DISCOMAX: A Proximity-Preserving Distance Correlation Maximization Algorithm

Praneeth Vepakomma and Ahmed Elgammal

May 7, 2014

Abstract

In a regression setting we propose algorithms that reduce the dimensionality of the features while simultaneously maximizing a statistical measure of dependence known as distance correlation between the low-dimensional features and a response variable. This helps in solving the prediction problem with a low-dimensional set of features. Our setting is different from subset-selection algorithms where the problem is to choose the best subset of features for regression. Instead, we attempt to generate a new set of low-dimensional features as in a feature-learning setting. We attempt to keep our proposed approach as model-free and our algorithm does not assume the application of any specific regression model in conjunction with the low-dimensional features that it learns. The algorithm is iterative and is formulated as a combination of the majorization-minimization and concave-convex optimization procedures. We also present spectral radius based convergence results for the proposed iterations.

1 Introduction

In problems of high-dimensional nonparametric regression, it is known that the number of samples required to attain a reliable generalization error rapidly increases with the increase in dimensionality. This is also referred to as the curse of dimensionality and the following is an intuitive example for this phenomenon: For a hypercube with a fixed side length, as the dimension of the space increases the ratio of the volume of an inscribed hypersphere to the volume of the hypercube rapidly decreases to an infinitesimal value thereby indicating that in a uniform sample, the number of points that lie within a hypersphere around a fixed center and fixed radius happens to decrease with an increase in dimension thus requiring a greater sample complexity to generalize the phenomenon of the underlying distribution. Recently there has been work around the assumption that the high-dimensional features may lie on a smooth manifold in a lower-dimension. A characterization of this assumption is presented in detail in [1]. There has been a significant research in developing methods like [2], [3] and [4] that try to recover the low-dimensional manifold from high-dimensional representations of data. In this paper we propose algorithms that instead focus on reducing the dimensionality of the covariates (features / predictor variables) in a regression setting while maximizing a measure of statistical dependency between the covariates and the response variable. The statistical dependency maximization approach presented in this paper is model-free and the dimensionality reduction does not require
any prior assumption on the type of regression model that needs to be used in conjunction with
the low-dimensional covariates produced by the method. This is in contrast to model-dependent
supervised dimensionality reduction methods such as [5] where a supervised dimensionality
reduction algorithm is presented based on an assumption that a generalized linear model would
be applied on the appropriate features obtained after the dimensionality reduction. Similarly, the
model-based approaches in [6] and [8] aim to learn low-dimensional features that can be used
to learn Gaussian mixture and Bayesian mixture based predictive models respectively. We shall
first introduce basic notations used in the paper. Let the high-dimensional covariates in a regres-
sion setting be represented by a matrix $X$ where the columns are the covariates and let the re-
sponse be represented by the matrix $Y$. We use $\text{Degree}(A(G))$ to represent the degree matrix of
a weighted graph $G$ having an adjacency matrix $A(G)$ where $\text{Degree}_{i,i}(G) = \sum_j A_{ij}(G)$ and
the degree matrix is a diagonal matrix. Similarly, the Laplacian matrix of a graph $G$ denoted by
$L(A(G))$ is given by $\text{Degree}(A(G)) - A(G)$. Given a matrix of features $X$ and a corresponding
response $Y$ we define the corresponding squared Euclidean distance matrices $E^X$ and $E^Y$ such
that for $k,l \in 1, ..., n$, $E^X_{kl} = (|X_k - X_l|^2)$ and $E^Y_{kl} = (|Y_k - Y_l|^2)$. The framework presented
in this paper might be generalized for prediction with multiple response variables but we focus
our evaluations in this paper in the case of a univariate response. A line of research which has a
greater similarity to our proposed approach is the setting in sufficient dimensionality reduction
methods like Inverse Regression Estimation (IRE) [?], Principal Hessian Directions (pHD) [9],
Sliced Inverse Regression (SIR) [10] and Sliced Average Variance Estimation (SAVE) [11] as
these methods do not make assumptions about the regression model that can be applied over
the low-dimensional features. These techniques are based on the principle of ‘sufficiency’ as
described in [?] and however assume that the distribution of the covariates is elliptic. We now
give a brief overview about the structure of this paper. In section 2 we cite the definitions for the
population Distance Correlation and the corresponding sample statistics as proposed by [12],
[?]. In section 3 we propose a graph-theoretic formulation of sample distance correlation and
sample distance covariance and show that they can be formulated using Laplacian matrices.
In section 4 we propose a loss function for supervised dimensionality reduction based on the lapla-
cian formulation of sample distance correlation. In section 5 we investigate the convexity and
differentiability of this loss-function. In section 6 we present an update to optimize the proposed
loss based on the convexity properties presented in section 5. In section 7 we propose an algo-
 rbith for optimizing the loss without requiring a matrix inversion. In section 8 we investigate
the convergence properties of the loss function based on spectral radius and the differentiability
properties presented in section 5. In section 9 we present experimental results on 5 regression
datasets and compare our technique with other supervised dimensionality reduction techniques
like IRE, SIR, pHD, SAVE and KDR. We evaluate the techniques by running regression tech-
niques like Support Vector Machines (SVM), Random Forests (RF), Lasso, Node Harvest (NH),
Bayesian Additive Regression Trees (BART) over the low-dimensional features learnt by the
above mentioned dimensionality reduction techniques, and compare the cross-validated pre-
dictive performances of the regression methods across low-dimensional features produced by
different dimensionality reduction techniques. We also present empirical results showing con-
vergence along with some simple empirical results evaluating the proposed conditions required
to achieve convergence. In section 10 we present the conclusion and some discussions on future
work.

