DISCRIMINANT SIMPLEX ANALYSIS

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ABSTRACT

Image representation and distance metric are both significant for learning-based visual classification. This paper presents the concept of k-Nearest-Neighbor Simplex (kNNS), which is a simplex with the vertices as the k nearest neighbors of a certain point. kNNS contributes to the image classification problem in two aspects. First, a novel distance metric between a point to its kNNS within a certain class is provided for general classification problem. Second, we develop a new subspace learning algorithm, called Discriminant Simplex Analysis (DSA), to pursue effective feature representation for image classification. In DSA, the within-locality and between-locality are both modeled by kNNS distance, which provides a more accurate and robust measurement of the probability of a point belonging to a certain class. Experiments on real-world image classification demonstrate the effectiveness of both DSA as well as kNNS based classification approach.

Index Terms— subspace learning, graph embedding, *k*-nearest-neighbor simplex, discriminant simplex analysis.

1. INTRODUCTION

Image classification is an extensively discussed topic in computer vision and pattern recognition fields. For a given query image, the basic idea is to classify it into a predefined class associated with the top-matched training image. In general, there are two most important subproblems in conducting image classification in practice: 1) how to seek effective image feature representation for discriminant analysis; and 2) how to choose appropriate distance measurement favoring such features to enhance the classifier's discriminating power.

Recent studies reveal that locality features and intrinsic geometric structures in the input space take on discriminating power for classification. The representative algorithms, such as LLE [12], Isomap [16], Laplacian Eigenmaps [2], LEA [6], and LPP [10], assume that high-dimensional data can be considered as a set of geometrically related points lying on or nearly on a smooth low-dimensional manifold. The manifold embedding is closely related to preserving the local neighborhood connections without assumption on the data distribution. Graph Embedding [18] has shown that these methods can all be unified within the same framework including their linear/ kernel/ tensor extensions [9, 3]. To further boost the discriminating power of such techniques, recent discriminant learning methods, such as MFA [18], LDE [4], LDG [8], and CEA [7], combine the Fisher criterion [1] with manifold criterion to explicitly aim at the classification capacity and discriminating efficiency of the embedding. These algorithms are more general since the data distributions are modelled with affinity graphs. Such Nearest-Neighbor type of distance measure strategy considers the membership style for isolated data points in the feature space. However, it is often more accurate to make the subspace modeling based on several nearest neighbors of each datum when they are available [11, 5].

Aiming to improve discriminant feature representation and distance measurement, we present a new idea, called Discriminant Simplex Analysis (DSA), for image classification. DSA is designed from a novel theoretical perspective on the graph embedding descriptor via the concept of k-Nearest-Neighbor Simplex(kNNS). For discriminant feature representation, DSA models both within-locality and between-locality data distribution structures by graph embedding in a manner of kNNS criterion. A linear subspace is then learned by optimizing the DSA objective function via a closed-form eigenvalue decomposition method. It does not require any data distribution assumptions and provides more possible projection directions for discriminant learning. For distance measurement of the classifier, the distance from a query to a particular class is measured by the distance from the query to the nearest point in its kNNS constituted by the samples from the class, which provides a more accurate and robust measure of its possibility belonging to a certain class. Extensive comparisons between DSA and most popular algorithms in real-world experiments reveal the effectiveness of the proposed framework.

2. K-NEAREST-NEIGHBOR SIMPLEX

Suppose we have the original data set $\mathcal{X} = {\mathbf{x}_i : \mathbf{x}_i \in \mathbb{R}^D}_{i=1}^n$. Assume only considering the locality in the data space, the *k*-Nearest-Neighbor Simplex (*k*NNS) is a set of

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Fig. 1. *k*NNS vs. NFL for two-class classification. *k*NNS metric correctly classifies all the data points whereas NFL misclassifies the round point located in the center. Note that c < b < a in this case.

infinite data generated by the linear combination of k local points x_1, x_2, \dots, x_k as

$$\mathcal{S}(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_k) = \Big\{ \sum_{i=1}^k \ell_i \mathbf{x}_i \mid \sum_{i=1}^k \ell_i = 1, \ell_i \ge 0 \Big\}.$$
(1)

