Discriminative Cluster Analysis

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Abstract

Clustering is one of the most widely used statistical tools for data analysis. Among all existing clustering techniques, k-means is a very popular method because of its ease of programming and because it accomplishes a good trade-off between achieved performance and computational complexity. However, k-means is prone to local minima problems, and it does not scale too well with high dimensional data sets. A common approach to dealing with high dimensional data is to cluster in the space spanned by the principal components (PC). In this paper, we show the benefits of clustering in a low dimensional discriminative space rather than in the PC space (generative). In particular, we propose a new clustering algorithm called Discriminative Cluster Analysis (DCA). DCA jointly performs dimensionality reduction and clustering. Several toy and real examples show the benefits of DCA versus traditional PCA+k-means clustering. Additionally, a new matrix formulation is proposed and connections with related techniques such as spectral graph methods and linear discriminant analysis are provided.

1. Introduction

Clustering is one of the most widely used statistical methods in data analysis (e.g. multimedia content-based retrieval, molecular biology, text mining, bioinformatics, ...). Recently, with an increasing number of database applications that deal with very large high dimensional datasets, clustering has emerged as a very important research area in many disciplines. Unfortunately, many known algorithms tend to break down in high dimensional spaces because of the sparsity of the points. In such high dimensional spaces not all the dimensions might be relevant for clustering, outliers are harder to detect, and it is not necessarily clear which is the right distance measure to choose. On the other hand when handling large amounts of data points, time complexity becomes a serious issue.

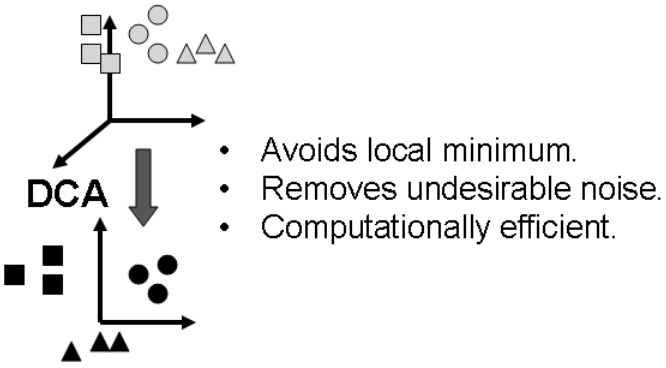

Figure 1. DCA finds a low dimensional projection beneficial for clustering.

There exist basically two types of clustering algorithms: Partitional and Hierchical (Jain et al., 1999). Partitional methods (e.g. k-means, mixture of Gaussians, graph theoretic, mode seeking) produce just one partition of the data, whereas hierarchical ones (e.g single link, complete link) produce several of them. In particular, k-means (MacQueen, 1967) is one of the simplest unsupervised learning algorithms that has been extensively studied and extended (Jain, 1988). Although an extremely popular technique because of its ease of programming and performance in large high dimensional data sets, k-means suffers from many drawbacks: it is sensitive to initial conditions; it does not remove undesirable noise (e.g. variables that are

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not useful for clustering); and it is only optimal for hyper-spherical clusters. In addition, its complexity in time is $O(nkl)$ and in space is $O(k)$, where n is the number of patterns, k the number of clusters and l the number of iterations. This complexity can be a problem for large datasets.

In this paper, we propose Discriminative Cluster Analysis (DCA) that alleviates some of the previous problems. DCA jointly optimizes for clustering and dimensionality reduction. In a first step, DCA finds a low dimensional projection of the data well suited for clustering by encouraging the preservation of distances between neighboring data points. Once the data is projected into a low dimensional space, DCA finds a "soft" clustering of the data. Later, this information is fed back into the dimensionality reduction step until convergence. Clustering in this subspace is less prone to local minima, it is faster to compute (especially for high dimensional data), and noisy dimensions not useful for clustering are removed. On the other hand, it is often difficult to model correlations in high dimensional spaces, but by projecting them into a low dimensional space, these correlations are able to be modeled. Figure 1, shows the main benefits of DCA.

2. Previous work

This section reviews, in a unified matrix framework, previous work on k-means clustering, spectral methods and linear discriminant analysis, pointing out the relationship between them.

2.1. K-means and spectral graph methods: a unified framework

k-means (MacQueen, 1967; Jain, 1988) is one of the simplest and most popular unsupervised learning algorithms to solve the clustering problem. Clustering refers to the partition of n data points into c disjoint clusters. k-means clustering splits a set of n objects into c groups by maximizing the between-clusters variation relative to within-cluster variation. That is, k-means clustering finds the partition of the data that is a local optimum of the following energy function:

$$J(\boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_n) = \sum_{i=1}^{c} \sum_{j \in C_i} ||\mathbf{d}_j - \boldsymbol{\mu}_i||_2^2 \qquad (1)$$

where $\mathbf{d}_j$ (see notation [1]) is a vector representing the j^{th} data point and $\boldsymbol{\mu}_i$ is the geometric centroid of the data points for class i. The optimization criteria in eq. 1 can be rewritten in matrix form as:

$$E_1(\mathbf{M}, \mathbf{G}) = ||\mathbf{D} - \mathbf{M}\mathbf{G}^T||_F \qquad (2)$$
$$subject\ to\ \mathbf{G}\mathbf{1}_c = \mathbf{1}_n \ \ and \ \ g_{ij} \in \{0, 1\}$$

where $\mathbf{G} \in \Re^{n \times c}$ and $\mathbf{M} \in \Re^{d \times c}$. $\mathbf{G}$ is a dummy indicator matrix, such that $\sum_j g_{ij} = 1$, $g_{ij} \in \{0, 1\}$ and g_{ij} is 1 if $\mathbf{d}_i$ belongs to class C_j, c denotes the number of classes and n the number of samples. The columns of $\mathbf{D} \in \Re^{d \times n}$ contain the original data points, d is the dimension of the data. Recall that the equivalence between the k-means error function eq. 1 and eq. 2 is only valid if $\mathbf{G}$ strictly satisfies the constraints.

