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Pairwise-Covariance Linear Discriminant Analysis

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Abstract

In machine learning, linear discriminant analysis (LDA) is a popular dimension reduction method. In this paper, we first provide a new perspective of LDA from an information theory perspective. From this new perspective, we propose a new formulation of LDA, which uses the pairwise averaged class covariance instead of the globally averaged class covariance used in standard LDA. This pairwise (averaged) covariance describes data distribution more accurately. The new perspective also provides a natural way to properly weigh different pairwise distances, which emphasizes the pairs of class with small distances, and this leads to the proposed pairwise covariance properly weighted LDA (pcLDA). The kernel version of pcLDA is presented to handle nonlinear projections. Efficient algorithms are presented to efficiently compute the proposed models.

Introduction

In the big data era, a large number of high-dimensional data (i.e., DNA microarray, social blog, image scenes, etc) are available for data analysis in different applications. Linear Discriminant Analysis (LDA) (Hastie, Tibshirani, and Friedman 2001) is one of the most popular methods for dimension reduction, which has shown state-of-the-art performance. The key idea of LDA is to find an optimal linear transformation which projects data into a low-dimensional space, where the data achieves maximum inter-class separability. The optimal solution to LDA is generally achieved by solving an eigenvalue problem.

Despite the popularity and effectiveness of LDA, however, in standard LDA model, instead of emphasizing the pairwise-class distances, it simply takes an *average* of metrics computed in different pairs (i.e., computation of between-class scatter matrix $\mathbf{S}_b$ or within-class scatter matrix $\mathbf{S}_w$). Thus, some pairwise class distances are depressed, especially for those pairs whose original class distances are relatively large.

To overcome this issue, in this paper, we present a new formulation for pairwise linear discriminant analysis. To obtain a discriminant projection, the proposed method considers all the pairwise between-class and with-class distances. We call it "pairwise-covariance LDA (pcLDA)". Then, the pcLDA problem is cast into solving an optimization problem, which maximizes the class separability computed from pairwise distance. An efficient algorithm is proposed to solve the resultant problem, and experimental results indicate the good performance of the proposed method.

A new perspective of LDA

The standard linear discriminant analysis (LDA) is to seek a projection $\mathbf{G} = (\mathbf{g}_1, \cdots, \mathbf{g}_{K-1}) \in \Re^{p\times(K-1)}$ which maximizes the class separability by solving,

$$\max_{\mathbf{G}} \mathrm{Tr}\Big(\frac{\mathbf{G}^T\mathbf{S}_b\mathbf{G}}{\mathbf{G}^T\mathbf{S}_w\mathbf{G}}\Big) = \max_{\mathbf{G}} \mathrm{Tr}(\mathbf{G}^T\mathbf{S}_b\mathbf{G})(\mathbf{G}^T\mathbf{S}_w\mathbf{G})^{-1}, \qquad (1)$$

where $\mathbf{S}_w$ is the within-class scatter matrix, and $\mathbf{S}_b$ is the between-class scatter matrix, and given by

$$\mathbf{S}_b = \frac{1}{n}\sum_{k=1}^{K} n_k(\mu_k - \mu)(\mu_k - \mu)^T,$$

$$\mathbf{S}_w = \Sigma = \frac{1}{n}\sum_{k=1}^{K} n_k\Sigma_k,\ \Sigma_k \triangleq \frac{1}{n_k}\sum_{\mathbf{x}_i\in C_k}(\mathbf{x}_i - \mu_k)(\mathbf{x}_i - \mu_k)^T,$$

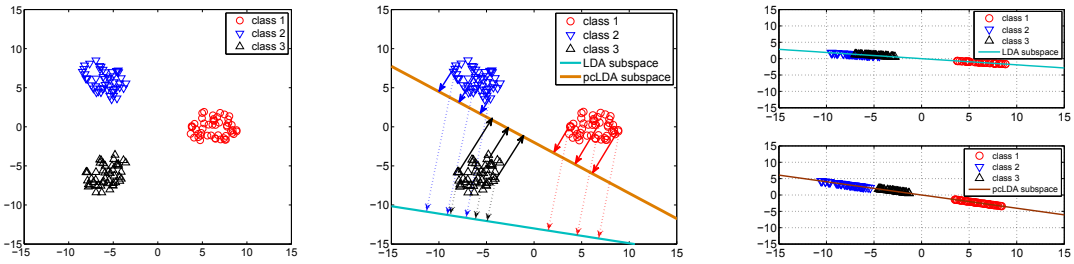
where n_k is the number of data in class C_k, $\mu_k \in \Re^{p\times 1}$ is the mean for the data from class C_k, μ is the global mean for all the data. In the history of LDA (Hastie, Tibshirani, and Friedman 2001), the objective function of LDA is evolved from Fisher's initial 2-class LDA:

$$\max_{\mathbf{g}} \frac{\mathbf{g}^T\mathbf{S}_b\mathbf{g}}{\mathbf{g}^T\mathbf{S}_w\mathbf{g}}. \qquad (2)$$

For multi-class LDA, this can be generalized to either the *trace-of-ratio* of Eq.(1), or the following *ratio-of-traces* objective:

$$\max_{\mathbf{G}} \frac{\mathrm{Tr}(\mathbf{G}^T\mathbf{S}_b\mathbf{G})}{\mathrm{Tr}(\mathbf{G}^T\mathbf{S}_w\mathbf{G})}. \qquad (3)$$

Mathematically, both generalization are natural; there is no clear difference in terms of machine learning. The trace-of-ratio objective Eq.(1) is the most widely used one. However, the ratio-of-trace objective of Eq.(3) has been used by many researches, *e.g.*, (Wang et al. 2007), (Kong and Ding 2012), *etc*. To our knowledge, there exist no clear explanations of the differences between these two different LDA objectives. In this paper, we bridge this gap, by providing theoretical support to the LDA objective of Eq.(1) from KL-divergence perspective, which is described in Theorem 1 below.