2 Distance Correlation

Pearson’s product-moment correlation is a measure of monotone or linear dependencies between two random variables of the same dimension. Distance Correlation introduced by [12], [?] is a measure of monotone as well as nonlinear dependencies between random vectors of arbitrary dimensions. For random variables $P \in \mathbb{R}^h$ and $Q \in \mathbb{R}^m$, the population distance covariance for a suitable weight function $\phi(t, s)$ proposed in [12], is given by

$$\nu^2(P, Q; \phi) = \int_{\mathbb{R}^{h+m}} |f_{P,Q}(t, s) - f_P(t)f_Q(s)|^2 \phi(t, s)dtds$$

where $f_P, f_Q$ are the characteristic functions of $P, Q$ and $f_{P,Q}$ is the joint characteristic function. It is clear from the above definition that the distance covariance can be zero, only when $P, Q$ are independent. The weight function $\phi(t, s)$ has special properties that allow for $\nu^2(P, P; \phi)$ to be defined as

$$\nu^2(P, P; \phi) = \int_{\mathbb{R}^{2h}} |f_{P,P}(t, s) - f_P(t)f_P(s)|^2 \phi(t, s)dtds$$

and hence a standardized version of the distance covariance was shown to be obtainable as

$$\frac{\nu^2(P, Q; \phi)}{\sqrt{\nu^2(P, P; \phi)\nu^2(Q, Q; \phi)}}$$

and this is the Distance Correlation of $P, Q$.

2.1 Sample Distance Correlation and Sample Distance Covariance:

The authors in [12], [?] propose a non-negative sample distance covariance, defined over a random sample

$$(P, Q) = \{(P_k, Q_k) : k = 1, ..., n\}$$

of $n$ i.i.d random vectors $(P, Q)$ from the joint distribution of random vectors $P$ in $\mathbb{R}^h$ and $Q$ in $\mathbb{R}^m$. For this they compute the Euclidean distance matrices $D^P$ and $D^Q$ where for $k, l \in 1, ..., n$ the distance matrices are formed as $(D^P_{kl}) = (|P_k - P_l|_2)$ and $(D^Q_{kl}) = (|Q_k - Q_l|_2)$ and the distance matrices $D^P, D^Q$ are double-centered to make their row and column means to be zero. The double-centered Euclidean distance matrices denoted by $A, B$ are obtained using the double-centering matrix, $J = I - n^{-1}ee^T$ with $I$ being the Identity matrix and $e_{n \times 1}$, a vector of one’s as $A = -0.5JD^PJ$ and $B = -0.5JD^QJ$. This is equivalent to performing the following operation on the entries of $D^P, D^Q$: If we denote the row $i$ of matrix $D^P$ by $D^P_i$ and the column $j$ by $D^P_j$ and $\overline{D^P}$ denotes the average of the elements in $D^P_i$ and similarly the average of all the elements in $D^P$ by $\overline{D^P}$, then the entries in $A$ and $B$ can be represented as: $A_{kl} = D^P_{kl} - D^P_k - D^P_l + \overline{D^P}$ and $B_{kl} = D^Q_{kl} - D^Q_k - D^Q_l + \overline{D^Q}$. Given these representations, the sample distance covariance is defined as $\hat{\nu}^2(P, Q) = \frac{1}{n^2} \sum_{k,l=1}^n A_{kl}B_{kl}$ and the sample distance correlation $\hat{\rho}^2(P, Q)$ is given by $\hat{\rho}^2(P, Q) = \frac{\hat{\nu}^2(P, Q; \phi)}{\sqrt{\hat{\nu}^2(P, P; \phi)\hat{\nu}^2(Q, Q; \phi)}}$.
3 Graph Laplacian formulation of Sample Distance Correlation

In this section we propose a Laplacian matrix based formulation of the sample distance covariance and sample distance correlation and in the next section we propose a loss-function for supervised dimensionality reduction based on the Laplacian formulation we propose here.