The k-means algorithm performs coordinate descent in $E_1(\mathbf{M}, \mathbf{G})$. Given the actual value of the means $\mathbf{M}$, the first step finds for each data point $\mathbf{d}_j$, the $\mathbf{g}^j$ such that one of the columns is one and the rest 0 and minimizes eq. 2. The second step optimizes over $\mathbf{M} = \mathbf{D}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}$, equivalent to compute the mean of each cluster. Although it can be proved that alternating these two steps will always terminate, the k-means algorithm does not necessarily find the optimal configuration over all possible assignments. The algorithm is significantly sensitive to the initial randomly selected clusters' centers; it typically runs multiple times and the best solution is chosen. Despite these limitations, the algorithm is used fairly frequently as a result of its ease of implementation and effectiveness.

Eliminating $\mathbf{M}$, eq. 2 can be rewritten as:

$$E_2(\mathbf{G}) = ||\mathbf{D} - \mathbf{D}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T||_F = tr(\mathbf{D}^T\mathbf{D})$$
$$-tr((\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{D}^T\mathbf{D}\mathbf{G}) \geq \sum_{i=c+1}^{min(d,n)} \lambda_i \qquad (3)$$

where λ_i are the eigenvalues of $\mathbf{D}^T\mathbf{D}$. Minimizing eq. 3 is equivalent to maximizing $tr((\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{D}^T\mathbf{D}\mathbf{G})$. Ignoring the special structure of $\mathbf{G}$ and considering the continuous domain, the optimum $\mathbf{G}$ value that optimizes eq. 3 is given by the eigenvectors of the covariance matrix $\mathbf{D}^T\mathbf{D}$ and the error is $E_2 = \sum_{i=c+1}^{min(d,n)} \lambda_i$. A similar reasoning has been reported by (Ding & He, 2004; Zha et al., 2001), where they show that a lower bound of eq. 3 is given by the residual eigenvalues. The continuous solution of $\mathbf{G}$ lies in the $c-1$ subspace spanned by the first

[1] Bold capital letters denote a matrix $\mathbf{D}$, bold lower-case letters a column vector $\mathbf{d}$. $\mathbf{d}_j$ represents the j column of the matrix $\mathbf{D}$. d_{ij} denotes the scalar in the row i and column j of the matrix $\mathbf{D}$ and the scalar i-th element of a column vector $\mathbf{d}_j$. d_{ji} is the i-th scalar element of the vector $\mathbf{d}^j$. All non-bold letters will represent variables of scalar nature. $diag$ is an operator that transforms a vector to a diagonal matrix or takes the diagonal of the matrix into a vector. $\circ$ denotes the Hadamard or point-wise product. $\mathbf{1}_k \in \Re^{k \times 1}$ is a vector of ones. $\mathbf{I}_k \in \Re^{k \times k}$ is the identity matrix. $tr(\mathbf{A}) = \sum_i a_{ii}$ is the trace of the matrix $\mathbf{A}$ and $|\mathbf{A}|$ denotes the determinant. $||\mathbf{A}||_F = tr(\mathbf{A}^T\mathbf{A}) = tr(\mathbf{A}\mathbf{A}^T)$ designates the Frobenious norm of a matrix.

$c-1$ eigenvectors with highest eigenvalues (Ding & He, 2004) of $\mathbf{D}^T\mathbf{D}$.

Finally, it is worthwhile to point out the connections (Dhillon et al., 2004) between k-means and standard spectral graph algorithms, such as Normalized Cuts (Shi & Malik, 2000), by means of kernel methods. The kernel trick is a standard way of lifting the points of a dataset to a higher dimensional space, where points are more likely to be linearly separable (assuming that the right mapping is found). Let us consider a lifting of the original points to a higher dimensional space, $\mathbf{\Gamma} = [\ \boldsymbol{\phi}(\mathbf{d}_1)\ \boldsymbol{\phi}(\mathbf{d}_2)\ \cdots\ \boldsymbol{\phi}(\mathbf{d}_n)\ ]$ where $\boldsymbol{\phi}$ is a high dimensional mapping. The kernelized version of eq. 2 will be:

$$E_3(\mathbf{M},\mathbf{G}) = ||(\mathbf{\Gamma} - \mathbf{M}\mathbf{G}^T)\mathbf{W}||_F \quad (4)$$

where we have introduced a weighting matrix $\mathbf{W}$ for normalization purposes. Eliminating $\mathbf{M} = \mathbf{\Gamma}\mathbf{W}\mathbf{W}^T\mathbf{G}(\mathbf{G}^T\mathbf{W}\mathbf{W}^T\mathbf{G})^{-1}$, it can be shown that:

$$E_3 \propto -tr((\mathbf{G}^T\mathbf{W}\mathbf{W}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{W}\mathbf{W}^T\mathbf{\Gamma}^T\mathbf{\Gamma}\mathbf{W}\mathbf{W}^T\mathbf{G}) \quad (5)$$

where $\mathbf{\Gamma}^T\mathbf{\Gamma}$ is the standard affinity matrix in Normalized Cuts (Shi & Malik, 2000). After a change of variable $\mathbf{Z} = \mathbf{G}^T\mathbf{W}$, the previous equation can be expressed as $E_3(\mathbf{Z}) \propto -tr((\mathbf{Z}\mathbf{Z}^T)^{-1}\mathbf{Z}\mathbf{W}^T\mathbf{\Gamma}^T\mathbf{\Gamma}\mathbf{W}\mathbf{Z}^T)$. Choosing $\mathbf{W} = diag(\mathbf{\Gamma}^T\mathbf{\Gamma}\mathbf{1}_n)^{-0.5}$ the problem is equivalent to solving the Normalized Cuts problem. Observe that this formulation is more general since it allows for arbitrary kernels and weights. Also, observe that the weight matrix could be used to reject the influence of a pair of data points with unknown similarity (i.e. missing data).

