a λ close to zero practically ignores the number of non-zero dimensions and concentrate on just fitting the data). However, note that λ does not imply dimensionality since the dimensionality depends on the dataset itself. This automatic choice of dimensionality is a valuable property of the method presented, and to the best of our knowledge is not present in the related methods (with the exception, to some degree, of [1]). Fig. 1 shows the average optimal number found by this process in a 10 fold experiment and the corresponding one-standard-deviation error bars. Note than in some cases the reduction is considerable large and this reduction depends on the properties of the dataset.

Fig. 1 shows the percentage correct averaged over 10 random splits of the data along with one-standard-deviation bars. For each of the 10 fold, 1000 triples from the test set are randomly chosen. When comparing the performance of both methods, we note that, except for dataset 5, our method clearly outperforms the competing approach. Interestingly, for this dataset, the optimal dimension was determined to always (for all randomly chosen data splits) be equal to the original dimensionality (four dimensions).

Since both methods can be seen as trying to learn a Mahalanobis distance so that distance constraints are satisfied, we believe the main reason for a superior performance is related to the possibility to identify a lower dimensional projection spaces. The method presented in this paper always attempt to reduce the dimensionality while the competing method always use all the dimensions. Given the results obtained, this reduction appears to provide an important advantage at the time of generalization. It is generally accepted that a simpler model (*i.e.,* one with less parameters) is preferable (*e.g.,* [3]) and it can reduce overfitting.

From a computational efficiency perspective, being able to represent the original data more succinctly is also advantageous. In particular, when distances can be calculated directly using a low dimensional representation, computation time savings are critical for on-line applications. The projection step in this approach can be precomputed off-line; for example in retrieval applications (*e.g.,* query-by-example), the objects can be stored in their low dimensional representation. From a conceptual point of view, our approach also has the advantage, over other methods, of providing a more effective tool for understanding the data since it can identify whether variables (dimensions) are of high or low relevance.

6. CONCLUSIONS

We have developed a new approach for learning distance functions from a set of relative distance relationships. An important property of this approach is that it targets lower dimensional representations, and the dimensionality is determined automatically depending on the characteristics of dataset in question and a balancing parameter λ. A key distinction is that, unlike a large number of dimensional-

Table 3: Benchmark Datasets

Name	Points (N)	Dimensions (D)	Classes
1 Housing-Boston	506	13	2
2 Ionosphere	351	34	2
3 Iris	150	4	3
4 Wine	178	13	3
5 Balance Scale	625	4	3
6 Breast-Cancer Wisconsin	569	30	2
7 Soybean Small	47	35	4
8 Protein	116	20	6
9 Pima Diabetes	768	8	2

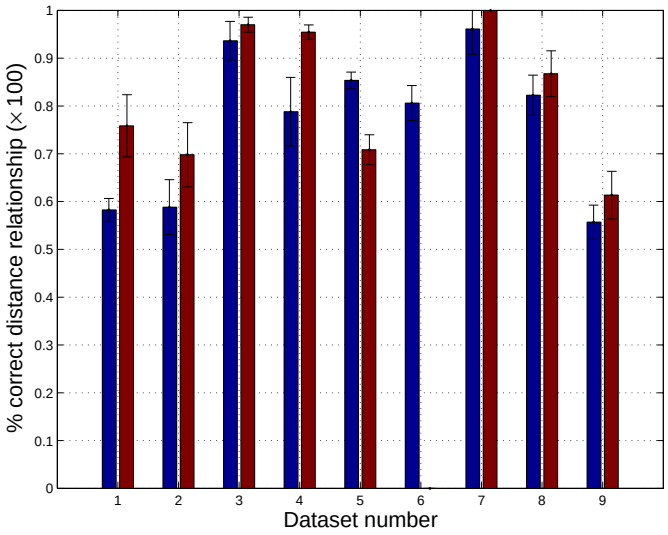

Figure 1: Performance comparison between competing approach and our approach in nine UCI datasets. Bars show performance results on 10 random splits of training/test points. Performance is measured in terms of the percentage of randomly chosen points (1000) from test set whose distance relationship respect the class labels. The number of triples used for training for all runs was 5000. Error bars show one standard deviation.

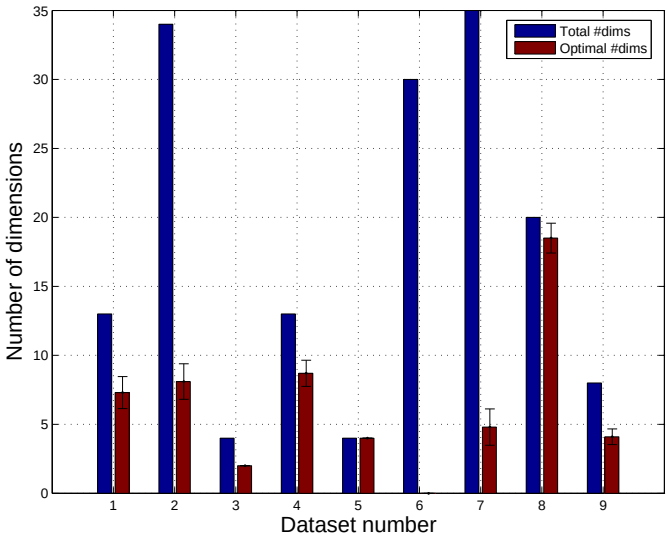

Figure 2: Total number of dimensions and average number of dimensions (along with one-standard-deviation error bars) found by our algorithm for each dataset.

ity reduction approaches, our approach does not attempt to build an isometry or distance preserving mapping[6], but to respect the proximity relationships between pairs of points. We believe this allows for more freedom at finding lower dimensional representations.

We considered the general problem and then designed specific formulations that allow the use of efficient convex optimization algorithms. In particular, we showed how the diagonal dominance constraint on $B = A^\top A$ leads to a general formulation that can be solved very efficiently using linear programming methods.

Our approach can also be seen as a form of supervised dimensionality reduction, where the supervision comes in the form of distance rankings.

The results from the experimental evaluation show that our method can outperform in accuracy state-of-the-art approaches, with the additional benefit of finding low dimensional representations.

Being able to find a distance that depends on a relatively *small* number of features allows to define kernels and/or similarity matrices for classification (in kernel methods like SVM, logistic regression, etc.) also depending in an small number of features. For example, instead of using the standard Gaussian kernel (μ is the Gaussian kernel parameter):

$$(K(X,Y))_{ij} = e^{-\mu \| {X_i}^\top - Y_{\cdot j} \|^2},\ i = 1 \ldots, m,\ j = 1 \ldots, k,$$

that depends on all the features, including irrelevant features for classification, we could use a modified Gaussian kernel as follows:

$$(\bar{K}(X,Y))_{ij} = e^{-\mu \| A({X_i}^\top - Y_{\cdot j}) \|^2},\ i = 1 \ldots, m,\ j = 1 \ldots, k,$$

that would only depends on relevant features. This simple

[6]For example by minimizing distortion

but powerful change may increase classification performance considerably. This is part of our future work.

Another idea worth exploring is the application of LP-boost algorithms [2] to allow our method the handling of datasets in very high dimensional spaces.

To finalize, we would like to highlight the fact that the technique applied in this paper to approximate an SDP problem by a linear programming problem (which is much easier to solve) has the potential to be applied to other recently proposed machine learning related problems involving PSD formulations.

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