We now give the main result of this section:

**Lemma 3.1** Given matrices of squared Euclidean distances $E^X$ and $E^Y$ the square of the sample distance correlation, $\hat{\rho}^2(X,Y)$ can be expressed using the graph laplacians $L_X = L(\frac{1}{2}JE^X J)$ and $L_Y = L(\frac{1}{2}JE^Y J)$ formed over adjacency matrices $\frac{1}{2}JE^X J$, $\frac{1}{2}JE^Y J$ as:

$L_X = \text{Degree} \left( \frac{1}{2}JE^X J \right) - \frac{1}{2}JE^X J$, $L_Y = \text{Degree} \left( \frac{1}{2}JE^Y J \right) - \frac{1}{2}JE^Y J$ and any scalar $\alpha$ where $L_Y \neq \alpha L_X$ with $k = \frac{n}{2Tr(Y^TLY)}$ as

$$\hat{\rho}^2(X,Y) = \frac{kTrX^TL_YY}{(TrX^TLXX)}$$  \hspace{1cm} (2)

**Proof 3.1** Let $R = \frac{1}{2}JE^X J$ and $S = \frac{1}{2}JE^Y J$ be the matrices obtained by double-centering $E^X$ and $E^Y$. $R$, $S$ are positive semi-definite and are related to $X$, $Y$ as $R = XX^T$, $S = YY^T$. Also, as $Re = 0$ and $Se = 0$, the mean of each column in $X$ and $Y$ is zero. $L_X$ and $L_Y$ can be viewed as Laplacian matrices constructed using the weighted adjacency matrices $R$, $S$. Now for any graph with a weighted adjacency matrix $W$ and a corresponding laplacian matrix $L$ along with a real matrix $X$ the term $TrX^TLX$ can be represented using Euclidean distances between the rows in $X$ as:

$$TrX^TX = \sum_{i,j} W_{ij}d_{ij}^2(X)$$  \hspace{1cm} (3)

Thus we can represent the term $Tr(X^TLYX)$ in terms of $S$ as

$$Tr(X^TLYX) = \frac{1}{2}\sum_{i,j} S_{ij}d_{ij}^2(X) = \frac{1}{2}\sum_{i,j} S_{ij}(R_{ii} + R_{jj} - 2R_{ij})$$

$$= -\sum_{i,j} R_{ij}S_{ij} + \frac{1}{2}\sum_{j} R_{jj}\sum_{i} S_{ij} + \frac{1}{2}\sum_{i} R_{ii}\sum_{j} S_{ij}$$

Since $R$ and $S$ are double centered, $\sum_{i} S_{ij} = \sum_{j} S_{ij} = 0$ and therefore,

$$\frac{2}{n^2}Tr(X^TLYX) = \sum_{i,j} S_{ij}d_{ij}^2(X) = \nu^2(X,Y)$$

With a similar argument we can express the sample distance covariance using both $L_Y, L_X$ as

$$\hat{\nu}^2(X,Y) = \left( \frac{2}{n} \right) Tr \left( X^TLYX \right) = \left( \frac{2}{n} \right) Tr \left( Y^TLXXY \right)$$  \hspace{1cm} (4)

and the sample distance variances can be expressed as $\hat{\nu}^2(X,X) = \left( \frac{2}{n} \right) Tr \left( X^TLYX \right)$ and $\hat{\nu}^2(Y,Y) = \left( \frac{2}{n} \right) Tr \left( Y^TLXXY \right)$ and so we can now represent the sample distance correlation in terms of $L_X$, $L_Y$ as in $[2]$. 

4
4 Low-Dimensional Distance Correlation:

In this section we propose a loss-function which we minimize over a low-dimensional \( \hat{X} \) inorder to maximize the distance correlation \( \hat{\rho}^2(\hat{X}, Y) \) and evaluate this setting in the later sections. The proposed loss function \( G(\cdot) \) that we would like to minimize over \( \hat{X} \) with \( w_{xy} \) being a fixed scalar when given a feature matrix \( X \) and a corresponding response variable \( Y \) is

\[
G(\hat{X}|X, Y, w_{xy}) = \text{Tr}(\hat{X}^T L_X \hat{X}) - w_{xy} \text{Tr}(\hat{X}^T L_Y \hat{X})
\]  

(5)