2.2. Linear Discriminant Analysis

The aim of most discriminant analysis methods (e.g. LDA) is to project the data into a space of lower dimension so that the classes are projected as far as possible from each other and the projection is compact within each cluster. LDA can be calculated by maximizing several optimization criteria (Fukunaga, 1990), and most of them are based on relations between the following covariance matrices, conveniently expressed in matrix form (de la Torre & Kanade, 2005):

$$\begin{aligned} f\mathbf{S}_t &= \sum_{j=1}^{n}(\mathbf{d}_j-\mathbf{m})(\mathbf{d}_j-\mathbf{m})^T = \mathbf{D}\mathbf{P}_1\mathbf{D}^T \\ f\mathbf{S}_w &= \sum_{i=1}^{c}\sum_{\mathbf{d}_j\in C_i}(\mathbf{d}_j-\mathbf{m}_i)(\mathbf{d}_j-\mathbf{m}_i)^T = \mathbf{D}\mathbf{P}_2\mathbf{D}^T \\ f\mathbf{S}_b &= \sum_{i=1}^{c} n_i(\mathbf{m}_i-\mathbf{m})(\mathbf{m}_i-\mathbf{m})^T = \mathbf{D}\mathbf{P}_3\mathbf{D}^T \end{aligned}$$

where $f = n-1$, $\mathbf{P}_i$ are projection matrices (i.e $\mathbf{P}_i^T = \mathbf{P}_i$ and $\mathbf{P}_i^2 = \mathbf{P}_i$) with the following expressions:

$$\begin{aligned} \mathbf{P}_1 = \mathbf{I} - \tfrac{1}{n}\mathbf{1}_n\mathbf{1}_n^T \quad \mathbf{P}_2 = \mathbf{I} - \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T \\ \mathbf{P}_3 = \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T - \tfrac{1}{n}\mathbf{1}_n\mathbf{1}_n^T \end{aligned} \quad (6)$$

$\mathbf{S}_b$ is the between covariance matrix and represents the average of the distances between the mean of the classes. $\mathbf{S}_w$ represents the within covariance matrix and it is a measure of the average compactness of each class. Finally $\mathbf{S}_t$ is the total covariance matrix. With the matrix expressions, it is straightforward to show that $\mathbf{S}_t = \mathbf{S}_w + \mathbf{S}_b$. The upper bounds on the ranks of the matrices are $c-1,\ n-c,\ n-1$ for $\mathbf{S}_b, \mathbf{S}_w, \mathbf{S}_t$ respectively. Note that eq. 2 is $tr(\mathbf{S}_w)$.

LDA computes a linear transformation of the data $\mathbf{B} \in \Re^{d\times k}$ that maximizes the distance between the means of the classes and minimizes the variance within clusters. A Rayleigh-like quotient is among the most popular LDA optimization criteria (Fukunaga, 1990), some are: $J_1(\mathbf{B}) = \frac{|\mathbf{B}^T\mathbf{S}_1\mathbf{B}|}{|\mathbf{B}^T\mathbf{S}_2\mathbf{B}|}$ $J_2(\mathbf{B}) = tr((\mathbf{B}^T\mathbf{S}_1\mathbf{B})^{-1}\mathbf{B}^T\mathbf{S}_2\mathbf{B})$ $J_3(\mathbf{B}) = \frac{tr(\mathbf{B}^T\mathbf{S}_1\mathbf{B})}{tr(\mathbf{B}^T\mathbf{S}_2\mathbf{B})}$, where $\mathbf{S}_1 = \{\mathbf{S}_b, \mathbf{S}_b, \mathbf{S}_t\}$ and $\mathbf{S}_2 = \{\mathbf{S}_w, \mathbf{S}_t, \mathbf{S}_w\}$. A closed form solution to previous minimization problems is given by a generalized eigenvalue problem $\mathbf{S}_1\mathbf{B} = \mathbf{S}_2\mathbf{B}\Lambda$.

Previous Rayleigh quotient optimization procedures are not easy to modify in order to incorporate new constraints (e.g temporal constraints or geometric invariance). Formulating LDA as an error function will allow having a better understanding of the LDA limitations; moreover, it will be easier to formulate further generalizations. Consider the following weighted between-class covariance matrix, $\hat{\mathbf{S}}_b = \mathbf{D}\mathbf{G}\mathbf{G}^T\mathbf{D}^T = \sum_{i=1}^{C}(\frac{n_i}{n})^2(\mathbf{m}_i)(\mathbf{m}_i)^T$, that favors the classes with more samples. $\mathbf{m}_i$ is the mean vector for the class i and we consider the global mean (i.e. $\mathbf{m} = \frac{1}{n}\mathbf{D}\mathbf{1}_n$) to be zero. Following previous work on neural networks (Gallinari et al., 1991; Lowe & Webb, 1991), it can be shown that maximizing $J_4(\mathbf{B}) = tr((\mathbf{B}^T\hat{\mathbf{S}}_b\mathbf{B})^{-1}\mathbf{B}^T\mathbf{S}_t\mathbf{B})$ is equivalent to minimizing:

$$E_4(\mathbf{B},\mathbf{V}) = ||\mathbf{G}^T - \mathbf{V}\mathbf{B}^T\mathbf{D}||_F \quad (7)$$

