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LARGE MARGIN CLASSIFIERS BASED ON AFFINE HULLS

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Abstract

This paper introduces a geometrically inspired large-margin classifier that can be a better alternative to the Support Vector Machines (SVMs) for the classification problems with limited number of training samples. In contrast to the SVM classifier, we approximate classes with affine hulls of their class samples rather than convex hulls. For any pair of classes approximated with affine hulls, we introduce two solutions to find the best separating hyperplane between them. In the first proposed formulation, we compute the closest points on the affine hulls of classes and connect these two points with a line segment. The optimal separating hyperplane between the two classes is chosen to be the hyperplane that is orthogonal to the line segment and bisects the line. The second formulation is derived by modifying the ν -SVM formulation. Both formulations are extended to the nonlinear case by using the kernel trick. Based on our findings, we also develop a geometric

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interpretation of the Least Squares SVM classifier and show that it is a special case of the proposed method. Multi-class classification problems are dealt with constructing and combining several binary classifiers as in SVM. The experiments on several databases show that the proposed methods work as good as the SVM classifier if not any better.

Keywords: Affine hull, classification, convex hull, kernel methods, large margin classifier, quadratic programming, support vector machines.

1 1. Introduction

The Support Vector Machine (SVM) classifier is a successful binary classifica-2 tion method that simultaneously minimizes the empirical classification error and 3 maximizes the geometric margin, which is defined as the distance between the separating hyperplane and closest samples from the classes [2, 8]. To do so, SVM 5 first approximates each class with a convex hull and finds the closest points in 6 these convex hulls [1]. Then, these two points are connected with a line segment. 7 The hyperplane, orthogonal to the line segment that bisects the line, is chosen to 8 be the separating hyperplane. From the geometrical point of view, in the sepa-9 rable case, the two closest points on the convex hulls determine the separating 10 hyperplane, and the SVM margin is merely equivalent to the minimum distance 11 between the convex hulls that represent classes. However, convex hull approxima-12 tions tend to be unrealistically tight in high-dimensional spaces since the classes 13 typically extend beyond the convex hulls of their training samples. For example, 14 a convex hull constructed by randomly sampled points from a high-dimensional 15 hypersphere can include only a negligible fraction of the volume of the sphere 16 even if the chosen samples are well spaced and close to the surface of the sphere 17

[3]. This situation may also be observed when the low-dimensional data samples
are mapped to a higher-dimensional feature space through kernel mapping during
estimation of the nonlinear decision boundaries between classes.

As opposed to the convex hulls, affine hulls (i.e., spanning linear subspaces 21 that have been shifted to pass through the centroids of the classes) give rather 22 loose approximations to the class regions, because they do not constrain the po-23 sitions of the training points within the affine subspaces. Therefore, they may 24 be better alternatives to convex hulls for some pattern classification problems es-25 pecially when the data samples lie in high-dimensional spaces. In the context 26 of classification, affine hulls are first used as global classifiers of isolated word 27 and hand-written digits giving good classification performance [11, 14]. In these 28 methods, each class is approximated with an affine hull constructed from its train-29 ing samples, and the label of a test sample is determined based on the distance to 30 the nearest affine hull. Vincent and Bengio [26] used affine/convex hulls in a local 31 sense by constructing them using k-nearest neighbors of a test sample for classi-32 fication problems with complex nonlinear decision boundaries. They report that 33 affine hulls usually give higher classification accuracy than convex hulls and that 34 using both models for classification significantly improves the k-nearest neighbor 35 classification performance [26]. We extended local linear affine/convex hull clas-36 sifiers to the nonlinear case in [4]. More recently, we compared different convex 37 class models for high-dimensional classification problems, then found that affine 38 hull approximations are typically more accurate than convex hull approximations 39 [3]. These results are not surprising due to the fact that high-dimensional ap-40 proximations tend to be simple: For a fixed sample size, the amount of geometric 41 details that can be resolved usually decreases rapidly as the dimensionality in-42

43 creases. Therefore, affine hulls tend to be better models for high-dimensional data
44 approximations.

Besides the classification, approximations based on affine hulls have also been 45 used for dimensionality reduction. Mixtures of Principal Component Analyzers 46 [12] use local affine hulls to estimate nonlinear data manifolds. Similarly, Lo-47 cally Linear Embedding [18] approximates the nonlinear structure of the high-48 dimensional data by exploiting local affine hull reconstructions. Verbeek [25] 49 combined several locally valid affine hulls to obtain a global nonlinear map-50 ping between the high-dimensional sample space and low-dimensional manifold. 51 Many applications of affine hulls in the context of classification and dimension-52 ality reduction can be attributed in part to their simplicity and computational ef-53 ficiency. Finding distances from test samples to affine hulls requires only simple 54 linear algebra. On the other hand, computing distances to nonlinear complex mod-55 els can be problematic. Even if the models are restricted to being convex hulls, 56 distance computations require the solution of a quadratic optimization problem. 57