This formulation contains a difference of the trace terms observed in 2. Note that the \( L_X \) and \( L_Y \) we use in this loss-function is computed over a high-dimensional \( X \) and the corresponding response \( Y \). This can also be expressed as

\[
\sum_{i,j} [(X_i, X_j) d_{ij}^2(\hat{X})] - \sum_{i,j} [(Y_i, Y_j) d_{ij}^2(\hat{X})]
\]

(6)

Similar formulations for solving a maximization of a ratio of trace functions, but under orthogonality constraints were studied in the Fisher Linear Discriminant Analysis Problem [14] where the ratio maximization is formulated as a minimization of a difference, just as in \( G(\cdot) \). [7] proved that the maximum of the ratio of trace functions under an orthogonality constraint can be achieved by optimizing a difference based formulation as in [5]. Their iterative solution for the difference formulation under the orthogonality constraints requires an eigen decomposition at every iteration. In our proposed solution for the optimization of \( G(\cdot) \) we do not fix any orthogonality constraints and that is the key difference between the two settings. We use \( L_X \) instead of \( L_{\hat{X}} \) because we are trying to find a Euclidean embedding that preserves the neighborhood relations within the inner-products of the rows (points) in \( X \) and \( Y \) while maximizing the distance correlation. We empirically show in the convergence plots in the later sections that minimizing the above loss which contains \( L_X \), maximizes the distance correlation between the optimal \( \hat{X} \) and \( Y \).

Under \( L_{\hat{X}} \), the first term \( Tr(\hat{X}^T L_{\hat{X}} \hat{X}) \) in the loss function is non-convex but in the case where we use \( L_X \), this term becomes convex. This leads to the loss being a sum of convex and concave functions which we utilize inorder to minimize it using the Concave Convex Procedure (CCCP) [15]. We will go into more details on optimizing this loss in later sections of this paper where we provide an iterative algorithm. We also choose the fixed number of iterations for which we run the optimization algorithm by cross-validation in a prediction setting.

5 Concave convex formulation:

In an iterative optimization framework we represent the above loss function as a sum of a convex function \( h_{\text{vex}}(\cdot) \) and a concave function \( h_{\text{cave}}(\cdot) \) at any iteration \( \varphi \) as

\[
G \left( \hat{X}_\varphi | X, Y, w_{xy} \right) = \left[ h_{\text{vex}}(\hat{X}_\varphi) + w_{xy} h_{\text{cave}}(\hat{X}_\varphi) \right]
\]

where the individual functions are \( h_{\text{vex}}(\hat{X}_\varphi) = Tr(\hat{X}_\varphi^T L_X \hat{X}_\varphi) \) and \( h_{\text{cave}}(\hat{X}_\varphi) = -Tr(\hat{X}_\varphi^T L_Y \hat{X}_\varphi) \)

Based on the concave-convex procedure [15] such a loss function can be iteratively minimized.
with guaranteed monotone convergence to the minimum or a saddle point by the following update:
\[ \nabla h_{\text{vex}}(X_\varphi) = -w_{xy}\nabla h_{\text{cave}}(X_{\varphi-1}) \] (7)
which gives the update using the Moore-Penrose inverse as
\[ X_\varphi = w_{xy}L^\dagger Y X_{\varphi-1} \] (8)

6 Algorithm without Matrix Inversion:

In this section we formulate a solution for the proposed supervised learning loss, in such a way that the iterative update does not require a matrix inversion.

We denote by \( \text{Diag}(L_X) \), a diagonal matrix whose diagonal is the diagonal of \( L_X \). Now, we can build a majorization function [16] over \( \text{Tr} \hat{X}^T L_X \hat{X} \), based on the fact that \( 2\text{Diag}[L_X] - L_X \) is diagonally dominant. This leads to the following inequality for any matrix \( M \) with real entries and of the same dimension as \( \hat{X} \):
\[ (\hat{X} - M)^T[2\text{Diag}[L_X] - L_X](\hat{X} - M) \succeq 0 \] (9)