After some linear algebra it can be shown (Gallinari et al., 1991; Lowe & Webb, 1991) that:

$$E_4(\mathbf{B}) \propto -tr(((\mathbf{B}^T\mathbf{D}\mathbf{D}^T\mathbf{B})^{-1})\mathbf{B}^T\mathbf{D}\mathbf{G}\mathbf{G}^T\mathbf{D}^T\mathbf{B}) \quad (8)$$

This approach is appealing, since Baldi and Hornik have shown that the surface of eq. 7 has a unique local minima (Baldi & Hornik, 1989), although several saddle points.

3. Discriminative Cluster Analysis

In the previous section, we have shown a matrix formulation for a generative approach to understand the error function of k-means algorithm (unsupervised), and a matrix expression to derive an approximation of LDA (supervised). The aim of DCA is to combine clustering and dimensionality reduction in an unsupervised manner. In this section, we show how DCA finds a low dimensional projection that preserves the local structure of the data, improving clustering by iteratively computing $\mathbf{B}$ and $\mathbf{G}$.

3.1. Error function for LDA

The key aspect to simultaneously perform dimensionality reduction and clustering consists of analyzing eq. 7. Ideally one would like to optimize eq. 7 w.r.t. $\mathbf{B}, \mathbf{G}$; however directly optimizing eq. 7 has several drawbacks. First, eq. 7 biases the solution towards the classes that have more samples, since it maximizes $\hat{\mathbf{S}}_b = \mathbf{D}\mathbf{G}\mathbf{G}^T\mathbf{D}^T = \sum_{i=1}^{c}(\frac{n_i}{n})^2(\mathbf{m}_i)(\mathbf{m}_i)^T$. Secondly, it does not encourage sparseness in $\mathbf{G}$ if $g_{ij} > 0$. Let $\mathbf{C} = \mathbf{B}^T\mathbf{D} \in \Re^{k\times n}$, eq. 7 is equivalent to $E_4 = tr(\mathbf{G}^T\mathbf{G}) - tr(\mathbf{G}^T\mathbf{C}^T(\mathbf{C}\mathbf{C}^T)^{-1}\mathbf{C}\mathbf{G})$. If g_{ij} are positive, minimizing $tr(\mathbf{G}^T\mathbf{G})$ does not encourage sparsitivity in $\mathbf{g}^i\ \forall i$ (recall $\mathbf{g}^i$ represents the i row of $\mathbf{G}$, see notation).

In this section, we show that Eq. 7 can be corrected to obtain the original LDA criteria by normalizing the error as follows:

$$E_5(\mathbf{B},\mathbf{V},\mathbf{G}) = ||(\mathbf{G}^T\mathbf{G})^{-\frac{1}{2}}(\mathbf{G}^T - \mathbf{V}\mathbf{B}^T\mathbf{D})||_F \quad (9)$$

subject to the constraint that $g_{ij} \in \{0,1\}$ and $\mathbf{G}\mathbf{1}_c = \mathbf{1}_n$. After eliminating $\mathbf{V}$, eq. 9 is equivalent to:

$$E_5(\mathbf{B},\mathbf{G}) = ||(\mathbf{G}^T\mathbf{G})^{-\frac{1}{2}}\mathbf{G}^T(\mathbf{I}_n - \mathbf{C}^T(\mathbf{C}\mathbf{C}^T)^{-1}\mathbf{C})||_F \quad (10)$$

$$\propto tr((\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{D}^T\mathbf{B}(\mathbf{B}^T\mathbf{D}\mathbf{D}^T\mathbf{B})^{-1}\mathbf{B}^T\mathbf{D}\mathbf{G}) \quad (11)$$

Equation eq. 11 can be re-written as $tr\big((\mathbf{B}^T\mathbf{D}\mathbf{D}^T\mathbf{B})^{-1}(\mathbf{B}^T\mathbf{D}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{D}^T\mathbf{B})\big)$.
If $\mathbf{G}$ is known eq. 11 is the exact expression for LDA.

If we relax the constraints on $\mathbf{G}$, an algorithm to minimize eq. 11 will alternate between solving the following eigenvalue problems:

$$\mathbf{D}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{D}^T\mathbf{B} = \mathbf{D}\mathbf{D}^T\mathbf{B}\mathbf{\Lambda}_1 \quad (12)$$

$$\mathbf{C}^T(\mathbf{C}\mathbf{C}^T)^{-1}\mathbf{C}\mathbf{G} = \mathbf{G}\mathbf{\Lambda}_2 \quad (13)$$

Observe that there is an ambiguity, since for any invertible matrix $\mathbf{T}_1 \in \mathbf{R}^{k\times k}$ $E_5(\mathbf{B}) = E_5(\mathbf{B}\mathbf{T}_1)$, similarly for any invertible matrix $\mathbf{T}_2 \in \mathbf{R}^{c\times c}$ $E_5(\mathbf{G}) = E_5(\mathbf{G}\mathbf{T}_2)$.