Instead of only considering the similarity between sample pairs for classification, distance measurement for an individual sample and a set of multiple samples can be derived by using kNNS concept. For a particular sample x_i , the distance between x_i and its kNNS is measured by minimizing the following objective function

$$\|\mathbf{x}_{i} - \sum_{j=1}^{k} \ell_{\mathcal{N}(j)}^{(i)} \mathbf{x}_{\mathcal{N}(j)}^{(i)}\|,$$
 (2)

where set $\{N(j)\}_{j=1}^k$ is the index set of the k nearest neighbors of the sample \mathbf{x}_i in local.

Inspired by the above discussion, a new multi-class classification algorithm, kNNS classification, can be designed via the concept of kNNS. Let $\mathcal{L} = \{l_i : l_i \in \{1, 2, ..., m\}\}_{i=1}^n$ be the corresponding class label for \mathcal{X} (m classes in total). For a given query \mathbf{x}_t : 1) calculate its k nearest neighbors $\{\mathbf{x}_{N(j)}^{(l)} : l \in 1, 2, ..., m\}_{j=1}^k$ from each class; 2) build simplex for each set of k nearest neighbors and calculate the distance $\{d_{kNNS}^{(l)} : l \in 1, 2, ..., m\}$ between \mathbf{x}_t and its kNNS by Eq. 2; 3) infer the label l_t of \mathbf{x}_t with

$$l_t^* = \arg\min_l d_{k\rm NNS}^{(l)}.$$
(3)

The difference between kNNS and Nearest Feature Line (NFL) [11] is obvious. Fig. 1 shows the two-class classification toy example using kNNS and NFL. In this case, the space of kNNS is inside the triangle area whereas the space of NFL consists of the three feature lines covering the three sides of the triangle. Since the feature lines could be infinite long, some feature lines from the different class may intersect and induce misclassifications. However, in such a geometric point of view, kNNS can measure the distances between data and classes more accurately for better classification.



Fig. 2. Two-class classification example for DSA embedding.

3. DISCRIMINANT SIMPLEX ANALYSIS

The kNNS concept is not only appropriate to define distance metric, but also effective to design graph-embedding-based feature extraction algorithm, such as Discriminant Simplex Analysis (DSA), which is favoring the assumption that the geometric relationship among high-dimensional data can be described by the distance measurement between data point and kNNS. The motivation of DSA is to keep the class relation reflected by the known labels after embedding or subspace learning. In other words, in the derived low-dimensional DSA subspace, we expect to preserve neighboring points close if they have the same locality label, while preventing points of other classes from entering the neighborhood. This basic learning strategy is consistent with the existing methods such as MFA [18], LDE [4], LDG [8], and CEA [7].

Define two types of k-nearest neighbors for each data point in \mathcal{X} : within-locality graph k_w -NN and between-locality graph k_b -NN. Note that k_w and k_b can be different. Given a label set $\mathcal{L} = \{l_i : l_i \in \mathbb{R}\}_{i=1}^n$, for each point \mathbf{x}_i with label $l^{(i)}$, we search its within-locality k_w -NNs from \mathcal{X} and obtain a set $\mathcal{X}_w^{(i)} = \{\mathbf{x}_{w(j)}^{(i)}\}_{j=1}^{k_w}$ satisfying $l_{w(j)}^{(i)} = l^{(i)}$. On the other hand, we find the set of \mathbf{x}_i 's between-locality k_b -NNs as $\mathcal{X}_b^{(i)} = \{\mathbf{x}_{b(j,p)}^{(i)}\}_{j,p=1}^{k_b,m-1}$, satisfying $l_{b(j,p)}^{(i)} \neq l^{(i)}$ and $l_{b(j_1,p)}^{(i)} = l_{b(j_2,p)}^{(i)}$ for $j_1, j_2 = 1, 2, \dots, k_b$, where *m* denotes the number of classes in the data space.