We now get the following majorization inequality over \( \text{Tr}(X^T L_X X) \), by separating it from the above inequality:
\[ \text{Tr}(\hat{X}^T L_X \hat{X}) + b(Y) \leq \text{Tr}[\hat{X}^T 2\text{Diag}(L_X) \hat{X}] - 2\text{Tr}[\hat{X}^T (2\text{Diag}(L_X) - L_X) M] = \lambda(\hat{X}, M) \]

which is quadratic in \( \hat{X} \) where, \( b(M) = \text{Tr}(M^T L_X M) - \text{Tr}(M^T 2\text{Diag}(L_X) M) \). Let, \( h(\hat{X}, M) = \lambda(\hat{X}, M) - w_{xy} \text{Tr} \hat{X}^T L_Y \hat{X} \). This leads to the following bound over our loss function with \( \text{const}(M) \) being a function that only depends on \( M \):
\[ G(\hat{X}|S,Y,w_{xy}) + \text{const}(M) \leq h(\hat{X}, M), \forall \hat{X} \neq M \]

\[ = h(\hat{X}, \hat{X}), \text{ when } \hat{X} = M \]

that satisfies the supporting point requirement, and hence \( h(.) \) touches the objective function at the current iterate and forms a majorization function. Now the following majorization-minimization iteration holds true for an iteration \( \varphi \):
\[ \hat{X}_{\varphi+1} = \arg \min_{\hat{X}} h(\hat{X}, M_\varphi) \text{ and } M_{\varphi+1} = \hat{X}_\varphi \] (10)

It is important to note that these inequalities occur amongst the presence of additive terms, \( \text{const}(M) \) that are independent of \( X \) unlike a typical majorization-minimization framework and hence, it is a relaxation. The majorization function \( h(\hat{X}, M_\varphi) \) can be expressed as a sum of a convex function \( e_{\text{vex}}(\hat{X}) = \lambda(X, M_\varphi) \) and a concave function \( e_{\text{cave}}(\hat{X}) = -w_{xy} \text{Tr} \hat{X}^T L_Y \hat{X} \).

By the concave-convex formulation, we get the iterative solution by solving for \( \nabla e_{\text{vex}}(X_\varphi) = -\nabla e_{\text{cave}}(X_{\varphi-1}) \) which gives us:
\[ X_n = \frac{w_{xy}}{2} \text{Diag}(L_X)^\dagger L_Y X_{\varphi-1} + M_\varphi - \frac{1}{2} \text{Diag}(L_X)^\dagger L_X M_\varphi \] (11)
Proposition 7.1 For any pair of real matrices $X, Y$ we can find a real scalar $\gamma$ that satisfies the above condition as $\frac{||Y||^2_F}{8} \leq ||\gamma X||^2_F \leq ||Y||^2_F$. Rearranging the terms we have that choosing any $\gamma$ from the interval $|\gamma| \in \left[\frac{1}{\sqrt{\frac{5}{3} ||X||^2}}, \frac{1}{\sqrt{||X||^2}}\right]$ would ensure that $\rho(T'(\hat{X}^*), X, Y) < 1$ for any pair of real matrices $X, Y$ and any stationary point $\hat{X}^*$. 

7 Spectral radius based convergence properties:

Notation: In this section we use $\rho(\cdot)$ to denote the spectral-radius as it has been a standard notation in literature. So, is the case with using $\rho(\cdot)$ for denoting distance correlation in the previous sections. We would like the reader to interpret notation in this case, based on context.

Definition 7.1 Strong Attraction. A fixed point $\hat{X}^*$ of $T(\hat{X}|X,Y)$ is said to be a point of strong attraction of the iteration if $T(\hat{X}|X,Y)$ is differentiable at $\hat{X}^*$ and the spectral radius $\rho(T'(\hat{X}^*)), X, Y) < 1$.

We now study the conditions under which the twice Fretchet differentiable iterative update in $6$ converges with $\rho(T'(Z^*)), X, Y) < 1$.

Proposition 7.1 For any pair of real matrices $X, Y$ along with a real scalar $|\gamma| \in \left[\frac{1}{\sqrt{\frac{5}{3} ||X||^2}}, \frac{1}{\sqrt{||X||^2}}\right]$ and laplacians $L_X, L_Y$ constructed over $\gamma X, Y$ respectively the spectral radius $\rho(T'(\hat{X}^*),|\gamma X, Y) \leq 1$ for any stationary point $\hat{X}^*$.

Proof 7.1 The gradient of the iterative update of the majorization based approach can be represented using the hessian of $G(.)$ as

$$T'(\hat{X}^*) = I - 0.25 * Diag(L_X)\|\nabla^2 G(\hat{X}^*|X,Y)\|$$

$$= I + 0.25 * Diag(L_X)\|L_Y - L_X\|$$

(12)

By the extension to the Ostrowski’s theorem in [17] $\rho(T'(\hat{X}^*)), X, Y) \leq 1$ when $0 \leq 2(L_Y - L_X) \leq 8Diag(L_X)$ On representing $L_X$ and $L_Y$ in terms of $X$ and $Y$ using equations 3.1, 3.1 we have the following two positive semi-definiteness conditions that need to be satisfied: $XX^T + 4Diag(XXT) - YY^T + 0$ and $YY^T - XX^T \geq 0$ which we represent using the trace function as

$$Tr(XX^T) + 4 \sum_{i=1}^{n} ||X_i|| \geq Tr(YY^T) \geq Tr(XX^T)$$

(13)