At this point, it is interesting to make a connection of the error function 11 with previous clustering techniques. Let $\mathbf{B} = \mathbf{I}_d \in \Re^{d\times d}$ be the identity matrix (no projection is done). Assuming $\mathbf{G}$ is continuous, the low dimensional embedding for clustering will be computed as the eigenvectors of $\mathbf{D}^T(\mathbf{D}\mathbf{D}^T)^{-1}\mathbf{D}$. If $n >> d$ $\mathbf{D} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ (i.e. SVD), where $\mathbf{U} \in \Re^{d\times d}$ $\mathbf{V} \in \Re^{n\times d}$ and $\mathbf{\Sigma} \in \Re^{d\times d}$, and assuming $\mathbf{D}\mathbf{D}^T$ is full rank, $\mathbf{D}^T(\mathbf{D}\mathbf{D}^T)^{-1}\mathbf{D} = \mathbf{V}\mathbf{V}^T$, which is the affinity matrix used previously in motion segmentation problems (Costeira & Kanade, 1995).

3.2. Updating B

The optimal $\mathbf{B}$ given $\mathbf{G}$ can be computed in closed form by solving the following generalized eigenvalue problem (eq. 12) $\mathbf{D}\mathbf{R}\mathbf{D}^T\mathbf{B} = \mathbf{D}\mathbf{D}^T\mathbf{B}\mathbf{\Lambda}_1$, where $\mathbf{R} = \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$. If $d << n$ and $\mathbf{D}\mathbf{D}^T$ is full rank, standard packages for generalized eigenvalue problems can be applied. However, for high dimensional data ($d >> n$) solving directly previous equation is not computationally efficient in either space or time. Fortunately, using the fact that the solutions of $\mathbf{B}$ are linear combinations of the data (i.e. $\mathbf{B}$=$\mathbf{D}\boldsymbol{\alpha}$), multiplying both sides by $\mathbf{D}^T$ and assuming $\mathbf{D}^T\mathbf{D}$ is invertible, the original eigenvalue problem is equivalent to solve $\mathbf{R}\mathbf{D}^T\mathbf{D}\boldsymbol{\alpha} = \mathbf{D}^T\mathbf{D}\boldsymbol{\alpha}\mathbf{\Lambda}_1$, which is of much lower dimension ($n \times n$).

There are many ways of efficiently solving this generalized eigenvalue problem (e.g. subspace methods (de la Torre et al., 2005)). In this section, we explore closed form solutions that invert $\mathbf{D}^T\mathbf{D}$ and solve a regular eigenvalue problem (i.e. $(\mathbf{D}^T\mathbf{D})^{-1}\mathbf{R}\mathbf{D}^T\mathbf{D}\boldsymbol{\alpha} = \boldsymbol{\alpha}\mathbf{\Lambda}_1$). Assuming $\mathbf{D}^T\mathbf{D}$ is full rank, computing $(\mathbf{D}^T\mathbf{D})^{-1}$ can be a numerically unstable process, especially if $\mathbf{D}^T\mathbf{D}$ has some eigenvalues close to zero. A common approach to solve ill-condition is to regularize the solution by factorizing $\mathbf{\Sigma} = \mathbf{D}^T\mathbf{D}$ as the sum of the outer products plus a scaled identity matrix, that is $\mathbf{\Sigma} \approx \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T + \sigma^2\mathbf{I}_d$. $\mathbf{V} \in \Re^{n\times k}$, $\mathbf{\Lambda} \in \Re^{k\times k}$ is a diagonal matrix. The parameters σ^2, $\mathbf{V}$, $\mathbf{\Lambda}$ are estimated by following a fitting approach that minimizes $E_c(\mathbf{V},\mathbf{\Lambda},\sigma^2) = ||\mathbf{\Sigma} - \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T - \sigma^2\mathbf{I}_n||_F$. After optimizing the parameters, it can be shown (de la Torre & Kanade, 2005) that: $\sigma^2 = tr(\mathbf{\Sigma} - \mathbf{V}\hat{\mathbf{\Lambda}}\mathbf{V}^T)/d - k$, $\mathbf{\Lambda} = \hat{\mathbf{\Lambda}} - \sigma^2\mathbf{I}_d$, where $\hat{\mathbf{\Lambda}}$ are the eigenvalues of the covariance matrix $\mathbf{\Sigma}$ and $\mathbf{V}$ the eigenvectors. After the factorization is found, we apply the matrix inversion lemma (Golub & Loan, 1989) ($(\mathbf{A}^{-1}+\mathbf{V}\mathbf{C}^{-1}\mathbf{V}^T)^{-1} = \mathbf{A} - (\mathbf{A}\mathbf{V}(\mathbf{C}+\mathbf{V}^T\mathbf{A}\mathbf{V})^{-1})\mathbf{V}^T\mathbf{A}$) to invert $(\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T + \sigma^2\mathbf{I}_d)^{-1}$ which results in:

$$(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^T + \sigma^2\mathbf{I}_n)^{-1} = \frac{1}{\sigma^2}(\mathbf{I}_n - \frac{1}{\sigma^2}\mathbf{V}(\mathbf{\Lambda}^{-1} + \frac{\mathbf{I}_n}{\sigma^2})^{-1}\mathbf{V}^T)$$

Now solving $(\mathbf{I}_d - \frac{1}{\sigma^2}\mathbf{V}(\mathbf{\Lambda}^{-1} + \frac{\mathbf{I}_n}{\sigma^2})^{-1}\mathbf{V}^T)\mathbf{R}\mathbf{D}^T\mathbf{D}\boldsymbol{\alpha} = \boldsymbol{\alpha}\mathbf{\Lambda}$ becomes more computationally tractable and numerically stable process.

The number of bases (k) are bounded by the number of classes, since $rank(\mathbf{D}\mathbf{R}\mathbf{D}^T) = c$. We typically choose $c-1$ to be consistent with LDA. Moreover, we have experienced that the best clustering results are achieved by projecting the data into a space of $c-1$ dimensions.