(a) 2-dim Data distribution (b) LDA and pcLDA (c) Enlarged LDA and pcLDA

Figure 1: A synthetic data set of 150 data points, 50 data of each class. (a) data distribution; (b) 1-dimensional projection of LDA and pcLDA. Note that both the subspaces (lines) pass through (0,0). We shift them to avoid clutter. (c) Enlarged 1-dim LDA and pcLDA.

From the KL-divergence to classic LDA

LDA assumes that data points of each class k are a Gaussian distribution. The covariance matrix of this class Σ_k is called the within-class scatter matrix $\mathbf{S}_w^k$. In this paper, we use "covariance" or "averaged covariance" instead of the usual "within-class scatter matrix" $\mathbf{S}_w$ to emphasize the new perspective. The within-class scatter matrix defined in Eq.(2) is the globally averaged (*i.e.,* averaged over all k classes) covariance matrix. Furthermore, we propose the pairwise averaged covariance as a better formulation which is used in pcLDA.

We start with the KL-divergence between two Gaussian distributions $\mathcal{N}_k(\mu_k, \Sigma_k), \mathcal{N}_l(\mu_l, \Sigma_l)$ with the same covariances: $\Sigma_k = \Sigma_l = \Sigma_{kl}$. The KL-divergence of $\mathcal{N}_k$ and $\mathcal{N}_l$ is:

$$D_{KL}(\mathcal{N}_k||\mathcal{N}_l) = \frac{1}{2}(\mu_k - \mu_l)^T \Sigma_{kl}^{-1}(\mu_k - \mu_l). \tag{4}$$

KL-divergence is used as a measure of distance between two classes. When the data are transformed using projection $\mathbf{G}$, i.e., we project $\mathbf{x}_i$ to the subspace $\mathbf{y}_i = \mathbf{G}^T\mathbf{x}_i$, or $\mathbf{Y} = \mathbf{G}^T\mathbf{X}$, the KL-divergence in $\mathbf{Y}$-space is

$$D_{KL}^{\mathbf{Y}}(\mathcal{N}_k||\mathcal{N}_l) = \frac{1}{2}(\mu_k - \mu_l)^T \mathbf{G}(\mathbf{G}^T\Sigma_{kl}\mathbf{G})^{-1}\mathbf{G}^T(\mu_k - \mu_l). \tag{5}$$

We have the following results.

Theorem 1. *When the covariances of all K classes are identical, i.e., $\Sigma_k = \Sigma, k = 1 \cdots K$, the sum of all pairwise KL-divergences:*

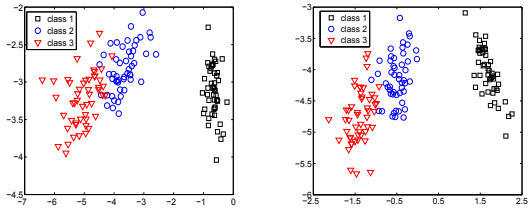
$$J_0^{\mathbf{Y}} = \sum_{k<l} n_k n_l D_{KL}^{\mathbf{Y}}(\mathcal{N}_k||\mathcal{N}_l) \tag{6}$$

is identical to the objective function of standard LDA of Eq.(1), where $\sum_{k<l} = \sum_{k=1}^{K}\sum_{l=k+1}^{K}$.

Proof: Note that $(\mu_k - \mu_l)^T\Sigma^{-1}(\mu_k - \mu_l)$
$= \mathrm{Tr}[(\mu_k - \mu_l)(\mu_k - \mu_l)^T\Sigma^{-1}]$
$= \mathrm{Tr}[(\mu_k\mu_k^T + \mu_l\mu_l^T - \mu_k\mu_l^T - \mu_l\mu_k^T)\Sigma^{-1}]$, we have

$$J_0^{\mathbf{X}} = \sum_{k=l}^{K}\sum_{l=1}^{K} n_k n_l \mathrm{Tr}[(\mu_k\mu_k^T + \mu_l\mu_l^T - \mu_k\mu_l^T - \mu_l\mu_k^T)\Sigma^{-1}]$$

$$= 2n\mathrm{Tr}[\sum_{k=1}^{K} n_k(\mu_k - \mu)(\mu_k - \mu)^T\Sigma^{-1}] = 2n\mathrm{Tr}[\mathbf{S}_b\Sigma^{-1}].$$



(a) Standard LDA. (b) Pairwise-covariance LDA.

Figure 2: Results on `Iris` dataset with 3 classes, each class has 50 data points. Original 4-dimensional data are projected into 2 dimensions. (a) Results of standard LDA; (b) Results of pairwise-covariance LDA.

Now we project $\mathbf{x}_i$ to the subspace $\mathbf{y}_i = \mathbf{G}^T\mathbf{x}_i$. The covariance in $\mathbf{Y}$-space is $\Sigma^{\mathbf{Y}} = \mathbf{G}^T\Sigma\mathbf{G}$ and the between-class scatter matrix becomes: $\mathbf{S}_b^{\mathbf{Y}} = \mathbf{G}^T\mathbf{S}_b\mathbf{G}$. Thus

$$J_0(\mathbf{G}) = 2n\mathrm{Tr}(\mathbf{G}^T\mathbf{S}_b\mathbf{G})(\mathbf{G}^T\Sigma\mathbf{G})^{-1} \tag{7}$$

is identical to the LDA objective function of Eq.(1) aside from the unimportant constant $2n$. □

Pairwise-covariance LDA

Motivation In standard LDA, covariances Σ_k of all K classes are assumed to be exactly identical. This results in a standard LDA of Eq.(1), as we can see from Theorem 1. In practice, data covariance for each class is often different. For 2-class problem, when $\Sigma_1 \neq \Sigma_2$, the quadratic discriminant analysis (QDA) (Hastie, Tibshirani, and Friedman 2001) can be used. However, in QDA, the boundary between different classes is a quadratic surface, and the discriminant space can *not* be represented by $\mathbf{G}^T\mathbf{X}$ explicitly. For multi-class, one can directly solve it using the Gaussian mixture density function with Bayes rules. In this paper, we seek a discriminant subspace that can be obtained by the linear transformation $\mathbf{G}^T\mathbf{X}$, which has not been studied before.

