

Extended Grassmann Kernels for Subspace-Based Learning

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Abstract

Subspace-based learning problems involve data whose elements are linear subspaces of a vector space. To handle such data structures, Grassmann kernels have been proposed and used previously. In this paper, we analyze the relationship between Grassmann kernels and probabilistic similarity measures. Firstly, we show that the KL distance in the limit yields the Projection kernel on the Grassmann manifold, whereas the Bhattacharyya kernel becomes trivial in the limit and is suboptimal for subspace-based problems. Secondly, based on our analysis of the KL distance, we propose extensions of the Projection kernel which can be extended to the set of affine as well as scaled subspaces. We demonstrate the advantages of these extended kernels for classification and recognition tasks with Support Vector Machines and Kernel Discriminant Analysis using synthetic and real image databases.

1 Paper Body

In machine learning problems the data often live in a vector space, typically a Euclidean space. However, there are many other kinds of non-Euclidean spaces suitable for data outside this conventional context. In this paper we focus on the domain where each data sample is a linear subspace of vectors, rather than a single vector, of a Euclidean space. Low-dimensional subspace structures are commonly encountered in computer vision problems. For example, the variation of images due to the change of pose, illumination, etc, is well-approximated by the subspace spanned by a few "eigenfaces". More recent examples include the dynamical system models of video sequences from human actions or time-varying textures, represented by the linear span of the observability matrices [1, 14, 13]. Subspace-based learning is an approach to handle the data as a collection of subspaces instead of the usual vectors. The appropriate data space for the subspace-based learning is the Grassmann manifold $G(m, D)$, which is defined as the set of m -dimensional linear subspaces in \mathbb{R}^D . In particular, we can define positive definite kernels on the Grassmann manifold, which allows

us to treat the space as if it were a Euclidean space. Previously, the Binet-Cauchy kernel [17, 15] and the Projection kernel [16, 6] have been proposed and demonstrated the potential for subspace-based learning problems. On the other hand, the subspace-based learning problem can be approached purely probabilistically. Suppose the set of vectors are i.i.d samples from an arbitrary probability distribution. Then it is possible to compare two such distributions of vectors with probabilistic similarity measures, such as the KL distance¹, the Chernoff distance, or the Bhattacharyya/Hellinger distance, to name a few [11, 7, 8, 18]. Furthermore, the Bhattacharyya affinity is indeed a positive definite kernel function on the space of distributions and have nice closed-form expressions for the exponential family [7].¹

by distance we mean any nonnegative measure of similarity and not necessarily a metric.

¹

In this paper, we investigate the relationship between the Grassmann kernels and the probabilistic distances. The link is provided by the probabilistic generalization of subspaces with a Factor Analyzer which is a Gaussian blob that has nonzero volume along all dimensions. Firstly, we show that the KL distance yields the Projection kernel on the Grassmann manifold in the limit of zero noise, whereas the Bhattacharyya kernel becomes trivial in the limit and is suboptimal for subspace-based problems. Secondly, based on our analysis of the KL distance, we propose an extension of the Projection kernel which is originally confined to the set of linear subspaces, to the set of affine as well as scaled subspaces. We will demonstrate the extended kernels with the Support Vector Machines and the Kernel Discriminant Analysis using synthetic and real image databases. The proposed kernels show the better performance compared to the previously used kernels such as Binet-Cauchy and the Bhattacharyya kernels.

²

Probabilistic subspace distances and kernels

In this section we will consider the two well-known probabilistic distances, the KL distance and the Bhattacharyya distance, and establish their relationships to the Grassmann kernels. Although these probabilistic distances are not restricted to specific distributions, we will model the data distribution as the Mixture of Factor Analyzers (MFA) [4]. If we have $i = 1, \dots, N$ sets in the data, then each set is considered as i.i.d. samples from the i -th Factor Analyzer $x \sim \pi(x) = N(u_i, C_i)$, $C_i = Y_i Y_i^T + \sigma^2 I_D$, $(1) D$ where $u_i \in \mathbb{R}^D$ is the mean, Y_i is a full-rank $D \times m$ matrix ($D \geq m$), and σ^2 is the ambient noise level. The FA model is a practical substitute for a Gaussian distribution in case the dimensionality D of the images is greater than the number of samples n in a set. Otherwise it is impossible to estimate the full covariance C nor invert it. More importantly, we use the FA distribution to provide the link between the Grassmann manifold and the space of probabilistic distributions. In fact a linear subspace can be considered as the “flattened” ($\sigma^2 \rightarrow 0$) limit of a zero-mean ($u_i = 0$), homogeneous ($Y_i^T Y_i = I_m$) FA distribution. We will look at the limits of the KL distance and the Bhattacharyya kernel under this condition. ^{2.1}