3.3. Updating G

Let $\mathbf{A} = \mathbf{C}^T(\mathbf{C}\mathbf{C}^T)^{-1}\mathbf{C} \in \Re^{n\times n}$, recall $\mathbf{C} = \mathbf{B}^T\mathbf{D}$, eq. 11 is equivalent to:

$$E_5(\mathbf{G}) \propto tr((\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{A}\mathbf{G}) \tag{14}$$

To impose non-negativity constraints in g_{ij}, we parameterize $\mathbf{G}$ as the product of two matrices $\mathbf{G} = \mathbf{V} \circ \mathbf{V}$ (Liu & Yi, 2003) and use a gradient descent strategy to search for an optimum:

$$\mathbf{V}^{n+1} = \mathbf{V}^n - \eta\frac{\partial G(\mathbf{V}^n)}{\partial \mathbf{V}} \tag{15}$$
$$\frac{\partial G(\mathbf{V}^n)}{\partial \mathbf{V}} = (\mathbf{I}_c - \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T)\mathbf{A}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1} \circ \mathbf{V}$$

The major problem with the update of eq. 15 is to determine the optimal η. In our case, η is determined with a line search strategy. To impose $\mathbf{G}\mathbf{1}_c = \mathbf{1}_n$ in each iteration, the $\mathbf{V}$ is normalized to satisfy the constraint. Because eq. 15 is prone to local minima, we start from several random initial points and select the solution with minimum error.

At this point, observe that this optimization problem is similar in spirit to recent work on clustering with non-negative matrix factorization (Zass & Shashua, 2005; Ding et al., 2005; Lee & Seung, 2000). However, we optimize a discriminative criteria rather than a generative one. On the other hand, we simultaneously compute the dimensionality reduction and clustering and a different optimization technique is used.

3.4. Initialization

At the beginning neither $\mathbf{G}$ or $\mathbf{B}$ are known, but the matrix $\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$ can be estimated from data. Similarly to (He & Niyogi, 2003), we compute local information (i.e. $\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T \in \Re^{n\times n}$) from data. We assume that $(\mathbf{G}^T\mathbf{G}) \approx s\mathbf{I}_c$, so that all the classes are equally distributed and s is the number of samples per class. $\mathbf{R} = \frac{1}{s}\mathbf{G}\mathbf{G}^T$ is a hard-affinity matrix, where r_{ij} will be 1 if $\mathbf{d}_i$ and $\mathbf{d}_j$ are considered to be neighbors (i.e. belong to the same class). $\mathbf{R}$ can be estimated by simply computing the k nearest neighbors for each data point using Euclidian distance. To make $\mathbf{R}$ symmetric, we filter out the cases where $\mathbf{d}_i$ is within the k-neighborhood of $\mathbf{d}_j$ but not the opposite. Figure 6.b shows an estimate of $\mathbf{R}$. In this example, there are 15 clusters (subjects), 10 samples per class and 9 nearest neighbors are selected. The samples are ordered by class. After factorizing (i.e. SVD) $\mathbf{R} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T$, we normalize $\mathbf{R}$ as $\hat{\mathbf{R}} \approx \mathbf{U}_c\mathbf{U}_c^T$, where $\mathbf{U}_c \in \mathbf{R}^{n\times c}$ are the first c eigenvectors of $\mathbf{R}$. $\hat{\mathbf{R}}$ will be the initial neighbor matrix.

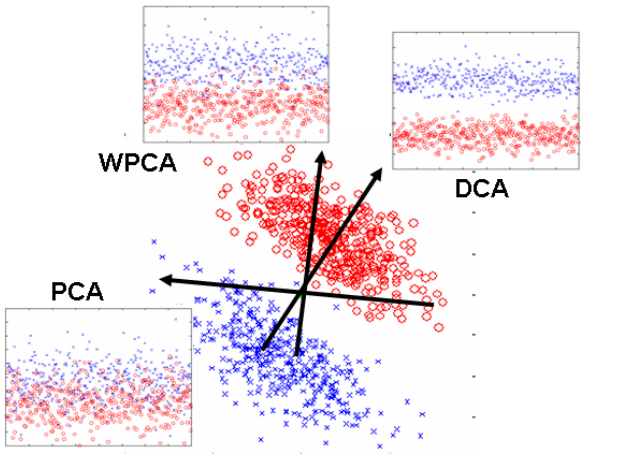

Figure 2. Two class toy problem. PCA, WPCA and DCA projections into 1 dimensional space.

3.5. Interpreting the weighted covariance matrix

A key aspect to interpret DCA is the understanding of the weighted covariance matrix $\mathbf{D}\mathbf{R}\mathbf{D}^T = \sum_{i=1}^n\sum_{j=1}^n r_{ij}\mathbf{d}_i\mathbf{d}_j^T$. Principal Component Analysis (PCA) (Jolliffe, 1986) computes a basis $\mathbf{B}$ that maximize the variance of the projected samples, i.e. PCA finds an orthonormal basis that maximizes $tr(\mathbf{B}^T\mathbf{D}\mathbf{D}^T\mathbf{B}) = \sum_{i=1}^N ||\mathbf{B}^T\mathbf{d}_i||_2^2$. The PCA solution, $\mathbf{B}$, is given by the eigenvectors of $\mathbf{D}\mathbf{D}^T$. Finding the leading eigenvectors of $\mathbf{D}\mathbf{R}\mathbf{D}^T$ is equivalent to maximize $tr(\mathbf{B}^T\mathbf{D}\mathbf{R}\mathbf{D}^T\mathbf{B}) = \sum_{i=1}^N\sum_{i=1}^N r_{ij}\mathbf{d}_j^T\mathbf{B}\mathbf{B}^T\mathbf{d}_i$. If $\mathbf{R} = \mathbf{I}$ we have the standard PCA result; however, if $\mathbf{R}$ contains a block structure with the cluster information, the weighted covariance just maximizes the covariance within each cluster, finding a projection where the correlation between each pair of points within each cluster is maximized. Figure 2 shows a toy problem, where two Gaussian classes with an equal number of points are generated. The first eigenvector in PCA finds a direction of maximum variance that does not necessarily correspond to maximum discrimination (in fact, projecting the data into the first principal component the clusters overlap). If $\mathbf{R}$ is the initial matrix of neighbors, the first step of DCA finds a better projection for clustering.