Illustrative example In most datasets, data variance for each class is generally different, standard LDA uses the *pooled* (i.e., the global averaged) within-class scatter matrices of all classes. However, the global averaged covariance $\mathbf{S}_w$ could differ from each individual covariance sig-

nificantly. A simple example is shown in Fig.1, where a 2-dimensional data from three classes are shown in Fig.(1(a)). Each class has 50 data points. The covariance for data from each class is $\Sigma_1, \Sigma_2, \Sigma_3$:

$$\Sigma_1 = \begin{bmatrix} 2.336 & 0.015 \\ 0.015 & 1.097 \end{bmatrix}, \quad \Sigma_2 = \begin{bmatrix} 1.704 & -0.539 \\ -0.539 & 1.575 \end{bmatrix},$$
$$\Sigma_3 = \begin{bmatrix} 1.514 & 0.512 \\ 0.512 & 1.531 \end{bmatrix}; \Sigma_{123} = \begin{bmatrix} 1.851 & -0.004 \\ -0.004 & 1.401 \end{bmatrix}.$$

These individual covariances are very different. In standard LDA, we average all the classes and obtain $\mathbf{S}_w = \Sigma_{123}$. In this paper, we propose a formulation of LDA that uses pairwise classes. The three pairwise averaged class-covariance: Σ_{12}, Σ_{13} and Σ_{23} are

$$\Sigma_{12} = \begin{bmatrix} 2.020 & -0.262 \\ -0.262 & 1.336 \end{bmatrix}, \quad \Sigma_{13} = \begin{bmatrix} 1.925 & 0.264 \\ 0.264 & 1.314 \end{bmatrix},$$
$$\Sigma_{23} = \begin{bmatrix} 1.609 & -0.013 \\ -0.013 & 1.553 \end{bmatrix}.$$

We see that the pairwise averaged covariance are *much closer* to the two individual covariances as compared to the global average.

Formulation For simplicity, we define the distance $d_{k,l}(\mathbf{G})$ between two classes k, l as

$$d_{k,l}(\mathbf{G}) = 2D_{KL}^{\mathbf{Y}}(\mathcal{N}_k, \mathcal{N}_l),$$

where $D_{KL}^{\mathbf{Y}}(\mathcal{N}_k, \mathcal{N}_l)$ is defined in Eq.(5), and Σ_{kl} is a pairwise covariance matrix (average of the pair of classes) and defined as

$$\Sigma_{kl} = \beta \frac{n_k \Sigma_k + n_l \Sigma_l}{n_k + n_l} + (1 - \beta)\Sigma. \tag{8}$$

Here we use the globally averaged covariance $\Sigma = \mathbf{S}_w$ as a regularization. Parameter $0 \leq \beta \leq 1$ controls the balance of global covariance matrix Σ and local pairwise covariance matrix Σ_k, Σ_l.

The pairwise-covariance LDA is defined the same as that in Theorem 1:

$$\max_{\mathbf{G}} \; J_1(\mathbf{G}) = \sum_{k<l} n_k n_l d_{kl}(\mathbf{G}), \tag{9}$$

where $\mathbf{G} \in \Re^{p \times (K-1)}$ is the projection. The objective in Eq.(9) is similar to standard LDA (except that we use pairwise covariance instead of global averaged covariance).

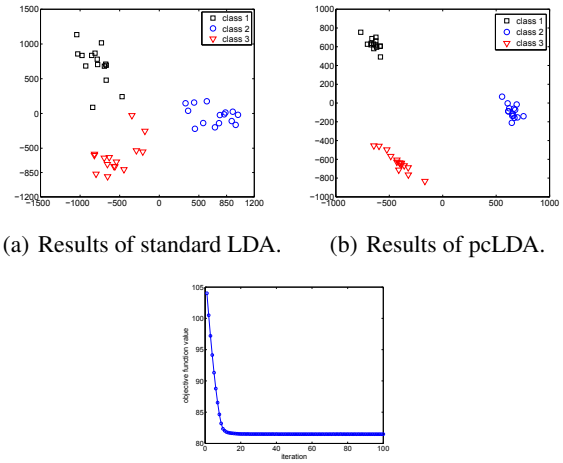
The proposed new model

Back to the form of Eq.9, it is easy to see that we can define a better objective. In maximizing J_1, all pairs of distances are treated equally. However, in classification, we wish the pair of classes with smaller distances to be given more weight, i.e., after projecting to $\mathbf{Y} = \mathbf{G}^T\mathbf{X}$ subspace, they are more separated (as compared to other pairs of classes). On the other hand, if two classes are already well-separated, i.e., their distances are large, they can have less weight in the objective function. Therefore, we propose the following pairwise covariance *properly weighted* objective function:

$$\min_{\mathbf{G}} \; J_2(\mathbf{G}) = \sum_{k<l} \frac{n_k n_l}{[d_{kl}(\mathbf{G})]^q}, \;\; s.t. \;\; \mathbf{G}^T\mathbf{G} = \mathbf{I}, \tag{10}$$

where $q \geq 1$ is a hyper-parameter. In this objective function, the pair of classes with smaller distances contribute more than the pair of classes with larger distances. Parameter q controls how much the pair of classes with smaller distances are weighted. The larger q is, the stronger that pair of classes is weighted. In practice, we found that $q = \{1, 2\}$ are good choices. This model is our final proposed model. For simplicity, we call it **pairwise-covariance LDA (pcLDA)** with the proper weighting implicit.