KL distance in the limit

Extension to affine subspaces

An affine subspace in \mathbb{R}^D is a linear subspace with an "offset". In that sense a linear subspace is simply an affine subspace with a zero offset. Analogously to the (linear) Grassmann manifold, we can define an affine Grassmann manifold as the set of all m -dim affine subspaces in \mathbb{R}^D space. The affine span is defined from the orthonormal basis $Y \in \mathbb{R}^{D \times m}$ and an offset $u \in \mathbb{R}^D$ by $\text{aspan}(Y, u) = \{x \mid x = Yv + u, v \in \mathbb{R}^m\}$.

(10)

By definition, the representation of an affine space by (Y, u) is not unique and there is an invariant condition for the equivalent of representations: Definition 1 (invariance to representations). $\text{aspan}(Y_1, u_1) = \text{aspan}(Y_2, u_2)$ if and only if $\text{span}(Y_1) = \text{span}(Y_2)$ and $Y_1^T (Y_1^T)^{-1} u_1 = Y_2^T (Y_2^T)^{-1} u_2$, where Y is any orthonormal basis for the orthogonal complement of $\text{span}(Y)$. Similarly to the definition of Grassmann kernels [6], we can now formally define the affine Grassmann kernel as follows. Let $k : (\mathbb{R}^{m \times D} \times \mathbb{R}^D) \times (\mathbb{R}^{m \times D} \times \mathbb{R}^D) \rightarrow \mathbb{R}$ be a real valued symmetric function $k(Y_1, u_1, Y_2, u_2) = k(Y_2, u_2, Y_1, u_1)$. The Grassmann manifold is defined as a quotient space $O(D)/O(m) \times O(D \times m)$ where O is the orthogonal group. The affine Grassmann manifold is similarly defined as $E(D)/E(m) \times O(D \times m)$, where E is the Euclidean group. For more explanations, please refer to [5].

3

Definition 2. A real valued symmetric function k is an affine Grassmann kernel if it is positive definite and invariant to different representations: $k(Y_1, u_1, Y_2, u_2) = k(Y_3, u_3, Y_4, u_4)$ for any Y_1, Y_2, Y_3, Y_4 , and u_1, u_2, u_3, u_4 such that $\text{aspan}(Y_1, u_1) = \text{aspan}(Y_3, u_3)$ and $\text{aspan}(Y_2, u_2) = \text{aspan}(Y_4, u_4)$. With this definition we check if the KL distance in the limit suggests an affine Grassmann kernel. The KL distance with the homogeneity condition only $Y_1^T Y_1 = Y_2^T Y_2 = I_m$ becomes, $\frac{1}{2} \text{tr}(Y_1^T Y_2 Y_2^T Y_1) + (u_1^T - u_2^T)(2I_D - Y_1 Y_1^T - Y_2 Y_2^T)(u_1 - u_2)$. Ignoring the multiplicative factor, the first term is the same as the original Projection kernel, which we will denote as the "linear" kernel to emphasize the underlying assumption: $k_{\text{Lin}}(p_1, p_2) = \text{tr}(Y_1 Y_1^T Y_2 Y_2^T)$.

$$k_{\text{Lin}}(Y_1, Y_2) = \text{tr}(Y_1 Y_1^T Y_2 Y_2^T), \quad (11)$$

The second term give rise to a new "kernel" $k_u(Y_1, u_1, Y_2, u_2) = u_1^T (2I_D - Y_1 Y_1^T - Y_2 Y_2^T) u_2$.

$$(12) \quad Y_2 Y_2^T.$$

which measures the similarity of the offsets u_1 and u_2 scaled by $2I$. However, this term is not invariant under the invariance condition unfortunately. We instead propose the slight modification: $k(Y_1, u_1, Y_2, u_2) = u_1^T (I - Y_1 Y_1^T)(I - Y_2 Y_2^T) u_2$. The proof of the proposed form being invariant and positive definite is straightforward and is omitted. Combined with the linear term k_{Lin} , this defines the new "affine" kernel $k_{\text{Aff}}(Y_1, u_1, Y_2, u_2) = \text{tr}(Y_1 Y_1^T Y_2 Y_2^T) + u_1^T (I - Y_1 Y_1^T)(I - Y_2 Y_2^T) u_2$.

$$(13)$$

As we can see, the KL distance with only the homogeneity condition has two terms related to the subspace Y and the offset u . This suggests a general construction rule for affine kernels. If we have two separate positive kernels for subspaces and for offsets, we can add or multiply them together to construct new kernels [10].