The classification methods using affine hulls or other convex sets described 58 above are "nearest convex model" classifiers and they are instance-based in na-50 ture. In other words, decision boundaries are not explicitly created during a train-60 ing phase. Instead, the decision boundaries remain implicit, and new examples 61 are classified online based on the distances to the nearest convex class models. 62 This paper investigates an alternative "margin between convex model" strategy 63 that is based on explicitly building maximum margin separators between pairs 64 of affine hulls. As a first example of the power of this approach, note that the 65 SVM itself is the maximum margin separator between the convex hulls of the 66 training samples of the two classes. One motivation for replacing nearest-convex-67

model approaches with margin-based ones is that for all of the above cited nearest-68 convex-model classifiers, the decision boundaries (surfaces equidistant from the 69 two convex models) are generically at least quadratic or piecewise quadratic in 70 complexity. For example, for affine hulls they are generically hyperboloids. Such 71 decision boundaries are more flexible than linear ones, but in high dimensions 72 when the training data is scarce this may lead to overfitting, thus damaging gener-73 alization to unseen examples. Linear margin based approaches have fewer degrees 74 of freedom, so they are typically less sensitive to the precise arrangement of the 75 training samples. For example, for an SVM classifier, motions of the SVM support 76 vectors parallel to the SVM decision surface do not alter the margin and hence do 77 not invalidate the classifier, whereas they do typically change piece-wise quadratic 78 decision surface of the equivalent nearest convex hull classifier. Another motiva-79 tion for studying margin-between-affine hulls approach is their potential flexibility 80 and compactness. In linear case, affine models allow each class to be fitted indi-81 vidually and represented compactly, following which the linear separator between 82 any two classes can be found quickly by simple linear algebra. 83

In our preliminary work [5] we showed how to construct maximum margin 84 classifier that separates linear affine hulls. Another study addressing the same 85 problem was independently given in [29]. Here we extend the method such that 86 it can be used when the class samples lie on nonlinear manifolds that cannot be 87 modeled with linear affine hulls. To this end, we map the samples in each class 88 into a much higher-dimensional feature space through kernel mapping and then 89 construct the linear affine hulls in the mapped space. Since the problem is cast 90 in a much higher-dimensional space, it is more likely that class regions can now 91 be approximated with linear affine hulls. Although the constructed linear affine 92

⁹³ hulls in the mapped space corresponds to nonlinear manifolds in the input space,
⁹⁴ finding the maximum separating hyperplane between these nonlinear manifolds is
⁹⁵ still straightforward because of their linear nature in the mapped space. In case
⁹⁶ of outliers, to allow soft margin solutions, we first reduce affine hulls in order
⁹⁷ to alleviate the effects of those outliers and then search for the best separating
⁹⁸ hyperplane between these reduced robust models.

The rest of the paper is organized as follows: In Section II, we introduce the proposed method. Section III describes the experimental results. Concluding remarks are given in Section IV.

102 **2. Method**

Consider a binary classification problem with the training data given in the 103 form $\{\mathbf{x}_i, y_i\}$, i = 1, ..., n, $y_i \in \{-1, +1\}$, $\mathbf{x}_i \in \mathbb{R}^d$. To separate classes, SVM 104 classifier finds a separating hyperplane that maximizes the margin, which is de-105 fined as the distance between the hyperplane and closest samples from the classes. 106 To do so, SVM first approximates each class with a convex hull [1]. A convex hull 107 consists of all points that can be written as a convex combination of the points in 108 the original set, and a convex combination of points is a linear combination of data 109 points where all coefficients are nonnegative and sum up to 1. More formally, the 110 convex hull of samples $\{\mathbf{x}_i\}_{i=1,...,n}$ can be written as 111

$$H^{convex} = \left\{ \mathbf{x} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i | \sum_{i=1}^{n} \alpha_i = 1, \alpha_i \ge 0 \right\}.$$
 (1)

¹¹² Convex hulls of two classes are illustrated in Fig. 1. Following this approximation,
¹¹³ SVM finds the closest points in these convex hulls. Then, these two points are

¹¹⁴ connected with a line segment. The plane, orthogonal to the line segment that bisects the line, is selected to be the separating hyperplane as shown in Fig. 1.



Figure 1: Two closest points on the convex hulls determine the separating hyperplane.

115



Figure 2: Comparison of convex and affine hulls of samples.

In contrast to the SVM classifier, the proposed method approximates each class (positive and negative classes) with an affine hull of its training samples. An affine hull of a class is the smallest affine subspace containing them. This is an unbounded, and hence typically rather loose model for each class, thus affine hull modeling can be a better choice than convex hull modeling for highdimensional data. Affine and convex hulls of four samples are illustrated in Fig. 2. The affine hull of samples $\{\mathbf{x}_i\}_{i=1,...,n}$ contains all points of the form $\sum_{i=1}^{n} \alpha_i \mathbf{x}_i$ with $\sum_{i=1}^{n} \alpha_i = 1$. More formally affine hull of a class with samples $\{\mathbf{x}_i\}_{i=1,\dots,n}$ can be written as

$$H^{aff} = \left\{ \mathbf{x} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i \mid \sum_{i=1}^{n} \alpha_i = 1 \right\}.$$
 (2)

Our goal is to find the maximum margin linear separating hyperplane between 125 affine hulls of classes. The points x which lie on the separating hyperplane satisfy 126 $\langle \mathbf{w}, \mathbf{x} \rangle + b = 0$, where w is the normal of the separating hyperplane, $|b|/||\mathbf{w}||$ 127 is the perpendicular distance from the hyperplane to the origin, and ||w|| is the 128 Euclidean norm of w. For any separating hyperplane, all points x_i in the posi-129 tive class satisfy $\langle \mathbf{w}, \mathbf{x}_i \rangle + b > 0$ and all points \mathbf{x}_i in the negative class satisfy 130 $\langle \mathbf{w}, \mathbf{x}_i \rangle + b < 0$ so that $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) > 0$ for all training data points. Finding 131 the best separating hyperplane between affine hulls can be solved by computing 132 the closest points on them. The optimal separating hyperplane will be the one that 133 bisects perpendicularly the line segment connecting the closest points as in SVM 134 classifier. The offset (also called threshold), b, can be chosen as the distance from 135 the origin to the point halfway between the closest points along the normal w. 136 Once the best separating hyperplane is determined, a new sample x is classified 137 based on the sign of the decision function, $f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b$. 138