For any pair of real matrices we can find a real scalar $\gamma$ that satisfies the above condition as $\frac{||Y||^2_F}{8} \leq ||\gamma X||^2_F \leq ||Y||^2_F$. Rearranging the terms we have that choosing any $\gamma$ from the interval $|\gamma| \in \left[\frac{1}{\sqrt{\frac{5}{3} ||X||^2}}, \frac{1}{\sqrt{||X||^2}}\right]$ would ensure that $\rho(T'(\hat{X}^*),|X, Y) < 1$ for any pair of real matrices $X, Y$ and any stationary point $\hat{X}^*$. 


8 Experimental Results

8.1 Comparison/Experiment Setup:

To evaluate our technique we ran experiments using 5 standard regression datasets. We performed a dimensionality reduction of the features in each of these datasets using our technique (SDR-DCM) and also with other supervised dimensionality reduction techniques like Sliced Average Variance Estimation (SAVE), Principal Hessian Directions (pHd), Sliced Inverse Regression (SIR), Inverse Regression Estimation (IRE), Kernel Sliced Inverse Regression (KSIR) and No Dimensionality Reduction (Without DR) giving us low-dimensional feature sets obtained from seven different techniques across the 5 datasets. We then ran regression models using Support Vector Machines (SVM), Lasso, Random Forests (RF), Node Harvest (NH) and Bayesian Additive Regression Trees (BART) utilizing the low-dimensional feature set obtained from each dimensionality reduction techniques across each dataset. The parameters of the regression models were tuned using 5-fold cross-validation. Also, the 5-fold cross-validated Root Mean Square Error (R.M.S.E) was computed for each combination of the supervised dimensionality reduction technique, regression model and dataset. These cross-validated R.M.S.E values are presented in Table 1. Also, for our proposed technique we choose the number of iterations for which we run the algorithm based on cross-validation. The overlaid vertical, black lines in Figure 1 show the iteration at which the minimal cross-validation error was achieved for each of these datasets. The dimensionality to which the covariates in each dataset was reduced to is mentioned in the following sub-section.

8.2 Datasets

We now give a terse description of each of the 5 regression datasets used.

a) **Boston Housing** is a dataset available at the UCI ML repository. The data consists of 506 census tracts of Boston from the 1970 census and contains information collected by the U.S Census Service and the task is to predict the median value of a home. This dataset contains 14 features. The dimensionality was reduced to 3 covariates.

b) **Concrete Compressive Strength** is a dataset also available from the UCI ML repository and the task is to predict the concrete compressive strength based on the age and other ingredients. Some of these ingredients include cement, blast furnace slag, fly ash, water, superplasticizer, coarse aggregate, and fine aggregate. This dataset consists of 1090 samples and 9 features. The dimensionality was reduced to 3 covariates.

c) **Windspeed** data at a candidate site in Northern South Dakota was collected every six hours for all of 2002, except that of the month of May and a few other observations that are missing. Wind speed and direction data corresponding to the candidate site was also collected at four reference sites. The task is to predict the wind speed at the candidate site. The data consists of 1114 observations and 14 variables and was collected by WindLogics, Inc. The dimensionality was reduced to 3 covariates.

d) **Voting Record** Dataset was scraped from [http://www.senate.gov/](http://www.senate.gov/) and is also available on CRAN R repository. It consists of 598 samples and 96 variables. The task is to predict the voting record of the California Democrat Junior Senator Barbara Boxer from the voting records.
of other Senators. The senators included in the dataset consists of those who were in office for the entire session. The dimensionality was reduced to 6 covariates.

e) **Breast Cancer Gene Expression** data from [13] was studied. It consists of gene signature data with 144 breast cancer patients and 77 covariates. The task is to predict the survival time of the patients based on the combination of gene expression measurements and the clinical covariates. The dimensionality was reduced to 6 covariates. As seen in the table 1, our supervised dimensionality reduction technique (SDR-DCM) performed well in comparison to the other supervised dimensionality reduction techniques. Figure 1 shows the convergence of the maximization of Distance Correlation, and in Figure 2 the convergence plots of a Gamma chosen from Proposition 8.1 for the Voting Record Dataset and three Gamma choices outside the suggested interval are shown. The green line shows that convergence was reached when Gamma was in the suggested interval unlike the rest of the choices of the Gamma.