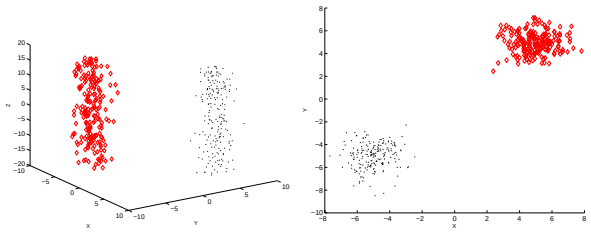

Figure 3. a) 2 classes of 3 dimensional data. b) Projection onto XY space.

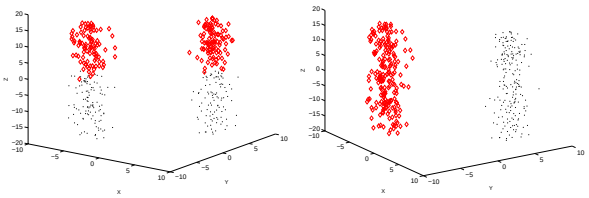

Figure 4. a) k-means clustering. b) DCA clustering.

Another possible unsupervised technique for dimensionality reduction preserving topological relations is Weighted Principal Component Analysis. WPCA minimizes $E_5(\mathbf{B},\mathbf{C}) = ||(\mathbf{D} - \mathbf{BC})\mathbf{R}^{\frac{1}{2}}||_F$. After eliminating $\mathbf{C}$, minimizing the previous equation is equivalent to maximizing $E_5(\mathbf{B}) = tr((\mathbf{B}^T\mathbf{B})^{-1}(\mathbf{B}^T\mathbf{DRD}^T\mathbf{B}))$. WPCA will be closely related to local preserving projection (He & Niyogi, 2003) with the right choice of weights. The optimum is achieved by solving the following eigenvalue problem $\mathbf{DRD}^T\mathbf{B} = \mathbf{B}\mathbf{\Lambda}$, where $\mathbf{B}$ will be given by the eigenvectors of $\mathbf{DRD}^T$.

4. Experiments

4.1. Removing undesirable dimensions

The first experiment demonstrates the ability of DCA to deal with undesired dimensions not relevant for clustering. A toy problem is created as follows: 200 samples from a two-dimensional Gaussian distribution with mean $[-5,-5]$ and another 200 samples from another Gaussian with mean $[5,5]$ are generated (x and y dimensions). We add a third dimension generated with uniform noise between [0..35] (z dimension). Figure 3 shows the 200 samples of each class, in the original space (fig. 3.a) and the projection (fig. 3.b) onto x and y. k-means algorithm gets confused by the noise(fig. 4.a). Similarly, by projecting the data into the first two principal components, the wrong clustering is achieved, since PCA preserves the energy of the uniform noise which is not relevant for clustering. However, DCA (projecting into two dimensional space) is able to remove the noise and it achieves the correct clustering, fig. 4.b. In this particular example 15 neighbors were selected initially and $\mathbf{B} \in \Re^{3\times 2}$. Also, observe that k-means is optimal for spherical clusters, whereas DCA is able to deal with oriented clusters ($E_5(\mathbf{TD}) = E_5(\mathbf{D})$) for any invertible matrix $\mathbf{T} \in \Re^{d\times d}$.

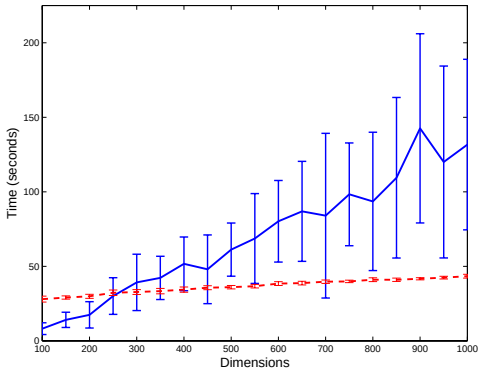

Figure 5. Time (seconds) versus number of dimensions. Blue straight line PCA+k-means, red dotted line DCA.

4.2. Computational efficiency

In this experiment, we have generated 400 samples of four x-dimensional Gaussians, with the dimension x ranging from 100 to 1000 in increments of 50. For two of the Gaussians, the means are 10 and -10 respectively, whereas the other two have half of the dimensions as 10 and the other half -10, and vice versa. For each dimension and each Gaussian, we synthetically generate 400 samples and cluster them using k-means and DCA. Figure 5 shows the results of the time spent in clustering with k-means in the original spaces versus DCA. As we can observe, DCA is more computationally efficient as the number of samples increase.