¹³⁹ Next, we will first show how to find the best separating hyperlane for linearly ¹⁴⁰ separable affine hulls and then extend the idea for inseparable case. After that, we ¹⁴¹ explain kernelization process. This is followed by introducing a second equivalent ¹⁴² formulation based on a variation of ν -SVM [20]. Lastly we show the relation ¹⁴³ between the proposed method and the Least Squares SVM (LS-SVM) [24, 23] ¹⁴⁴ and derive a geometric intuition for LS-SVM.

145 2.1. Linearly Separable Case

Suppose that affine hulls belonging to the positive and negative classes are linearly separable. The affine hulls of two classes do not intersect, i.e., they are linearly separable, if the affine combinations of their samples satisfy the rule

$$\sum_{i:y_i=+1} \alpha_i \mathbf{x}_i \neq \sum_{j:y_j=-1} \alpha_j \mathbf{x}_j \quad \text{for} \quad \sum_{i:y_i=+1} \alpha_i = \sum_{j:y_j=-1} \alpha_j = 1.$$
(3)

It should be noted that linear separability of data points does not necessarily guarantee the separability of corresponding affine hulls of classes. For linearly separable case, it is more convenient to write an affine hull as

$$\{\mathbf{x} = \mathbf{U}\mathbf{v} + \mu \,|\, \mathbf{v} \in \mathbb{R}^l\},\tag{4}$$

where $\mu = (1/n) \sum_i \mathbf{x}_i$ is the mean of the samples (or any other reference 152 point in the hull) and \mathbf{U} is an orthonormal basis for the directions spanned by 153 the affine subspace. The vector v contains the reduced coordinates of the point 154 within the subspace, expressed with respect to the basis U. Numerically, U can 155 be found as the U-matrix of the 'thin' Singular Value Decomposition (SVD) of 156 $[\mathbf{x}_1 - \boldsymbol{\mu}, ..., \mathbf{x}_n - \boldsymbol{\mu}]$. Here, 'thin' indicates that we take only the columns of U 157 corresponding to "significantly non-zero" singular values λ_k ; l is the number of 158 such non-zero singular values. This subspace estimation process is essentially or-159 thogonal least squares fitting. Discarding near-zero singular values corresponds to 160 discarding directions that appear to be predominantly "noise". As an alternative, 161 samples can be fitted with some other more robust subspace estimation processes 162 such as L1 norm based subspace fitting procedures described in [10, 13]. But, we 163 will consider only the least squares fitting (L2 norm) in this study. 164

Now suppose that we have two affine hulls with point sets $\{U_+ v_+ + \mu_+\}$ and $\{U_- v_- + \mu_-\}$. (These can be estimated with either L2 or L1 fitting and they may

have different numbers of dimensions l). A closest pair of points between the two hulls can be found by solving

$$\min_{\mathbf{v}_{+},\mathbf{v}_{-}} ||(\mathbf{U}_{+}\mathbf{v}_{+}+\boldsymbol{\mu}_{+}) - (\mathbf{U}_{-}\mathbf{v}_{-}+\boldsymbol{\mu}_{-})||^{2}.$$
 (5)

Defining $\mathbf{U} \equiv \begin{pmatrix} \mathbf{U}_+ & -\mathbf{U}_- \end{pmatrix}$ and $\mathbf{v} \equiv \begin{pmatrix} \mathbf{v}_+ \\ \mathbf{v}_- \end{pmatrix}$, this can be written as the standard least squares problem

$$\min_{\mathbf{v}} ||\mathbf{U}\mathbf{v} - (\boldsymbol{\mu}_{-} - \boldsymbol{\mu}_{+})||^{2}.$$
 (6)

If we take the derivative of the objective function (6) with respect to v and equate
it to zero, then we obtain

$$\mathbf{U}^{\mathsf{T}}\mathbf{U}\mathbf{v} - \mathbf{U}^{\mathsf{T}}(\boldsymbol{\mu}_{-} - \boldsymbol{\mu}_{+}) = \mathbf{0}$$
(7)

Subsequently, we get the solution of the problem as $\mathbf{v} = (\mathbf{U}^{\mathsf{T}} \mathbf{U})^{-1} \mathbf{U}^{\mathsf{T}} (\boldsymbol{\mu}_{-} - \boldsymbol{\mu}_{+})$. Taking the decision boundary $f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b$,

$$\mathbf{w} = \frac{1}{2}(\mathbf{x}_{+} - \mathbf{x}_{-}) = \frac{1}{2}(\mathbf{I} - \mathbf{P})(\boldsymbol{\mu}_{+} - \boldsymbol{\mu}_{-})$$
 (8)

where $\mathbf{P} = \mathbf{U} (\mathbf{U}^{\mathsf{T}} \mathbf{U})^{-1} \mathbf{U}^{\mathsf{T}}$ is the orthogonal projection onto the joint span of the directions contained in the two subspaces, $\mathbf{I} - \mathbf{P}$ is the corresponding projection onto the orthogonal complement of this span¹, and \mathbf{x}_{+} and \mathbf{x}_{-} denote the closest points on the positive and negative classes, respectively. Note that \mathbf{w} lies along the line segment joining the two closest points and it is half the line segment's size. The offset *b* of the separating hyperplane is given by

$$b = -\mathbf{w}^{\top}(\mathbf{x}_{+} + \mathbf{x}_{-})/2.$$
(9)