The objective of DSA is to learn a linear projection $P \in \mathbb{R}^{D \times d}$ of our desired subspace that minimizes the distance between each sample to its kNNS of the same class and at the same time maximizes the distance between each sample to its kNNS of another nearest different class. The objective function for modeling P is formulated as follows

$$\max \varepsilon_{\rm b}(\mathbf{P}) \text{ and } \min \varepsilon_{\rm w}(\mathbf{P}),$$
 (4)

where

$$\begin{cases} \varepsilon_{\mathbf{w}}(\mathbf{P}) = \sum_{i=1}^{n} \left\| \mathbf{P}^{T} \mathbf{x}_{i} - \sum_{j=1}^{k_{w}} c_{\mathbf{w}(j)}^{(i)} \mathbf{P}^{T} \mathbf{x}_{\mathbf{w}(j)}^{(i)} \right\|^{2} \\ \varepsilon_{\mathbf{b}}(\mathbf{P}) = \sum_{i=1}^{n} \left\| \mathbf{P}^{T} \mathbf{x}_{i} - \sum_{j=1}^{k_{\mathbf{b}}} c_{\mathbf{b}(j,l^{*})}^{(i)} \mathbf{P}^{T} \mathbf{x}_{\mathbf{b}(j,l^{*})}^{(i)} \right\|^{2} \end{cases}$$
(5)

Here, we define the index sets w(j), $b(j, l^*) = 1, 2, \cdots, n$, reconstruction coefficient set $C_w^{(i)} = \{c_{w(j)}^{(i)}\}_{j=1}^{k_w}$ for the withinlocality case and $C_b^{(i)} = \{c_{b(j,l^*)}^{(i)}\}_{j=1}^{k_b}$ for the between-locality case respectively. Fig. 2 is for better understanding this idea. The coefficient matrices is calculated in terms of the similar objective functions as Eq. 5 by removing the \mathbf{P}^T . Define the $k_{w} \times k_{w}$ local Gram matrix \mathbf{G}_i for each \mathbf{x}_i as $\mathbf{G}_i[u, v] = (\mathbf{x}_i - \mathbf{x}_{w(u)}^{(i)})^T (\mathbf{x}_i - \mathbf{x}_{w(v)}^{(i)})$, we want to solve the optimization

$$\min_{\mathbf{c}_{\mathbf{w}}^{(i)}} \mathbf{c}_{\mathbf{w}}^{(i)T} \mathbf{G}_{i} \mathbf{c}_{\mathbf{w}}^{(i)}, \text{ s.t. } \sum_{j=1}^{k_{\mathbf{w}}} c_{\mathbf{w}(j)}^{(i)} = 1, \text{ and } c_{\mathbf{w}(j)}^{(i)} \ge 0.$$
 (6)

Then $\mathbf{C}_{\mathbf{w}}[i, \mathbf{w}(j)] = \mathbf{c}_{\mathbf{w}}^{(i)}(j)$. This problem can be easily solved by using the optimization toolbox in Matlab, such as the function *quadprog* in Matlab 7.0. Since the number of $k_{\mathbf{w}}$ is usually small, this procedure is fast enough in practice. On the other hand, define the $k_{\mathbf{b}} \times k_{\mathbf{b}}$ local Gram matrix $\widetilde{\mathbf{G}}_i$ for each \mathbf{x}_i in its l^* -NN simplex as $\widetilde{\mathbf{G}}_i[u, v] = (\mathbf{x}_i - \mathbf{x}_{\mathbf{b}(u, l^*)}^{(i)})^T (\mathbf{x}_i - \mathbf{x}_{\mathbf{b}(v, l^*)}^{(i)})$, we have the same way to calculate $\mathbf{c}_{\mathbf{b}}^{(i)}$. Then $\mathbf{C}_{\mathbf{b}}[i, \mathbf{b}(j, l^*)] = \mathbf{c}_{\mathbf{b}}^{(i)}(j)$.