3.2 Extension to scaled subspaces

We have assumed homogeneous subspace so far. However, if the subspaces are computed from the PCA of real data, the eigenvalues in general will have non-homogeneous values. To incorporate these scales for affine subspaces, we now allow the Y to be non-orthonormal and check if the resultant kernel is still valid. Let Y_i be a full-rank $D \times m$ matrix, and $Y_{bi} = Y_i (Y_i^T Y_i)^{-1/2}$ be the orthonormalization of Y_i .

Ignoring the multiplicative factors, the limiting kernel from (3) becomes $\frac{1}{b} \text{tr}(Y_1^T Y_1 Y_2^T Y_2 + Y_1^T Y_{b1} Y_{b2}^T Y_{b2}) + u_0^T (I - Y_{b1} Y_{b1}^T - Y_{b2} Y_{b2}^T) u$, which is again not well-defined.

The second term is the same as (12) in the previous subsection, and can be modified in the same way to $u^T (I - Y_{b1} Y_{b1}^T - Y_{b2} Y_{b2}^T) u$. The first term is not positive definite, and there are several ways to remedy it. We propose to use the following form $k(Y_1, Y_2) =$

$\frac{1}{b} \text{tr}(Y_1^T Y_{b1} Y_{b2}^T Y_2 + Y_{b1}^T Y_1 Y_2^T Y_{b2}) = \text{tr}(Y_{b1} Y_{b2}^T Y_2 Y_1^T)$, among other possibilities. The sum of the two modified terms, is the proposed affine scaled kernel: $k_{\text{AffSc}}(Y_1, u_1, Y_2, u_2) = \text{tr}(Y_1^T Y_{b1} Y_{b2}^T Y_2) + u_0^T (I - Y_{b1} Y_{b1}^T - Y_{b2} Y_{b2}^T) u$. This is a positive definite kernel which can be shown from the definition.

(14)

Summary of the extended Projection kernels The proposed kernels are summarized below. Let Y_i be a full-rank $D \times m$ matrix, and let $Y_{bi} = Y_i (Y_i^T Y_i)^{-1/2}$ the orthonormalization of Y_i as before. $k_{\text{Lin}}(Y_1, Y_2)$

$$\begin{aligned}
 &= \\
 &k_{\text{Aff}}(Y_1, Y_2) \\
 &= \\
 &\text{tr}(Y_{b1} Y_{b2}^T Y_{b2} Y_{b1}) , k_{\text{LinSc}}(Y_1, Y_2) = \text{tr}(Y_{b1} Y_{b2}^T Y_2 Y_1^T) \\
 &\text{tr}(Y_{b1} Y_{b2}^T Y_{b2} Y_{b1}) + u_0^T (I - Y_{b1} Y_{b1}^T - Y_{b2} Y_{b2}^T) u \\
 &k_{\text{AffSc}}(Y_1, Y_2) \\
 &= \\
 &\text{tr}(Y_{b1} Y_{b2}^T Y_2 Y_1^T) + u_0^T (I - Y_{b1} Y_{b1}^T - Y_{b2} Y_{b2}^T) u
 \end{aligned}$$

(15)

We also spherize the kernels $e k(Y_1, u_1, Y_2, u_2) = k(Y_1, u_1, Y_2, u_2) k(Y_1, u_1, Y_1, u_1)^{-1/2} k(Y_2, u_2, Y_2, u_2)^{-1/2}$ so that $k(Y_1, u_1, Y_1, u_1) = 1$ for any Y_1 and u_1 . There is a caveat in implementing these kernels. Although we used the same notations Y and Y_b for both linear and affine kernels, they are different in computation. For linear kernels the Y and Y_b are computed from data assuming $u = 0$, whereas for affine kernels the Y and Y_b are computed after removing the estimated mean u from the data.

3.3 Extension to nonlinear subspaces

A systematic way of extending the Projection kernel from linear/affine subspaces to nonlinear spaces is to use an implicit map via a kernel function, where the latter kernel is to be distinguished from the former kernels. Note that the proposed kernels (15) can be computed only from the inner products of the column vectors of Y 's and u 's including the orthonormalization procedure. If we replace the inner products of those vectors $y_i^T y_j$ by a positive definite function $f(y_i, y_j)$ on Euclidean spaces, this implicitly defines a nonlinear feature space. This "doubly kernel" approach has already been proposed for the Binet-Cauchy kernel [17, 8] and for probabilistic distances in general [18]. We can adopt the trick for the extended Projection kernels as well to extend the kernels to operate on nonlinear subspaces.