¹If the two subspaces share common directions, $\mathbf{U}^{\mathsf{T}}\mathbf{U}$ is not invertible and the solution for $(\mathbf{v}_+, \mathbf{v}_-)$ and $(\mathbf{x}_+, \mathbf{x}_-)$ is non-unique, but the orthogonal complement remains well defined, giving a unique minimum norm separator \mathbf{w} . Numerically all cases can be handled by finding $\tilde{\mathbf{U}}$, the U matrix of the thin SVD of U, and taking $\mathbf{P} = \tilde{\mathbf{U}}^{\mathsf{T}}\tilde{\mathbf{U}}$.

175 2.2. Inseparable Case

A problem arises if the affine hulls of classes intersect, i.e., affine hulls are not 176 linearly separable. If the affine hulls of classes are close to being linearly separable 177 and they overlap because of a few outliers, we can restrict the influence of outlying 178 points by reducing affine hulls. Note that ignoring directions corresponding to the 179 overly small singular values during affine hulls constructions reduces the effects 180 of noise and outliers up to some degree. But, we will use a different approach 181 here in order to cope with the outliers. To this end, we use the initial affine hull 182 formulation (2) and introduce upper and lower bounds on coefficients α_i to reduce 183 affine hulls inspired by the idea that is introduced to reduce convex hulls in [1]. It 184 should be noted that the reduced affine hulls are not uniformly scaled versions of 185 the initial complete affine hulls. One may go further and choose different lower 186 and uper bounds, or define a different interval for every sample in the training 187 set if a-priori information is available. For instance, if the lower bound is set 188 to zero, then the method will be equivalent to the SVM classifier. Finding the 189 closest points on the reduced affine hulls can be written as a quadratic optimization 190 problem 191

$$\min_{\alpha} || \sum_{i:y_i=+1} \alpha_i \mathbf{x}_i - \sum_{i:y_i=-1} \alpha_i \mathbf{x}_i ||^2$$
s.t.
$$\sum_{i:y_i=+1} \alpha_i = 1, \quad \sum_{i:y_i=-1} \alpha_i = 1, \quad -\tau \le \alpha_i \le \tau,$$
(10)

where τ is the user-chosen bound. This optimization problem (10) can be written in a more compact form as

$$\min_{\alpha} \sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$
s.t.
$$\sum_{i} \alpha_i y_i = 0, \sum_{i} \alpha_i = 2, \quad -\tau \le \alpha_i \le \tau.$$
(11)

This is a quadratic programming problem that can be solved using standard optimization techniques. Note that the Hessian matrix, $\mathbf{G} = [G_{ij}] = y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$, is a positive semi-definite matrix, thus the objective function is convex and a global minimum exists as in SVM classifier. Moreover, if the Hessian matrix is strictly positive definite, the solution is unique and it is guaranteed to be the global minimum.

Since the coefficients are bounded between $-\tau$ and $+\tau$, the solution is determined by more points and no extreme point or noisy point can excessively influence the solution for well-chosen τ . Once we compute the optimal values of coefficients α_i , the normal and the offset of the separating hyperplane can be computed as in the linearly separable case

$$\mathbf{w} = \frac{1}{2} \left(\sum_{i:y_i=+1} \alpha_i \mathbf{x}_i - \sum_{i:y_i=-1} \alpha_i \mathbf{x}_i \right), \tag{12}$$

205

$$b = -\frac{1}{2} \mathbf{w}^{\top} (\sum_{i:y_i=+1} \alpha_i \mathbf{x}_i + \sum_{i:y_i=-1} \alpha_i \mathbf{x}_i),$$
(13)

We call this method Large Margin Classifier of Affine Hulls (LMC-AH) since it uses affine hulls to approximate class regions and finds the optimal separating hyperplane yielding the largest margin between the affine hulls.

If the underlying geometry of the classes is highly complex and nonlinear, and 209 approximating classes with linear affine hulls is not appropriate, we can map the 210 data into a higher-dimensional space where the classes can be approximated with 211 linear affine hulls. Note that the objective function of (11) is written in terms of 212 the dot products of samples, which allows the use of the kernel trick. Thus, by 213 using kernel trick, – i.e., replacing $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ with the kernel function $k(\mathbf{x}_i, \mathbf{x}_j) =$ 214 $\langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$ where $\phi : \mathbb{R}^d \to \Im$ is the mapping function from the input space 215 to the mapped space \Im – we can find the best seperating hyperplane parameters 216

in the mapped space. As a result, more complex nonlinear decision boundaries
between classes can be approximated by using this trick.