As defined in Eq.(10), the objective is invariant under any non-singular transformation using $\mathbf{A} \in \Re^{(K-1)\times(K-1)}$, i.e., $J_2(\mathbf{GA}) = J_2(\mathbf{G})$. To fix this uncertainty, we require $\mathbf{G}^T\mathbf{G} = \mathbf{I}$.



(a) Results of standard LDA. (b) Results of pcLDA.

(c) Convergence of algorithm.

Figure 3: Data: 45 data points (images) from 3 classes on `mnist` dataset. Original 784-dimensional data are projected into 2-dimension. (a) Results of standard LDA; (b) Results of pcLDA; (c) Convergence of algorithm on `mnist`. Shown are objective function vs. iterations.

Illustrations of pcLDA

We illustrate pcLDA on synthetic and real data. In Fig.1, LDA and pcLDA results on a synthetic 2D dataset of 150 data points (50 data of each class) are shown. We show the data distribution and 1-dimensional projection results using LDA and pcLDA. The point here is that the globally averaged covariance $\mathbf{S}_w$ is a poor representation of the individual covariances, but the pairwise-covariance approach seems to give a better representation such that a single pcLDA dimension can clearly separate the 3 classes, while standard LDA needs 2-dimensions to separate data from different classes (results not shown).

In Fig.2, we show the results on the widely used `iris` data[1]. Iris has 150 data points with K=3 classes. Thus LDA project to K-1=2 dimensions. Fig.2 indicates that pcLDA gives clear discrimination between classes 2 and 3 while standard LDA has strong mixing between classes 2 and 3. In Fig.3, we show results on 45 images (from K=3 classes) from `mnist` handwritten digits image dataset. LDA projections to 2-dimension are shown. Result of pcLDA shows that

[1] http://archive.ics.uci.edu/ml/datasets/Iris

the 3 classes contract strongly and become more separated as compared to the LDA results. These results demonstrate the benefits of the pairwise-covariance properly weighted LDA. More experiments and comparisons with related methods are reported in §7.

Algorithm to solve Pairwise-covariance LDA

The key idea of our approach is to use gradient descent algorithm to solve pcLDA of Eq.(10). The gradient of $J_2(G)$ is

$$\nabla J_2 \triangleq \frac{\partial J_2}{\partial \mathbf{G}} = -\sum_{k<l} \frac{q n_k n_l}{[d_{kl}(\mathbf{G})]^{q+1}} \frac{\partial d_{kl}(\mathbf{G})}{\partial \mathbf{G}}. \quad (11)$$

For notational simplicity, we write

$$\mathbf{B}_{kl} = (\mu_k - \mu_l)(\mu_k - \mu_l)^T,$$
$$d_{kl}(\mathbf{G}) = \text{Tr}(\mathbf{G}^T \mathbf{B}_{kl} \mathbf{G})(\mathbf{G}^T \Sigma_{kl} \mathbf{G})^{-1}. \quad (12)$$

Using Eq.(12), the derivative of $d_{kl}(\mathbf{G})$ is

$$\frac{\partial d_{kl}(\mathbf{G})}{\partial \mathbf{G}} = 2[\mathbf{B}_{kl}\mathbf{G}(\mathbf{G}^T\Sigma_{kl}\mathbf{G})^{-1} - \Sigma_{kl}\mathbf{G}(\mathbf{G}^T\Sigma_{kl}\mathbf{G})^{-1}(\mathbf{G}^T\mathbf{B}_{kl}\mathbf{G})(\mathbf{G}^T\Sigma_{kl}\mathbf{G})^{-1}]. \quad (13)$$

Note that $(\mathbf{G}^T\Sigma_{kl}\mathbf{G})^{-1}$ is an inverse of a small (K-1)-by-(K-1) matrix. ∇J_2 can be efficiently computed using Algorithm 1.

Algorithm 1 Computation of $\nabla J_2(\mathbf{G})$ (i.e., Eq.11) or $\nabla J_2(\mathbf{A})$ (i.e., gradient of Eq.21).

Input: $\mathbf{G}$, $\{\Sigma_k, \mu_k\}$, q
Output: ∇J_2
Algorithm:
$\mathbf{F} = 0$
for $l = 1$ to K **do**
  for $k = l + 1$ to K **do**
    Compute $\mu_{kl} = \mu_k - \mu_l$.
    Compute $\mathbf{b} = \mathbf{G}^T \mu_{kl}$.
    Compute Σ_{kl} according to Eq.(8). % Σ^{ϕ}_{kl} according to Eq.(23)
    Compute $\mathbf{B} = \Sigma_{kl}\mathbf{G}$.
    Compute $\mathbf{b} = (\mathbf{G}^T\mathbf{B})^{-1}\mathbf{b}$.
    Compute $\mathbf{a} = n_k n_l(\mu_{kl} - \mathbf{B}\mathbf{b})/(\mu_{kl}^T \mathbf{G}\mathbf{b})^{q+1}$.
    Compute $\mathbf{F} = \mathbf{F} + \mathbf{a} \times \mathbf{b}^T$ % cross-product between vectors $\mathbf{a}$, $\mathbf{b}$
  end for
end for
$\nabla J_2 = -2q\mathbf{F}$.
Output: ∇J_2.