4

Experiments with synthetic data

In this section we demonstrate the application of the extended Projection kernels to two-class classification problems with Support Vector Machines (SVMs).

4.1 Synthetic data

The extended kernels are defined under different assumptions of data distribution. To test the kernels we generate three types of data: "easy", "intermediate" and "difficult" from MFA distribution, which cover the different ranges of data distribution. A total of $N = 100$ FA distributions are generated in $D = 10$ dimensional space. The parameters of each FA distribution $\pi_i(x) = N(u_i, C_i)$ are randomly chosen such that "Easy" data have well separated means u_i and homogeneous scales $Y_i^T Y_i$. "Intermediate" data have partially overlapping means u_i and homogeneous scales $Y_i^T Y_i$. "Difficult" data have totally overlapping means ($u_1 = \dots = u_N = 0$) and randomly chosen scales between 0 and 1. The class label for each distribution π_i is assigned as follows. We choose a pair of distribution p^+ and p^- which are the farthest apart from each other among all pairs of distributions. Then the labels of the remaining distributions π_i are determined from whether they are close to p^+ or p^- . The distances are measured by the KL distance J_{KL} .

the preimage corresponding to the linear subspaces in the RKHS via the feature map

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4.2

Algorithms and results

We compare the performance of the Euclidean SVM with linear/ polynomial/ RBF kernels and the performance of SVM with Grassmann kernels. To test the original SVMs, we randomly sampled $n = 50$ point from each FA distribution $\pi_i(x)$. We evaluate the algorithm with N -fold cross validation by holding out one set and training with the other $N - 1$ sets. The polynomial kernel used is $k(x_1, x_2) = (x_1^T x_2 + 1)^3$. To test the Grassmann SVM, we first estimated the mean u_i and the basis Y_i from $n = 50$ points of each FA distribution $\pi_i(x)$ used for the original SVM. The Y_i , σ_i and θ_i are estimated simply from the probabilistic PCA [12], although they can also be estimated by the Expectation Maximization approach. Six different Grassmann kernels are compared: 1)

the original and the extended Projection kernels (Linear, Linear Scaled, Affine, Affine Scaled), 2) the Binet-Cauchy kernel $k_{BC}(Y1R, Y2) = (\det Y10 Y2)^2 = \det Y10 Y2 Y20 Y1$, and 3) the Bhattacharyya kernel $k_{Bhat}(p1, p2) = [p1(x) p2(x)]^{1/2} dx$ adapted for FA distributions. We evaluate the algorithms with leave-one-out test by holding out one subspace and training with the other $N - 1$ subspaces.

Table 1: Classification rates of the Euclidean SVMs and the Grassmann SVMs. The BC and Bhat are short for Binet-Cauchy and Bhattacharyya kernels, respectively.

| | | | | | | | | | | | |
|-----------------------------|-------|-------|-------|-------|-------|-------|-------|-------|--|--|--|
| Easy Intermediate Difficult | | | | | | | | | | | |
| Euclidean Linear Poly | 84.63 | 79.85 | 62.40 | 61.76 | 52.00 | 63.74 | | | | | |
| Linear | 55.10 | 68.10 | 80.10 | | | | | | | | |
| Grassmann Lin Sc Aff Aff Sc | 55.30 | 92.70 | 92.30 | 67.50 | 85.20 | 83.60 | 81.00 | 80.30 | | | |
| | 81.20 | | | | | | | | | | |
| BC | 54.70 | 60.90 | 68.90 | | | | | | | | |
| Probabilistic Bhat | 46.10 | 59.00 | 77.30 | | | | | | | | |

Table 1 shows the classification rates of the Euclidean SVMs and the Grassmann SVMs, averaged for 10 trials. The results shows that best rates are obtained from the extended kernels, and the Euclidean kernels lag behind for all three types of data. Interestingly the polynomial kernels often perform worse than the linear kernels, and the RBF kernel performed even worse which we do not report. For the ‘‘difficult’’ data where the means are zero, the linear SVMs degrade to the chancelevel (50%), which agrees with the intuitive picture that any decision hyperplane that passes the origin will roughly halve the points from a zero-mean distribution. As expected, the linear kernel is inappropriate for data with nonzero offsets (‘‘easy’’ and ‘‘intermediate’’), whereas the affine kernel performs well regardless of the offsets. However, there is no significant difference between the homogeneous and the scaled kernels. The Binet-Cauchy and the Bhattacharyya kernels mostly underperformed. We conclude that under certain conditions the extended kernels have clear advantages over the original linear kernels and the Euclidean kernels for the subspace-based classification problem.