219 2.3. An Equivalent Formulation Based on Variation of ν -SVM Classifier

The ν -SVM formulation has been proposed as an alternative to the classical 220 SVM formulation [20]. A new parameter ρ' is introduced in this formulation, and 221 error penalty term C that appears in classical SVM formulation is removed. Here, 222 we introduce an alternative formulation to find the best separating hyperplane be-223 tween affine hulls based on a variation of ν -SVM formulation. A major advantage 224 of new formulation is that one can relate the parameter τ in (11) with the ex-225 pected error bounds and this may help us to find a more sophisticated procedure 226 for choosing unknown parameters that appear in both formulations. 227

The ν -SVM optimization is formulated as

$$\min_{\mathbf{w}',b',\xi',\rho'} \frac{1}{2} ||\mathbf{w}'||^2 - \nu \rho' + \frac{1}{n} \sum_i \xi'_i
s.t. \ y_i (\langle \mathbf{w}', \mathbf{x}_i \rangle + b') \ge \rho' - \xi'_i, \ \xi'_i \ge 0, \ \rho' \ge 0,$$
(14)

where w' represents the normal of the separating hyperplane, b' is the offset, ν 229 is a user-chosen parameter between 0 and 1, and ξ'_i , i = 1, ..., n, are the positive 230 slack variables. In this formulation, for linearly separable case, there exist two 231 parallel supporting hyperplanes positioned such that all points in the positive class 232 satisfy $\langle \mathbf{w}', \mathbf{x} \rangle + b' \geq \rho'$ and all points in the negative class satisfy $\langle \mathbf{w}', \mathbf{x} \rangle + b' \geq \rho'$ 233 $b' \leq -\rho'$ as shown in Fig. 3. Therefore, classes are separated by the margin 234 $2\rho'/||\mathbf{w}'||$ and it is shown that ν acts as an upper bound on the fraction of margin 235 errors and a lower bound on the fraction of support vectors [20]. Moreover, the 236 decision function produced by ν -SVM can also be produced by classical SVM for 237 appropriate choice of error penalty term C. 238



Figure 3: Illustration of the supporting and the best separating hyperplanes in linearly separable case for ν -SVM classifier.

The ν -SVM formulation can be interpreted as a maximal separation between the reduced convex hulls of classes [9]. Since we use affine hulls to model classes, we need to revise the optimization problem to accommodate this change. To this end, we first divide the objective function by $\nu^2/2$, the constraints by ν , and make the following substitutions as in [9]

$$\tau = \frac{2}{\nu n}, \quad \mathbf{w} = \frac{\mathbf{w}'}{\nu}, \quad b = \frac{b'}{\nu}, \quad \rho = \frac{\rho'}{\nu}, \quad \xi_i = \frac{\xi'_i}{\nu} \tag{15}$$

²⁴⁴ These modifications yield the equivalent formulation²

$$\min_{\mathbf{w},b,\xi,\rho} ||\mathbf{w}||^2 - 2\rho + \tau \sum_i \xi_i$$

$$s.t. \ y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \ge \rho - \xi_i, \ \xi_i \ge 0,$$
(16)

with the new decision function $f(\mathbf{x}) \equiv f'(\mathbf{x})/\nu$.

²Crisp and Burges [9] showed that the constraint $\rho' \ge 0$ in (14) is redundant and hence it can be removed.



Figure 4: Optimal separating hyperplane between affine hulls of two classes. Note that affine hulls lie on the supporting hyperplanes.

Note that two affine hulls are linearly separable if they lie parallel to each other 246 in the given input space since affine hulls extend to infinity in all directions. In this 247 case, the supporting hyperplanes yielding the largest margin between affine hulls 248 will entirely include them so that all affine combinations of samples belonging to 249 the positive class satisfy $\left< \mathbf{w}, \mathbf{x}_{+}^{a\!f\!f} \right> + b = \rho$ and all affine combinations of samples 250 belonging to the negative class satisfy $\left< \mathbf{w}, \mathbf{x}_{-}^{a\!\!f\!\!f} \right> + b = -\rho$ as illustrated in Fig. 251 4. Fig. 4 illustrates affine hulls of two classes where the affine hull of the first 252 class is a line and the affine hull of the second class is a plane. Note that affine 253 hulls are linearly separable if they lie parallel to each other. Therefore, all samples 254 of classes and their affine combinations lie on the supporting hyperplanes, which 255 yield the largest margin between the affine hulls. In case of outliers, we must 256 construct reduced compact affine hulls that will fit the data robustly. Therefore, we 257

should allow errors for outlier samples from all over the input space, not just the ones near the decision boundary as illustrated in Fig. 5. To do so, the inequality constraints in (16) is replaced with equality constraints $y_i(\langle \mathbf{w}, \mathbf{x} \rangle + b) = \rho - \delta_i \xi_i$, where δ_i is a term which takes values +1 or -1 based on the location of outliers with respect to the supporting hyperplanes. This leads to the new optimization problem

$$\min_{\mathbf{w},b,\xi,\rho} ||\mathbf{w}||^2 - 2\rho + \tau \sum_i \xi_i$$

$$s.t. \ y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) = \rho - \delta_i \xi_i, \ \xi_i \ge 0.$$
(17)

²⁶⁴ To derive the dual, we consider the Lagrangian

$$L(\mathbf{w}, b, \xi, \rho, \alpha, \beta) = ||\mathbf{w}||^2 - 2\rho + \tau \sum_i \xi_i - \sum_i \alpha_i \left[y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - \rho + \delta_i \xi_i \right] - \sum_i \beta_i \xi_i,$$
(18)

where $\beta_i \ge 0$. The Lagrangian *L* has to be maximized with respect to α_i , β_i and minimized with respect to \mathbf{w}, b, ξ , and ρ . The optimality conditions yield