The constraint $\mathbf{G}^T\mathbf{G} = \mathbf{I}$ enforces $\mathbf{G}$ on the Stiefel manifold. Variations of $\mathbf{G}$ on this manifold is parallel transport, which gives some restriction to the gradient. This has been been worked out in (Edelman, Arias, and Smith 1998). The gradient that preserves the manifold structure is

$$\nabla J_2 - \mathbf{G}[\nabla J_2]^T\mathbf{G}. \quad (14)$$

Thus the algorithm computes the new $\mathbf{G}$ as follows,

$$\mathbf{G} \leftarrow \mathbf{G} - \eta(\nabla J_2 - \mathbf{G}[\nabla J_2]^T\mathbf{G}) \quad (15)$$

The step size η is usually chosen as,

$$\eta = \rho\|\mathbf{G}\|_1\|/\|\nabla J_2 - \mathbf{G}(\nabla J_2)^T\mathbf{G}\|_1,\ \rho = 0.001 \sim 0.01. \quad (16)$$

where $\|\mathbf{A}\|_1 = \sum_{ij}|\mathbf{A}_{ij}|$. Occasionally, due to the loss of numerical accuracy, we do the projection: $\mathbf{G} \leftarrow \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-\frac{1}{2}}$ to restore $\mathbf{G}^T\mathbf{G} = \mathbf{I}$. Starting with the standard LDA solution of $\mathbf{G}$, this algorithm is iterated until the algorithm converges to a local optimal solution. Fig. 3(c) shows the convergence of algorithm on dataset `mnist`.

Pairwise-covariance Kernel LDA

Kernel LDA (Mika et al. 1999; Tao et al. 2004) is nonlinear generalization of LDA. We can derive the kernel version of pcLDA. Let $\mathbf{x}_i \rightarrow \phi(\mathbf{x}_i)$ or $\mathbf{X} \rightarrow \phi(\mathbf{X}) = (\phi(\mathbf{x}_1), \cdots, \phi(\mathbf{x}_n)$. For 2-class LDA, the projection vector is $\mathbf{g} = \sum_{i=1}^n \alpha_i\phi(\mathbf{x}_i) = \phi(\mathbf{X})\boldsymbol{\alpha}$, where $\boldsymbol{\alpha} = (\alpha_1 \cdots \alpha_n)^T$. For K-class LDA, the projection vector $\mathbf{g}_k = \sum_{i=1}^n \alpha_{ik}\phi(\mathbf{x}_i) = \phi(\mathbf{X})\boldsymbol{\alpha}_k$, thus, $\mathbf{G} = (\mathbf{g}_1 \cdots \mathbf{g}_{K-1}) = \phi(\mathbf{X})\mathbf{A}$, where $\mathbf{A} = (\boldsymbol{\alpha}_1 \cdots \boldsymbol{\alpha}_{K-1})$.

Under the transformation $\mathbf{X} \rightarrow \phi(\mathbf{X})$, $\mathbf{G} \rightarrow \phi(\mathbf{X})\mathbf{A}$, it is easy to see that the LDA objective of Eq.(1) transforms into

$$\text{Tr}(\mathbf{G}^T\mathbf{S}_b^{\phi}\mathbf{G})(\mathbf{G}^T\mathbf{S}_w^{\phi}\mathbf{G})^{-1} \rightarrow \text{Tr}(\mathbf{A}^T\mathbf{S}_b^{\phi}\mathbf{A})(\mathbf{A}^T\mathbf{S}_w^{\phi}\mathbf{A})^{-1} \quad (17)$$

where the kernel within-class scatter matrix is:

$$(\Sigma_k^{\phi})_{ij} = \phi(\mathbf{x}_i)^T[\frac{1}{n_k}\sum_{s\in C_k}\phi(\mathbf{x}_s)\phi(\mathbf{x}_s)^T]\phi(\mathbf{x}_j)$$
$$= \frac{1}{n_k}\sum_{s\in C_k}\mathcal{K}_{is}\mathcal{K}_{sj},\ \mathbf{S}_w^{\phi} = \frac{1}{n}\sum_{k=1}^K n_k(\Sigma_k^{\phi}) = \frac{1}{n}\mathcal{K}^2, \quad (18)$$

and the kernel between-class scatter matrix is:

$$(\mathbf{S}_b^{\phi})_{ij} = \phi(\mathbf{x}_i)^T[\frac{1}{n}\sum_{k=1}^K n_k(\bar{\phi}_k - \bar{\phi})(\bar{\phi}_k - \bar{\phi})^T]\phi(\mathbf{x}_j)$$
$$= \frac{1}{n}\sum_{k=1}^K n_k\big(\mathcal{K}_{i\bar{k}} - \mathcal{K}_{i\cdot}\big)\big(\mathcal{K}_{\bar{k}j} - \mathcal{K}_{\cdot j}\big), \quad (19)$$

where we use the shorthand notations:

$$\bar{\phi} = \frac{1}{n}\sum_{s=1}^n \phi(\mathbf{x}_s),\ \bar{\phi}_k = \frac{1}{n_k}\sum_{s\in C_k}\phi(\mathbf{x}_s),$$
$$\mathcal{K}_{i\cdot} = \mathcal{K}_{\cdot i} = \frac{1}{n}\sum_{s=1}^n \mathcal{K}_{is},\ \mathcal{K}_{\bar{k}i} = \mathcal{K}_{i\bar{k}} = \frac{1}{n_k}\sum_{s\in C_k}\mathcal{K}_{is}. \quad (20)$$

The solution of kernel LDA is given by the largest k eigenvectors of the eigen-equation $\mathbf{S}_b^{\phi}v = \lambda\mathbf{S}_w^{\phi}v$. When $K = 2$, this reduces to the familiar 2-class kernel LDA (Tao et al. 2004). Efficient computation of $\mathbf{S}_b^{\phi}$ is given in the end of §5.1.