9 Conclusion

The results produced by the proposed technique were reasonably competitive with regards to the results obtained on the without dimensionality reduction dataset apart from other techniques. As part of future-work, we believe that there may be a reasonable scope for generalizing this approach to prediction in a multi-task learning setting apart from applying this approach to classification problems.
| Method       | Boston Housing | Voting Record | Concrete Compressive Strength | Wind Speed | Van’t Veer Breast Cancer |
|--------------|----------------|---------------|-------------------------------|-----------|-------------------------|
|              | SDR-DCM       | SAVE          | IRE                          | pHd       | KSIR                    | Without DR |
| SVM          | 0.153         | 0.191         | 0.244                        | 0.198     | 0.208                   | 0.182       | 0.169 |
| Lasso        | 0.148         | 0.259         | 0.288                        | 0.236     | 0.280                   | 0.210       | 0.194 |
| Node Harvest | 0.163         | 0.241         | 0.277                        | 0.221     | 0.269                   | 0.174       | 0.184 |
| Random Forest| 0.166         | 0.213         | 0.257                        | 0.186     | 0.220                   | 0.192       | 0.170 |
| BART         | 0.148         | 0.259         | 0.288                        | 0.236     | 0.280                   | 0.179       | 0.194 |
|              | 0.091         | 0.262         | 0.262                        | 0.104     | 0.262                   | 0.193       | 0.228 |
|              | 0.134         | 0.456         | 0.372                        | 0.126     | 0.456                   | 0.231       | 0.184 |
|              | 0.106         | 0.287         | 0.290                        | 0.091     | 0.287                   | 0.227       | 0.198 |
|              | 0.162         | 0.237         | 0.294                        | 0.240     | 0.236                   | 0.186       | 0.187 |
|              | 0.148         | 0.259         | 0.288                        | 0.236     | 0.280                   | 0.193       | 0.194 |
|              | 5.697         | 6.530         | 12.468                       | 11.810    | 9.585                   | 8.362       | 6.301 |
|              | 8.538         | 10.403        | 13.226                       | 14.136    | 14.471                  | 10.832      | 10.382 |
|              | 6.381         | 10.064        | 13.219                       | 12.690    | 12.401                  | 9.917       | 8.386 |
|              | 6.216         | 8.040         | 12.273                       | 12.403    | 9.653                   | 7.806       | 5.341 |
|              | 7.813         | 10.589        | 10.716                       | 9.674     | 8.211                   | 7.215       | 5.683 |
|              | 2.135         | 2.278         | 2.248                        | 2.190     | 2.287                   | 2.263       | 2.276 |
|              | 3.443         | 2.182         | 2.224                        | 2.131     | 2.271                   | 2.241       | 2.152 |
|              | 1.837         | 2.437         | 2.517                        | 2.259     | 2.497                   | 2.972       | 2.275 |
|              | 2.051         | 2.291         | 2.354                        | 2.227     | 2.295                   | 2.085       | 2.176 |
|              | 1.928         | 2.269         | 2.681                        | 2.265     | 2.316                   | 2.164       | 2.183 |
|              | 2.234         | 3.826         | 4.819                        | 3.964     | 5.583                   | 3.749       | 4.153 |
|              | 3.074         | 5.416         | 4.397                        | 4.360     | 4.753                   | 3.249       | 3.965 |
|              | 2.160         | 4.813         | 4.265                        | 4.361     | 3.436                   | 4.186       | 3.702 |
|              | 2.203         | 3.261         | 3.974                        | 4.132     | 4.924                   | 3.134       | 3.986 |
|              | 2.627         | 3.563         | 3.298                        | 3.612     | 4.173                   | 2.937       | 3.641 |

Table 1: Comparison of Cross-Validated Root Mean Square Errors obtained by applying supervised learning (regression) methods on low-dimensional features obtained by different supervised dimensionality reduction techniques over five standard datasets. The row names in each table indicate the regression methods and the column names indicate the supervised dimensionality reduction techniques being compared.
References

[1] Z. Zhang, H. Zha Principal Manifolds and Nonlinear Dimensionality Reduction via Tangent Space Alignment, SIAM Journal on Scientific Computing, Volume 26 Issue 1, 2005, pp. 313 –338.

[2] R. R. Coifman, S. Lafon, Diffusion maps, Applied and Computational Harmonic Analysis, Volume 21, Issue 1, (2006) , pp. 5—30

[3] M. Bernstein, V. De Silva, J. C. Langford, J. B. Tenenbaum, Graph Approximations to Geodesics on Embedded Manifolds

[4] D. L. Donoho, C. Grimes, Hessian eigenmaps: Locally linear Embedding Techniques for High-Dimensional Data, Proc. Natl. Acad. Sci. USA, PNAS, (2003), vol. 100, no. 10, pp. 5591–5596

[5] I. Rish, G. Grabarnik, G. Cecchi, F. Pereira, G. J. Gordon Closed-Form Supervised Dimensionality Reduction with Generalized Linear Models, 25th International Conference on Machine Learning, (2008).