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{0} \to \mathbf{w} = \frac{1}{2} \sum_{i} \alpha_{i} y_{i} \mathbf{x}_{i},$$

$$\frac{\partial L}{\partial b} = 0 \to \sum_{i} \alpha_{i} y_{i} = 0,$$

$$\frac{\partial L}{\partial \rho} = 0 \to \sum_{i} \alpha_{i} = 2,$$

$$\frac{\partial L}{\partial \xi_{i}} = 0 \to \alpha_{i} = \frac{\tau - \beta_{i}}{\delta_{i}} \to -\tau \le \alpha_{i} \le \tau.$$
(19)

²⁶⁷ Thus, the dual of the optimization problem becomes

$$\min_{\alpha} \frac{1}{4} \sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$
s.t.
$$\sum_i \alpha_i y_i = 0, \quad \sum_i \alpha_i = 2, \quad -\tau \le \alpha_i \le \tau.$$
(20)

This optimization is equivalent to the one given in (11) - here 1/4 appears in the objective function, but rescaling objective function with a positive constant does not change the solution. Therefore, the new formulation based on modified ν -SVM is in fact equivalent to finding the best separating hyperplane between the reduced affine hulls that represent classes. We call this method ν -LMC-AH. Due to the Karush-Kuhn-Tucker (KKT) conditions, slack variables can occur only



Figure 5: To obtain better separating hyperplanes between affine hulls, we should allow errors for outlier samples from all over the input space.

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when $\alpha_i = \pm \tau$. To compute offset *b*, we use the primal constraints and take equal number of samples with coefficients $\alpha_i \neq \pm \tau$ from positive and negative classes. Assume that there are *l* selected samples. By using KKT conditions, we know that $\xi_i = 0$ for the samples with $\alpha_i \neq \pm \tau$. Thus, the offset will be

$$b = -\frac{1}{2l} \sum_{i=1}^{l} \sum_{j=1}^{n} \alpha_j y_j \langle \mathbf{x}_j, \mathbf{x}_i \rangle.$$
(21)

This offset is not necessarily equivalent to the one given in (13). Therefore, using 278 geometrically inspired formulation and ν -LMC-AH formulation create separating 279 hyperplanes with the same normal, but the positions (perpendicular distances from 280 the origin) of these hyperplanes may be different. It is not a-priori evident that 281 which offset is the best and one can use other principled methods to determine the 282 best b for a given problem, e.g., given w, b can be computed as value yielding the 283 smallest classification error on a validation set. As in the previous case, extension 284 to the nonlinear case can be done by using the kernel trick. 285

286 2.4. Geometric Interpretation of Least Squares SVM Classifier

Least Squares Support Vector Machines (LS-SVM) was initially proposed by 287 Suykens and Vandewalle [24] for classification and nonlinear function estimation 288 and then new variants of this method have been introduced [7, 21, 22]. The basic 289 motivation was to simplify the classical SVM formulation without losing much 290 generalization performance. To this end, inequality constraints in the SVM clas-291 sification formulation are heuristically replaced with equality constraints³, and 292 square of the slack variables are used in the objective function. More formally the 293 optimization problem is defined as 294

$$\min_{\mathbf{w},b,\xi} \frac{1}{2} ||\mathbf{w}||^2 + \frac{C}{2} \sum_i \xi_i^2$$
s.t. $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) = 1 - \xi_i,$
(22)

where C is a user-chosen error penalty term as in classical SVM classifier. It is shown that the solution is obtained by solving a set of linear equations rather than

³In fact, using equality constraints for nonlinear function estimation was introduced earlier in [19].

solving a quadratic programming problem [24]. Note that, in this formulation, 297 for the linearly separable case, there exist two parallel supporting hyperplanes po-298 sitioned such that all points in the positive class satisfy $\langle {f w}, {f x}
angle + b = 1$ and all 299 points in the negative class satisfy $\langle {\bf w}, {\bf x} \rangle + b = -1$ where the margin between 300 these hyperplanes is given by $2/||\mathbf{w}||$. As in ν -LMC-AH formulation, this cor-301 responds to approximating each class with an affine hull instead of a convex hull 302 since all samples and their affine combinations are forced to lie on the supporting 303 hyperplanes. In LS-SVM, L2 norm (squares) of the slack variables are used in 304 the optimization, but using L1 norm of the slack variables in the objective func-305 tion may be more appropriate for some applications since it allows more robust 306 fitting of data samples. If we use L1 norm of the slack variables, new optimization 307 problem becomes 308

$$\min_{\mathbf{w},b,\xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_i \xi_i$$
s.t. $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) = 1 - \delta_i \xi_i, \ \xi_i \ge 0,$
(23)

where δ_i is a term which takes values +1 or -1. The Lagrangian will be

$$L(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2} ||\mathbf{w}||^2 + C \sum_i \xi_i - \sum_i \alpha_i \left[y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 + \delta_i \xi_i \right] - \sum_i \beta_i \xi_i,$$
(24)

under the constraint $\beta_i \ge 0$. The optimality conditions yield

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{0} \to \mathbf{w} = \frac{1}{2} \sum_{i} \alpha_{i} y_{i} \mathbf{x}_{i},$$

$$\frac{\partial L}{\partial b} = 0 \to \sum_{i} \alpha_{i} y_{i} = 0,$$

$$\frac{\partial L}{\partial \xi_{i}} = 0 \to \alpha_{i} = \frac{C - \beta_{i}}{\delta_{i}} \to -C \le \alpha_{i} \le C.$$
(25)

³¹¹ Thus, the dual of the optimization problem becomes

$$\min_{\alpha} \frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_i \alpha_i$$
s.t.
$$\sum_i \alpha_i y_i = 0, \quad -C \le \alpha_i \le C.$$
(26)