We are now ready to present the pairwise-covariance kernel LDA. We apply the same transformation to the pairwise-covariance LDA. We have

Theorem 2. *Under the transformation* $\mathbf{X} \rightarrow \phi(\mathbf{X})$, $\mathbf{G} \rightarrow \phi(\mathbf{X})\mathbf{A}$, *the pairwise-covariance LDA of* $J_2(\mathbf{G})$ *becomes* $J_2(\mathbf{A})$*:*

$$\min_{\mathbf{A}} \sum_{k<l} \frac{n_k n_l}{[Tr(\mathbf{A}^T\mathbf{B}_{kl}^{\phi}\mathbf{A})(\mathbf{A}^T\Sigma_{kl}^{\phi}\mathbf{A})^{-1}]^q},\ s.t.\ \mathbf{A}^T\mathbf{A} = \mathbf{I}. \quad (21)$$

where

$$(\mathbf{B}^{\phi}_{kl})_{ij} = \phi(\mathbf{x}_i)^T(\bar{\phi}_k - \bar{\phi}_l)(\bar{\phi}_k - \bar{\phi}_l)^T\phi(\mathbf{x}_j)$$
$$= \left(\mathcal{K}_{i\bar{k}} - \mathcal{K}_{i\bar{l}}\right)\left(\mathcal{K}_{\bar{k}j} - \mathcal{K}_{\bar{l}j}\right) \quad (22)$$

where shorthand notations are defined in Eq.(20), Σ^{ϕ}_k is defined in Eq.(18), and

$$\Sigma^{\phi}_{kl} = \beta\frac{n_k\Sigma^{\phi}_k + n_l\Sigma^{\phi}_l}{n_k + n_l} + (1-\beta)\Sigma^{\phi}. \quad (23)$$

Algorithm for Kernel PC-LDA

We solve $J_2(\mathbf{A})$ of Eq.(21) using the same algorithm in computing pcLDA using $J_2(\mathbf{G})$ of Eq.(10). The derivative is the same as Eqs.(19,20) except $\mathbf{B}_{kl}$ is replaced by $\mathbf{B}^{\phi}_{kl}$, Σ_{kl} replaced by Σ^{ϕ}_{kl}, $\mathbf{G}$ by $\mathbf{A}$. The constraint $\mathbf{A}^T\mathbf{A} = \mathbf{I}$ is handled in same way as $\mathbf{G}^T\mathbf{G} = \mathbf{I}$ in Eqs.(20,21). The step size is given in Eq.(22). The remaining part is the efficient computation of the gradient $\nabla J_2(\mathbf{A})$. First, we note that $\{\mathbf{B}^{\phi}_{kl}\}, \{\Sigma^{\phi}_k\}$ of Eqs.(22,23) can be efficiently computed. Let $\mathbf{V}_k$ be a n-by-n_k matrix consisting of n_k columns of $\mathcal{K}$ belonging to class k. It is ready to see that in Eq.(21),

$$\Sigma^{\phi}_k = \frac{1}{n_k}\mathbf{V}_k\mathbf{V}_k^T,\ \mathbf{u}_k = \frac{1}{n_k}\mathbf{V}_k\mathbf{e}, \quad (24)$$

where $\mathbf{e} = (1\cdots1)^T$. Here for clarity, we use $\mathbf{u}_k$ to represent the vector $\mathcal{K}_{i,\bar{k}}, i = 1\cdots n$. Clearly, $\mathbf{B}^{\phi}_{kl} = (\mathbf{u}_k - \mathbf{u}_l)(\mathbf{u}_k - \mathbf{u}_l)^T$. Now $\nabla J_2(\mathbf{A})$ is computed using Algorithm 1, with the replacement

$$\mu_k \leftarrow \mathbf{u}_k,\ \ \Sigma_k \leftarrow \Sigma^{\phi}_k. \quad (25)$$

$\mathbf{S}^{\phi}_b$ can be efficiently computed as $\mathbf{S}^{\phi}_b = (1/n)\sum_k n_k(\mathbf{u}_k - \mathbf{v})(\mathbf{u}_k - \mathbf{v})^T$, $\mathbf{v} = (1/n)\phi(\mathbf{X})\mathbf{e}$.

Related Work

A detailed survey of recent LDA works can be found in (Ye and Ji 2008).

Other LDA formulation There exist earlier works (Li, Jiang, and Zhang 2003), (Yan et al. 2004) which maximize the difference of traces, a.k.a maximum margin criteria (MMC). Several LDA formulations with different constraints and overfit analysis are given in (Luo, Ding, and Huang 2011), (Yan et al. 2004). To solve the well-known singularity or under-sampled problem, there are many extensions of LDA methods proposed, such as Regularized LDA (RLDA) (Hastie, Tibshirani, and Friedman 2001), uncorrelated LDA (ULDA) (Ye 2005b), orthogonal LDA (OLDA) (Ye 2005a) and orthogonal centroid method (OCM) (Park, Jeon, and Z 2003), etc. Among these, ULDA extracts the feature vectors which are mutually uncorrelated in low-dimensional space.

Connection with metric learning David et.al. (Alipanahi, Biggs, and Ghodsi 2008) showed a strong relationship between distance metric learning methods and the Fisher Discriminant Analysis. Our pairwise-covariance LDA formulation of Eq.(10) and kernel pcLDA of Eq.(21) can serve for distance metric learning purpose, which can be used for many applications (e.g., (Kong and Yan 2013), (Kong et al. 2012), *etc*).

Table 1: Characteristics of datasets

Dataset	# data	#dimension	#Class
MSRCv1	210	432	7
Umist	360	644	20
Mnist	150	784	10
Binalpha	1014	320	36

There are also works discussing local discriminative Gaussian (LDG) dimensionality reduction (Parrish and Gupta 2012), local fisher discriminant analysis (Sugiyama 2006). Sparsity in the LDA solution (Clemmensen et al. 2011), (Zhang and Chu 2013) is also desirable for interpretation purpose, because it is robustness to the noise and will lead to efficient computation in prediction. However, to our knowledge, none of the above works consider the pairwise covariance by computing distance of the projection in a pairwise way, which is the focus of this paper.