After we get C_w and C_b , the projection matrix P can be calculated by solving the eigenvalue problem

$$\left(\mathbf{X}\mathbf{L}_{w}^{\mathrm{DSA}}\mathbf{X}^{T}\right)^{-1}\mathbf{X}\mathbf{L}_{b}^{\mathrm{DSA}}\mathbf{X}^{T}\mathbf{P}=\Lambda\mathbf{P},$$
(7)

where we define the quadratic Laplacian matrices $\mathbf{L}_{b}^{DSA} = \mathbf{L}_{b}^{T}\mathbf{L}_{b}$ and $\mathbf{L}_{w}^{DSA} = \mathbf{L}_{w}^{T}\mathbf{L}_{w}$. Typically, it is straightforward to define the Laplacian matrix pair [7] as

$$\begin{cases} \mathbf{L}_{w} = \mathbf{D}_{w} - \mathbf{C}_{w} \\ \mathbf{L}_{b} = \mathbf{D}_{b} - \mathbf{C}_{b} \end{cases},$$
(8)

where $\mathbf{D}_{w}[i, i] = \sum_{j=1}^{n} \mathbf{C}_{w}[i, j]$ and $\mathbf{D}_{w}[i, j] = 0$ for $\forall i \neq j$, also $\mathbf{D}_{b}[i, i] = \sum_{j=1}^{n} \mathbf{C}_{b}[i, j]$ and $\mathbf{D}_{b}[i, j] = 0$ for $\forall i \neq j$. The subspace \mathbf{P} is spanned with $\{\mathbf{p}_{1} \ \mathbf{p}_{2} \cdots \mathbf{p}_{d}\}$, the generalized eigenvectors that correspond to the *d* largest eigenvalues in Eq. 7. Any new input datum \mathbf{X}_{new} can be represented by the new coordinates $\mathbf{Y}_{new} = \mathbf{P}^T \mathbf{X}_{new}$ when \mathbf{P} is available from training. If we first project the data into the PCA subspace with projection matrix \mathbf{P}_{PCA} , the new coordinates of \mathbf{X}_{new} can be represented as $\mathbf{Y}_{new} = \mathbf{P}^T \mathbf{P}_{PCA}^T \mathbf{X}_{new}$. For a certain class, the data set can be roughly considered

For a certain class, the data set can be roughly considered as convex within locality. If $\mathbf{O}_{k_w}(\mathbf{x}_i) = \sum_{j=1}^{k_w} c_{w(j)}^{(i)} \mathbf{x}_{w(j)}^{(i)}$ and $\mathbf{O}_{k_b}^{(l^*)}(\mathbf{x}_i) = \sum_{j=1}^{k_b} c_{b(j,l^*)}^{(i)} \mathbf{x}_{b(j,l^*)}^{(i)}$ are the within-locality k_w -NN simplex and the l^* -th between-locality k_b -NN simplex, correspondingly, $\mathbf{P}^T \mathbf{O}_{k_w}(\mathbf{x}_i)$ and $\mathbf{P}^T \mathbf{O}_{k_b}^{(l^*)}(\mathbf{x}_i)$ will be the low-dimensional simplex representations. Then we have that the samples within the simplex $S(\{\mathbf{x}_{w(j)}^{(i)}\}_{j=1}^{k_w})$ can be considered all belonging to the same class. Then, the distance between \mathbf{x}_i and $\mathbf{O}_{k_w}(\mathbf{x}_i)$ can more accurately characterize the distance between \mathbf{x}_i and the class $l^{(i)}$. To boost the discriminating power, the distance between each sample to its corresponding class should be small, while the distance between each sample to a different class should be large, which leads to Eq. 4. Compared with the distance between a sample to

Table 1. Face recognition accuracy comparison on the ORL database using multiple-sample metric.

Method	Method 3-Train		5-Train	
Accuracy	(%)[Dim.]	%)[Dim.] (%)[Dim.]		
NFL + NN	76.79 [117]	79.58[58]	84.00 [133]	
2NNS + NN	78.21 [107]	82.5 [106]	87.5 [158]	
kNNS + NN	81.07 [119]	86.25 [84]	89.50 [111]	

its kNNS can better characterize the possibility of a sample belonging to a certain class, since the latter is robust to the small sample size issue, and the kNNS can better represent the distribution of the data.

4. EXPERIMENTS AND APPLICATIONS

We show as follows the comprehensive performance comparisons between DSA and other state-of-the-art subspace learning algorithms for face recognition.