Similar to the previous cases, this is a convex quadratic optimization problem with a global minimum. Due to the Karush-Kuhn-Tucker (KKT) conditions, slack variables can occur only when $\alpha_i = \pm C$. To compute offset *b*, we use the primal constraints and take equal number of samples with coefficients $\alpha_i \neq \pm C$ from positive and negative classes as in ν -LMC-AH. Assume that there are *l* selected samples. By using KKT conditions, we know that $\xi_i = 0$ for the samples with $\alpha_i \neq \pm C$. Thus, the offset will be

$$b = -\frac{1}{2l} \sum_{i=1}^{l} \sum_{j=1}^{n} \alpha_j y_j \langle \mathbf{x}_j, \mathbf{x}_i \rangle.$$
(27)

A new sample is classified based on the sign of the decision function $f(\mathbf{x}) =$ 319 $\langle \mathbf{w}, \mathbf{x} \rangle + b$. Nonlinearization can be done by replacing the dot products $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ 320 with the kernel function $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$. We call this method as C-321 LMC-AH since it uses error penalty term C. It follows from Proposition 6 of [20] 322 that for appropriate choices of C, the C-LMC-AH algorithm will yield identical 323 results to LMC-AH and ν -LMC-AH classifiers. More precisely, if ν -LMC-AH 324 classification leads to $\rho \geq 0$, then C-LMC-AH method with C set a priori to 325 $1/\rho' n$ (or $1/\rho \nu n$), leads to the same decision function as ν -LMC-AH [6, 20]. 326

327 2.5. Extension to the Multi-Class Classification Problems

To use the proposed methods in multi-class classification problems, we can use most of the strategies adopted for extending binary SVM classifiers to the multiclass cases. Here we will discuss the most popular two strategies: one-against-one

(OAO) and one-against-rest (OAR). For a *c*-class classification problem, the OAR 331 strategy trains c binary classifiers, in which each classifier separates one class 332 from the remaining c-1 classes. All classifiers are needed to be trained on the 333 entire training set, and the class label of a test sample is determined according to 334 the highest output of the classifiers in the ensemble. On the other hand, the OAO 335 strategy constructs all possible c(c-1)/2 binary classifiers out of c classes. The 336 decision of the ensemble is decided by max wins algorithm: Each OAO classifier 337 casts one vote for its preferred class, and the final decision is the class with the 338 most votes. In addition to these we can also use Directed Acyclic Graphs [17] or 339 Binary Decision Trees [28] for multi-class classification. 340

341 3. Experiments

We tested⁴ the linear and kernelized versions of the proposed methods LMC-342 AH, v-LMC-AH and C-LMC-AH (L1 norm based LS-SVM) on a number of 343 data sets and compared them to the SVM classifier. For the linearly separable 344 case, linear separator is determined by using affine subspace estimation formula-345 tion, and subspace dimensions are set by retaining enough leading eigenvectors 346 to account for 95-98% of the total energy in the eigen-decomposition. For the 347 inseparable and nonlinear cases, we used quadratic programming formulations. 348 Both one-against-rest (OAR) and one-against-one (OAO) approaches are used for 349 multi-class classification problems and we report the results of whichever yields 350 the best. 351

352

We first tested the linear LMC-AH method on multiple and single shot face

⁴For software see *http://www2.ogu.edu.tr/~mlcv/softwares.html*.

recognition problems to demonstrate that affine hull approximations are more appropriate than convex hull approximations when the dimensionality of the input space is high. To assess the generalization performances of kernelized versions of the methods, we tested them on seven low-dimensional databases chosen from the UCI repository.

358 3.1. Experiments on the Honda/UCSD Database

Honda/UCSD database [15] has been collected for video-based face recognition and it consists of 59 video sequences belonging to 20 individuals. Each video consists of approximately 300-500 frames. It is a fixed database so that 20 of the videos are allocated for training and the remaining 39 for testing. Here, we consider face recognition based on multiple images. In this scenario, face recognition problem is defined as taking a set of face images from an unknown person and finding the most similar set among the database of labeled image sets. We used



Figure 6: Some detected face images from videos belonging to two subjects.

365

the cascade face detector of Viola and Jones [27] to detect faces in each video sequence and resized the detected face images to the gray images of size 40×40

Methods	Clean	Corrup. Training	Corrupted Test	Corrup. Training+Test
LMC-AH	97.44	97.44	92.31	87.18
SVM	94.87	92.31	92.31	82.05

Table 1: Classification Rates (%) on the Honda/UCSD Database.

followed by histogram equalization. Then, these images are used to construct im-368 age sets of individuals. Some of the detected face images are shown in Fig. 6. 369 We used affine hulls and convex hulls to model image sets, and used the distances 370 between these models as a similarity measure. In other words, computed margins 371 between linear affine hulls and convex hulls are used to determine the label of 372 the tested image sets⁵. We performed several experiments in order to test the ro-373 bustness against outliers. In the first experiment, we computed classification rates 374 based on the clean image sets. Then, we systematically corrupted training and test 375 sets by adding images from other classes to each set. These images can be seen as 376 outliers and the changes in classification rates reflect the robustness of the meth-377 ods against these outliers. The results are given in Table 3.1. As can be seen from 378 the table, affine hull approximations yield better results than convex hull approx-379 imations in all cases except for the corrupted test where both models give same 380 results. Thus, affine hulls seem better and more robust models for approximating 381 image sets. 382

⁵For the affine hull case we simply used the minimum distance between the estimated affine subspaces using equation (6) whereas soft margin linear SVM algorithm is used to determine the distances between convex hulls.