Experiment results

Dataset We evaluate the proposed pairwise-covariance LDA using four data sets (see Table 1) for multi-class classification experiments, including one face dataset `umist`, two digit datasets `mnist` (Lecun et al. 1998), `binalpha`, one image scene dataset `MSRCv1` (Lee and Grauman 2009)[2] . Due to space limit, we omit more details of datasets. Table 1 summarizes the datasets.

Methods & Parameter Settings In our experiment, we use 5-round 5-fold cross validation to evaluate the classification performance. Each dataset is evenly partitioned into 5 parts. Only one part is used as testing and the other 4 parts are used for training. We report the average results for 5 rounds. Next, we give an overview of the dimension reduction and classification methods used in our experiment. The compared methods can be divided into several groups.

(1) LDA and MMC (Li, Jiang, and Zhang 2003; Yan et al. 2004), kernel LDA (KLDA) For LDA, maximum margin criterion(MMC) ((Li, Jiang, and Zhang 2003; Yan et al. 2004)), kernel-LDA of Eq.(17) method, we project original data into LDA-subspace, and k(k=3) nearest neighbor classifier is used for classification. For kernel LDA, we use RBF kernel to construct the pairwise similarity $\mathbf{W}_{ij} = \mathbf{e}^{-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2}$, where bandwidth γ is searched in the grid $\{10^{-4}, 10^{-3}, \cdots, 10^3, 10^4\}$.

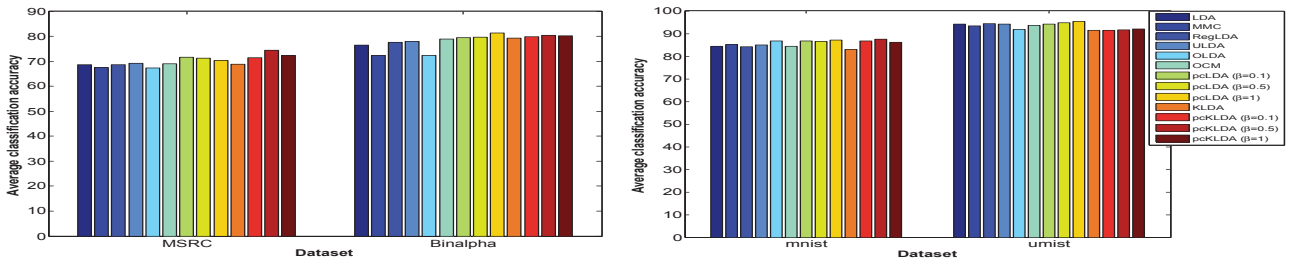
(2) Regularized LDA (RLDA) (Hastie, Tibshirani, and Friedman 2001), uncorrelated LDA (ULDA) (Ye 2005b), orthogonal LDA (OLDA) (Ye 2005a) and orthogonal centroid method (OCM) (Park, Jeon, and Z 2003). We compare our method against four methods of generalized LDA. It has been shown (Ye and Ji 2008) that these four LDA-extensions can be described in a unified framework for generalized LDA. However, there still exist subtle differences among them. The parameter μ in regularized LDA is determined by cross validation.

(3) Proposed pairwise-covariance LDA model of

[2]http://research.microsoft.com/en-us/projects/ObjectClassRecognition/

Table 2: Multi-class Classification Accuracy on 4 datasets using 9 different dimension reduction methods: LDA, kernel LDA(KLDA), pcLDA, kernel pcLDA (pcKLDA), and 5 other methods: MMC, RLDA, ULDA, OLDA, OCM.

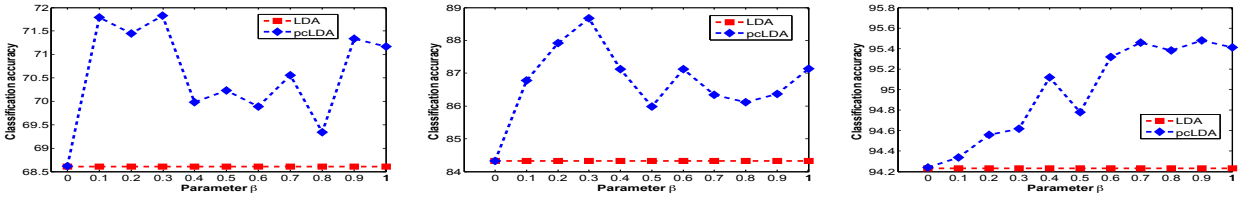
Data	LDA	MMC	RLDA	ULDA	OLDA	OCM	pcLDA (β=1)	KLDA	pcKLDA(β=1)
MSRC	68.57	67.45	68.54	69.11	67.34	68.91	71.32	68.78	**72.39**
Binalpha	76.37	72.38	77.66	77.95	72.30	78.89	**81.38**	79.23	80.12
Mnist	84.37	85.29	84.14	85.01	86.69	84.45	**87.10**	83.09	86.26
Umist	94.16	93.45	94.44	94.24	91.94	93.61	**95.35**	91.41	92.07



(a) Classification results on `MSRC, Binalpha`

(b) Classification results on `mnist, umist`

Figure 4: Classification results comparisons on 4 datasets, including our methods: pcLDA, pcKLDA at $\beta = \{0.1, 0.5, 1\}$ and seven other methods: LDA, KLDA, MMC, RLDA, ULDA, OLDA, OCM.



(a) pcLDA result on `MSRC`

(b) pcLDA result on `mnist`

(c) pcLDA result on `umist`

Figure 5: Classification accuracy w.r.t different parameter β for our model of Eq.(10) on dataset `MSRC, mnist, umist`. Red line gives LDA results, and blue line draws pcLDA results at $\beta = \{0, 0.1, \cdots, 0.9, 1.0\}$.