4.1. Distance Metric

The ORL [13] face database contains in total 400 images of 40 subjects with 10 gray-scale face images for each. The images show all frontal and slight tilt/rotation of the face up to 20 degrees. For some subjects, the images were taken at different time, varying the lighting, facial expressions (open or closed eyes, smiling or not smiling) and facial details (glasses or no glasses). The images are manually aligned, cropped and resized to 32×32 pixels, with 256 gray levels per pixel. Each image is represented by a 1024-dimensional column vector.

To demonstrate the advantage of kNNS in distance metric description, we conduct the face recognition experiments on ORL images and compare 2NNS and kNNS with NFL. We choose 2NNS for fairly comparing with NFL since NFL considers two points for each feature line. There are three different kinds of database partitions for the evaluation. The three training sets are formed by images of each individual with 3, 4, and 5 randomly picked samples respectively. The rest images of each case form the testing sets. The k of kNNS here is set to the same as the number of training samples of each individual, such as 3, 4, or 5. All the comparison methods are performed on the original image vectors with PCA dimensionality reduction (keeping all eigenvectors). Nearest neighbor classifier is used. We show the results in Table 1. It can be seen that kNNS + NN consistently outperforms others and significantly improves the NFL classification, which validates the discussions in the pervious sections.

4.2. Face Recognition

The CMU PIE [14] database contains in total 41,368 images of 68 subjects with 500+ images for each. The face images

were captured under varying pose, illumination, and expression. For each subject, we manually select 168 near frontal images which cover large illumination variation, pose of roll/ yaw/tilt head rotation and moderate variety in expression, constituting a challenging face database for recognition task. Face images are manually aligned, cropped out from the selected images and resized to be 20×20 , with 256 gray levels per pixel.

To further reduce the size of the database, we randomly choose around 1/5 samples for each individual and obtain a subdatabase with 34 images per individual. We finally have 2312 images in total. Random database partitions are done with 5, 10, 15, and 20 images per individual for training, and the rest of the database for testing. Different subspace learning methods, Eigenfaces [17], Fisherface [1], Laplacianface [10], and DSAface, are applied to represent the facial features for NN classification. All the results are from best tuning of the algorithm parameters. Table 2 shows the recognition results in terms of accuracy. As can be seen, Eigenface performs the worst and is comparable to the baseline, which uses the original image feature; Laplacianface is slightly better than Fisherface; DSAface consistently outperforms the other methods with highest recognition rates. One possible explanation of the superior performance of DSAface in the test lies on the large image variations of PIE database. DSA benefits from the robustness of both kNNS and Fisher criterion.

5. CONCLUSION

We have presented to use Discriminant Simplex Analysis for discriminating analysis on image classification and visual recognition. DSA is designed from a novel theoretical perspective on the graph embedding descriptor via the concept of k-Nearest-Neighbor Simplex. For discriminant feature representation, DSA models both within-locality and betweenlocality data structures by graph embedding in a manner of kNNS criterion. The superiority of DSA is embodied as that the distance between each sample to its kNNS of a certain class provides a more accurate and robust measure of its possibility belonging to the class. Real-world experiments on face recognition show that the algorithm design, benefiting from both Fisher criterion and kNNS criterion, can significantly boost the discriminating power. One future direction can focus on investigating the tensor form [15] of the DSA framework for discriminant analysis on high-order structures of multivariate data.

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Table 2. Face recognition accuracy on the PIE database.

Method	5-Train	10-Train	15-Train	20-Train
Accuracy	(%)[Dim.]	(%)[Dim.]	(%)[Dim.]	(%)[Dim.]
Baseline	24.34[400]	36.46[400]	45.20[400]	52.84[400]
Eigenface	24.34[200]	36.46[245]	45.20[285]	52.84[282]
Fisherface	51.27[70]	66.42[51]	73.22[46]	78.89[45]
Laplacianface	37.32[196]	63.85[67]	76.24[59]	82.35[66]
DSAface	52.54 [141]	67.28 [114]	78.10[51]	83.72 [54]

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