[6] Sajama, A. Orlitsky Supervised Dimensionality Reduction using Mixture Models, 22nd International Conference on Machine Learning, (2005).

[7] Huan Wang, Shuicheng Yan, Dong Xu, Xiaou Tang, Thomas Huang, Trace Ratio vs. Ratio Trace for Dimensionality Reduction, IEEE Conference on Computer Vision and pattern recognition, (2007).

[8] K. Mao, F. Liang, S. Mukherjee, Supervised Dimension Reduction Using Bayesian Mixture Modeling, Artificial Intelligence and Statistics, (2010), pp. 501–508.

[9] R. D. Cook, Journal of the American Statistical Association, Vol. 93, No. 441 (1998), pp. 84–94

[10] K. C. Li, Sliced Inverse Regression for Dimension Reduction, Journal of the American Statistical Association, Vol. 86, No. 414, (1991), pp. 316-327.

[11] Y. Li, L. X. Zhu, Asymptotics for sliced average variance estimation, The Annals of Statistics Vol. 35, No. 1 (Feb., 2007), pp. 41-69

[12] M. Rizzo, N. Bakirov Measuring and testing dependence by correlation of distances, Annals of Statistics, (2007) Vol. 35 No. 6, pp. 2769–2794.

[13] Van de Vijver, M. J. Y. D. He, L. J. van ’t Veer, H. Dai, A. A. M. Hart, D. W. Voskuil, G. J. Schreiber, J. L. Peterse, C. Roberts, M. J. Marton, M. Parrish, T. Rutgers, S. H. Friend, and R. Bernards, A gene- expression signature as a predictor of survival in breast cancer, New England Journal of Medicine , (2002), 347 (25), pp. 1999–2009.
10 Appendix:

10.1 Frechet differentiability of the distance correlation loss function:

Given that $\text{Mat}_n(\mathbb{R})$ denotes the space of linear functionals on matrices over reals, in order for a function $q: \text{Mat}_n(\mathbb{R}) \rightarrow \mathbb{R}$ to be Frechet differentiable at $Z \in \text{Mat}_n(\mathbb{R})$, it must satisfy for a direction $\Delta$, the condition

$$q(Z + \Delta) = q(Z) + q'(Z)\Delta + o(\Delta), \quad \Delta \rightarrow 0$$

for some linear map $q'(Z): \text{Mat}_n(\mathbb{R}) \rightarrow \mathbb{R}$. We check the Frechet differentiability of the loss function $G(\hat{X}|X,Y,w_{xy})$ in this section. We use $C := L_X - w_{xy}L_Y$ for brevity and also note that $C^T = C$ as the Laplacian matrices are symmetric. We check the above stated differentiability condition over our loss function $G(\hat{X}|X,Y,w_{xy})$ which gives us

$$G(\hat{X} + \Delta|X,Y,w_{xy}) = Tr(\hat{X}^T C \hat{X} + \Delta^T C \hat{X} + \hat{X}^T C \Delta + \Delta^T C \Delta) = Tr(\hat{X}^T C \hat{X}) + 2Tr(\Delta^T C \hat{X}) + Tr(\Delta^T C \Delta)$$

We have

$$|Tr\Delta^T C \Delta| \leq n||\Delta^T C \Delta||_2 \leq n||C||_2||\Delta||_2^2$$

Hence,

$$Tr(\Delta^T C \Delta) = o(\Delta) \text{ as } \Delta \rightarrow 0$$

and also the differential

$$G'(\hat{X}|X,Y,w_{xy}) \Delta = 2Tr(\Delta^T C \hat{X})$$

For showing that $G(\cdot)$ is twice differentiable, we have to prove that there is a linear

$$G''(\hat{X}): \text{Mat}_n(\mathbb{R}) \rightarrow \text{Mat}_n(\mathbb{R})^*$$
such that for a direction $K$

$$f'(\hat{X} + K) = f'(\hat{X}) + f''(\hat{X})K + o(K), \quad K \to 0$$  \hfill (20)

But now as $G'(\cdot)$ is linear, if we define $G''(\hat{X}) = G'$ for each $\hat{X}$, we have

$$G'(\hat{X} + K) = G'(X) + G'(K) = G'(X) + G''(X)K$$  \hfill (21)

So, the loss-function $G(\hat{X}|X,Y,w_{xy})$ is twice Frechet differentiable.