Eq.(10)(pcLDA) and kernel pairwise-covariance LDA model (pcKLDA) of Eq.(21) We set $q = 1$ for Eq.(10), Eq.(21) in our experiments. The parameter β is set to be $\{0.1, 0.5, 1\}$. To make a fair comparison, we project all original data to (C-1) dimension, and k(k=3) nearest neighbor classifier is used for classification purpose.

Classification Performance Analysis Table 2 and Fig.4 present the classification performance using different dimension reduction methods. We make several important observations from experiment results.

(1) As compared to standard LDA, MMC and other dimension reduction methods, pcLDA consistently provides better classification performance at different β values (e.g., $\beta = \{0.1, 0.5, 1\}$). For example, there is nearly 5% performance improvement on binalpha dataset when compared with standard LDA method. Note binalpha dataset is composed of data from K=36 classes, this indicates that the proposed pairwise pairwise-covariance LDA method gives much performance improvement at large class numbers.

(2) In kernel space, kernel version of LDA and pcLDA do not improve the classification performance quite a bit (sometimes even worse). However, pcKLDA still outperforms standard KLDA in kernel space.

(3) β controls the complexity of our model, i.e., when β approaches 1, pcLDA uses local pairwise covariance matrix, and when β approaches 0, pcLDA uses global covariance matrix which is equivalent to standard LDA. Fig.(5) shows the classification results on three datasets: MSRC, mnist and umist. The experiment results suggest that, generally, we tend to get better classification results for larger values of β. This further confirms our intuition, the pairwise covariance really helps to capture the data distribution as compared to globally averaged variance, and thus the projection and classification results are improved. Moreover, rather than maximizing the sum of inter-class distances, we minimize the sum of inverse inter-class distances. This choice makes classes that are close together have more influence on the LDA fit than those classes that are well-separated.

Conclusion

We present a pairwise-covariance model for linear discriminant analysis. The proposed model computes the projection by utilizing the pairwise class information. An efficient algorithm is present to solve the proposed model. Proposed method can be easily extended in kernel space. Experiment results indicate the good performance of proposed method.

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References

Alipanahi, B.; Biggs, M.; and Ghodsi, A. 2008. Distance metric learning vs. fisher discriminant analysis. In *AAAI*.

Clemmensen, L.; Hastie, T.; Wiiten, D.; and Ersboll, B. 2011. Sparse discriminant analysis. *Technometrics*.

Edelman, A.; Arias, T. A.; and Smith, S. T. 1998. The geometry of algorithms with orthogonality constraints. *SIAM J. MATRIX ANAL. APPL* 20(2):303–353.

Hastie, T.; Tibshirani, R.; and Friedman, J. 2001. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer.

Hoi, S. C. H.; Liu, W.; Lyu, M. R.; and Ma, W.-Y. 2006. Learning distance metrics with contextual constraints for image retrieval. In *CVPR*.

Kong, D., and Ding, C. H. Q. 2012. A semi-definite positive linear discriminant analysis and its applications. In *ICDM*, 942–947.

Kong, D., and Yan, G. 2013. Discriminant malware distance learning on structural information for automated malware classification. In *KDD*, 1357–1365.

Kong, D.; Ding, C. H. Q.; Huang, H.; and Zhao, H. 2012. Multi-label relieff and f-statistic feature selections for image annotation. In *CVPR*, 2352–2359.

Lecun, Y.; Bottou, L.; Bengio, Y.; and Haffner, P. 1998. Gradient-based learning applied to document recognition. In *Proceedings of the IEEE*, 2278–2324.

Lee, Y. J., and Grauman, K. 2009. Foreground focus: Unsupervised learning from partially matching images. *International Journal of Computer Vision* 85(2):143–166.

Li, H.; Jiang, T.; and Zhang, K. 2003. Efficient and robust feature extraction by maximum margin criterion. In *Proceedings of Advances in Neural Information Processing Systems(NIPS 2003)*.

Luo, D.; Ding, C.; and Huang, H. 2011. Linear discriminant analysis: New formulations and overfit analysis. In *AAAI2011*.

Mika, S.; Ratsch, G.; Weston, J.; Scholkopf, B.; and Muller, K. 1999. Fisher discriminant analysis with kernels.

Park, H.; Jeon, L. M.; and Z, J. B. R. 2003. Lower dimensional representation of text data based on centroids and least squares. *BIT* 43:2003.

Parrish, N., and Gupta, M. 2012. Dimensionality reduction by local discriminative gaussians. In *ICML*.

Sugiyama, M. 2006. Local fisher discriminant analysis for supervised dimensionality reduction. In *ICML*, 905–912.

Tao, X.; Ye, J.; Li, Q.; Janardan, R.; and Cherkassky, V. 2004. Efficient kernel discriminant analysis via qr decomposition. In *The Eighteenth Annual Conference on Neural Information Processing Systems (NIPS 2004)*, 1529–1536.

Wang, H.; Yan, S.; Xu, D.; Tang, X.; and Huang, T. 2007. Trace ratio vs. ratio trace for dimensionality reduction. In *CVPR*.

Xiang, S.; Nie, F.; and Zhang, C. 2008. Learning a mahalanobis distance metric for data clustering and classification.

Yan, J.; Zhang, B.; Yan, S.; Yang, Q.; and Li, H. 2004. Immc: incremental maximum margin criterion. In *Proceedings of the Tenth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*.

Ye, J., and Ji, S. 2008. *Discriminant Analysis for Dimensionality Reduction: An Overview of Recent Developments, Biometrics: Theory, Methods & Applications*. IEEE/Wiley.

Ye, J. 2005a. Characterization of a family of algorithms for generalized discriminant analysis on undersampled problems. *The Journal of Machine Learning Research* 6.

Ye, J. 2005b. Characterization of a family of algorithms for generalized discriminant analysis on undersampled problems. *Journal of Machine Learning* 6:483–502.

Zhang, X., and Chu, D. 2013. Sparse uncorrelated linear discriminant analysis. In *ICML*, 45–52.