4.3. Clustering faces

The last experiment shows results on clustering faces from the ORL face database (Samaria & Harter, 1994). The ORL face database is composed of 40 subjects and 10 images per subject. We randomly select k subjects from the database and add its 10 images to the data matrix $\mathbf{D} \in \Re^{d\times 10k}$ (e.g. fig. 6.a). Afterwards, we compute PCA, WPCA (with the initial matrix $\mathbf{R}$), PCA+LDA (preserving 95% of the energy in PCA) and DCA. After computing PCA, WPCA and PCA+LDA, we run the k-means (Matlab) on the projected samples 10 times and the best solution is chosen (the one with less error). This procedure is repeated

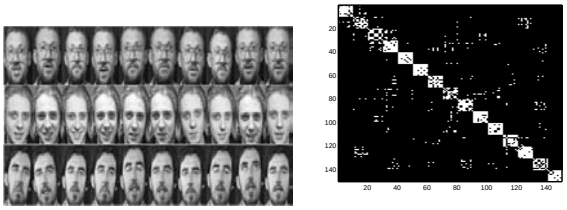

Figure 6. a) Some faces of the ORL data base. b) Estimate of $\mathbf{R}$ for 15 clusters (people), each cluster has 10 samples. The samples are ordered by clusters.

40 times for different numbers of classes (between 4 and 40 subjects). To perform a fair comparison, we project the data into $classes-1$ dimensions for all the methods. Fig. 7.a shows the PCA projection for the 10 classes case; fig. 7.b shows the DCA projection in the first step.

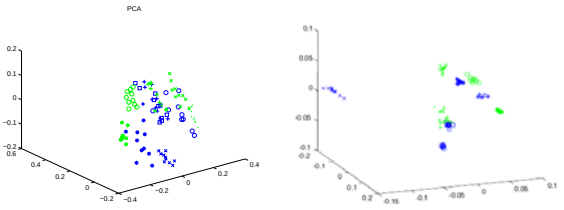

Figure 7. a) PCA projection. b)DCA projection.

To compute the accuracy of the results for a c cluster case, we compute a $c-by-c$ confusion matrix $\mathbf{C}$, where each entry c_{ij} is the number of faces in cluster i, which belong to class j. It is difficult to compute the accuracy by just using the confusion matrix $\mathbf{C}$ because we do not know which cluster matches which class. An optimal way to solve for it (Zha et al., 2001; Knuth, 1993) is to compute the following maximization problem:

$$\max\ tr(\mathbf{CP}) \mid \mathbf{P}\ is\ a\ permutation\ matrix \qquad (16)$$

and the accuracy is obtained by dividing the results for the number of data points to be clustered. To solve eq. 16, we use the classical Hungarian algorithm (Knuth, 1993). Table 1 shows the accuracy results (the mean and standard deviation over 40 runs) for different projection methods and different number of classes. As we can observe, DCA outperforms most of the methods when there are between 5 and 30 classes; for more classes $PCA+LDA$ performs marginally better.

Fig. 8 shows the accuracy in clustering for PCA+k-means vs. DCA. For a given number of clusters, we show the mean and variance of 40 realizations. DCA always outperforms PCA+k-means. Also observe how the accuracy drops with the number of classes (as expected).

C	PCA	WPCA	DCA	PCA+LDA
4	73±0%	1±0%	87±2%	**1**±0%
10	88±6%	95±6%	**97±4%**	88±8%
15	86±5%	88±4%	**96±1%**	82±6%
20	80±4%	84±4%	**87±2%**	83±4%
25	77±3%	80±4%	**87±2%**	80±4%
30	75±3%	79±3%	**81±3%**	81±4%
35	73±4%	77±3%	78±4%	**81±3%**
40	71±2%	74±3%	73±3%	**80±4%**

Table 1. Comparison of accuracy for several projection methods (same number of bases: classes-1).

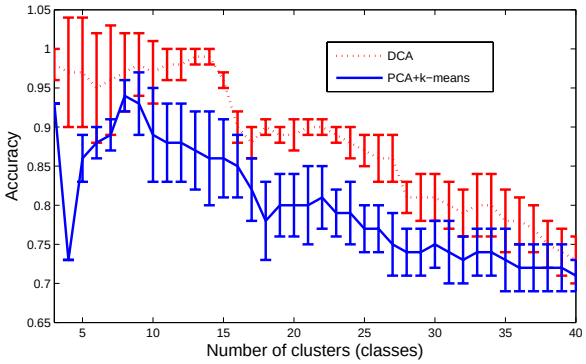

Figure 8. Accuracy of clustering versus the number of classes. Blue PCA and red DCA (dotted line).

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6. Discussion and future work

In this paper we have presented DCA, a new dimensionality reduction and clustering algorithm. DCA outperforms PCA+k-means, since it uses discriminative features for clustering rather than generative ones. Clustering in this space is less prone to local minima and removes unrelated dimensions for clustering. Moreover, clustering in this low dimensional discriminative space is more computationally efficient than

clustering in the original space. Additionally, we have constructed an error function for LDA.

However, several issues still need to be addressed. It still remains unclear how to select the optimal number of clusters; several model order selection (e.g. Minimum Description Length or Akaike information criterion) could be applied. On the other hand, DCA assumes that all the clusters have the same orientation (not necessarily spherical). Several extensions could be made in the case of non-Gaussian shape clusters, for instance using kernel methods. However, for huge amounts of high dimensional data ($d, n >> c$) the efficiency of the solution will be lost. Adding the constraint that $\mathbf{G}^T\mathbf{G} = \mathbf{I}$ will probably help the clustering process; an approximate manner to incorporate these constraints without transforming the problem into a quadratic programming one (that is computationally expensive) will be to add $\lambda tr(\mathbf{G}^T\mathbf{G})$ to eq. 11.

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