383 3.2. Experiments on the AR Face Database

The AR Face data set [16] contains 26 frontal images with different facial ex-384 pressions, illumination conditions and occlusions for each of 126 subjects, recorded 385 in two 13-image sessions spaced by 14 days. For this experiment, we randomly 386 selected 20 male and 20 female subjects. The images were down-scaled (from 387 768×576), aligned so that centers of the two eyes fell at fixed coordinates, 388 then cropped to size 105×78 . Some pre-processed images are shown in Fig. 389 7. Raw pixel values were used as features. For training we randomly selected 390 n = 7, 13, 20 samples for each individual, keeping the remaining 26 - n for test-391 ing. This process was repeated 10 times, with the final classification rate being 392 obtained by averaging the 10 results. The results are shown in Table 3.2. Best re-



Figure 7: Aligned images of one subject from the AR Face database.

393

³⁹⁴ sults are obtained by OAR strategy for both tested methods. The proposed method ³⁹⁵ gives better classification rates than soft-margin linear SVM classifier in all cases. ³⁹⁶ The performance difference is more apparent for n = 7. These results support our ³⁹⁷ claims, suggesting that affine hulls can be better models for representing classes ³⁹⁸ in high-dimensional spaces when the number of samples is limited.

Methods	n = 7	n = 13	n = 20
LMC-AH	95.19 ±0.6	98.95 ±0.3	99.62 ±0.3
SVM	94.54±0.6	98.66±0.2	99.58±0.3

Table 2: Classification Rates (%) on the AR Face Database.

399 3.3. Experiments on the UCI Databases

In this group of experiments, we tested the kernelized versions of the methods 400 (quadratic programming formulations) on seven lower-dimensional datasets from 401 the UCI repository: Ionosphere, Iris, Letter Recognition (LR), Multiple Features 402 (MF) - pixel averages, Pima Indian Diabetes (PID), Wine, and Wisconsin Diag-403 nostic Breast Cancer (WDBC). The key parameters of these datasets are summa-404 rized in Table 3.3. We used the Gaussian kernels, and all design parameters are set 405 based on random partitions of datasets into training and test sets. OAO strategy 406 was used for multi-class problems. Reported classification rates given in Table 407 3.3 are computed by 5-fold cross-validation. Although being quite mixed, results 408 indicate that generalization performances of LMC-AH and ν -LMC-AH methods 409 compare favorably with SVM classifier whereas C-LMC-AH generally yields the 410 worst classification accuracy. 411

412 **4. Summary and Conclusion**

We investigated the idea of basing large margin classifiers on affine hulls of classes as an alternative to the SVM (convex hull large margin classifier). Given two affine hull models, their corresponding large margin classifier is easily determined by finding a closest pair of points on these two models and bisecting the

Databases	Number of Classes	Data Set Size	Dimensionality
Ionosphere	2	351	34
Iris	3	150	4
LR	26	20000	16
MF	10	2000	256
PID	2	768	8
Wine	3	178	13
WDBC	2	569	30

Table 3: Low-Dimensional Databases Selected from UCI Repository

Table 4: Classification Rates (%) on the UCI Datasets.

UCI	LMC-AH	ν-LMC-AH	C-LMC-AH	SVM
Ionosphere	93.7 ±2.9	93.7 ±2.9	93.4±2.3	92.9±3.2
Iris	94.7±2.9	94.7±2.9	95.3 ±3.8	95.3 ±3.8
LR	99.98 ±0.02	99.98 ±0.02	99.89±0.13	99.64±0.12
MF	98.4 ±0.4	98.4 ±0.4	97.8±0.3	98.0±0.4
PID	99.9 ±0.3	99.9 ±0.3	99.9 ±0.3	99.9 ±0.3
Wine	98.8 ±1.6	98.8 ±1.6	94.8±2.6	98.2±1.6
WDBC	96.0±2.5	96.0±2.5	94.9±3.0	97.6 ±0.7

displacement between them. We also investigated another formulation obtained 417 by revising the ν -SVM classifier. This formulation yields a separating hyperplane 418 with the same normal as in our first formulation, but the offset is not necessarily 419 the same. This suggests that for a fixed hyperplane normal w in a specific prob-420 lem, there may be principled procedures to determine the best offset b. To allow 421 soft margin solutions, we first reduce affine hulls to alleviate the effects of outliers 422 and then find the best separating hyperplanes between these reduced models. Such 423 classifiers can also be kernelized, and extension to the multi-class classification is 424 straightforward using any of the standard approaches such as OAO or OAR. 425

The experimental results provided useful insights on the potential application 426 areas of the proposed method. The proposed method is much more efficient than 427 SVM classifier in terms of classification accuracy and real-time performance (test-428 ing time) when the dimensionality of the sample space is high and affine hulls are 429 linearly separable (in this case solution is easily determined based on subspace es-430 timation which requires simple linear algebra whereas SVM formulation requires 431 solving a quadratic programming). For the low-dimensional databases generaliza-432 tion performances of the proposed methods compare favorably with SVM classi-433 fier but SVM is more efficient in terms of testing time. This is because of the 434 fact that all training data points contribute to the affine hull models (almost all 435 computed α_i coefficients are nonzero), thus the proposed quadratic optimization 436 solutions lack sparseness, and we need more computations to evaluate decision 437 functions. Nevertheless, some pruning techniques can be employed to overcome 438 this problem. 439

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