5

Experiments with real-world data

In this section we demonstrate the application of the extended Projection kernels to recognition problems with the kernel Fisher Discriminant Analysis [10].

5.1

Databases

The Yale face database and the Extended Yale face database [3] together consist of pictures of 38 subjects with 9 different poses and 45 different lighting conditions. The ETH-80 [9] is an object database designed for object categorization test under varying poses. The database consists of pictures of 8 object categories and 10 object instances for each category, recored under 41 different poses.

These databases have naturally factorized structures which make them ideal to test subspace-based learning algorithms with. In Yale Face database, a

set consists of images of all illumination conditions a person at a fixed pose. By treating the set as a point in the Grassmann manifold, we can perform illumination-invariant learning tasks with the data. For ETH-80 database, a set consists of images of all possible poses of an object from a category. Also by treating such set as a point in the Grassmann manifold, we can perform pose-invariant learning tasks with the data. There are a total of $N = 279$ and 80 sets as described above respectively. The images are resized to the dimension of $D = 504$ and 1024 respectively, and the maximum of $m = 9$ dimensional subspaces are used to compute the kernels. The subspace parameters Y_i , u_i and θ_i are estimated from the probabilistic PCA [12].

Algorithms and results

We perform subject recognition tests with Yale Face, and categorization tests with ETH-80 database. Since these databases are highly multiclass (31 and 8 classes) relative to the total number of samples, we use the kernel Discriminant Analysis to reduce dimensionality and extract features, in conjunction with a 1-NN classifier. The six different Grassmann kernels are compared: the extended Projection (Lin/LinSc/Aff/Affsc) kernels, the Binet-Cauchy kernel, and the Bhattacharyya kernel. The baseline algorithm (Eucl) is the Linear Discriminant Analysis applied to the original images in the data from which the subspaces are computed. Figure 1 summarizes the average recognition/categorization rates from 9- and 10-fold cross validation with the Yale Face and ETH-80 databases respectively. The results shows that best rates are achieved from the extended kernels: linear scaled kernel in Yale Face and the affine kernel in ETH80. However the difference within the extended kernels are small. The performance of the extended kernels remain relatively unaffected by the subspace dimensionality, which is a convenient property in practice since we do not know the true dimensionality a priori. However the Binet-Cauchy and the Bhattacharyya kernels do not perform as well, and degrade fast as the subspace dimension increases. The analysis of the poor performance are given in the thesis [5].

6

Conclusion

In this paper we analyzed the relationship between probabilistic distances and the geometric Grassmann kernels, especially the KL distance and the Projection kernel. This analysis help us to understand the limitations of the Bhattacharyya kernel for subspace-based problems, and also suggest the extensions of the Projection kernel. With synthetic and real data we demonstrated that the extended kernels can outperform the original Projection kernel, as well as the previously used Bhattacharyya and the Binet-Cauchy kernels for subspace-based classification problems. The relationship between other probabilistic distances and the Grassmann kernels is yet to be fully explored, and we expect to see more results from a follow-up study.

2 References

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7

Yale Face 100

rate (%)

90 Eucl Lin LinSc Aff AffSc BC Bhat

80 70 60 50 40

1

3

5

7

9

subspace dimension (m)

ETH!80 100

rate (%)

90 Eucl Lin LinSc Aff AffSc BC Bhat

80 70 60 50 40

1

3

5

7

9

subspace dimension (m)

Figure 1: Comparison of Grassmann kernels for face recognition/ object categorization tasks with kernel discriminant analysis. The extended Projection kernels (Lin/LinSc/Aff/ AffSc) outperform the baseline method (Eucl) and the Binet-Cauchy (BC) and the Bhattacharyya (Bhat) kernels. [7] Tony Jebara and Risi Imre Kondor. Bhattacharyya expected likelihood kernels. In *COLT*, pages 57?71, 2003. [8] Risi Imre Kondor and Tony Jebara. A kernel between sets of vectors. In *Proc. of the 20th Int. Conf. on Mach. Learn.*, pages 361?368,

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