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Construction of Convex Hull Classifiers in High Dimensions

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Abstract

We propose an algorithm to approximate each class region by a small number of approximated convex hulls and to use these for classification. The classifier is one of non-kernel maximum margin classifiers. It keeps the maximum margin in the original feature space, unlike support vector machines with a kernel. The construction of an exact convex hull requires an exponential time in dimension, so we find an approximate convex hull (a polyhedron) instead, which is constructed in linear time in dimension. We also propose a model selection procedure to control the number of faces of convex hulls for avoiding over-fitting, in which a fast procedure is adopted to calculate an upper-bound of the leave-one-out error. In comparison with support vector machines, the proposed approach is shown to be comparable in performance but more natural in the extension to multi-class problems.

1 **1. Introduction**

2 Determining class regions directly in a feature space and classifying a
3 class-unknown sample to the class of which region is closest to the sample
4 seems a promising approach to classification. However, the efficacy of this
5 approach has not been established. In this paper, we address this issue,
6 specifically for a set of convex hulls as a class region.

7 Usually, class regions are determined indirectly by discriminant functions
8 or by an estimated decision boundary. Nevertheless, some classifiers are
9 connected to certain types of regions. For example, a linear support vector
10 machine (shortly, SVM) [1] is connected to the convex hulls of samples of
11 two classes [2] and the nearest neighbor classifier is connected to the Voronoi
12 diagram of samples [3]. Therefore, it is worth examining which type of re-
13 gions is most effective for a wide range of classification problems and how
14 such regions can be constructed. In this paper, we focus on a set of convex
15 hulls that include training samples of a class maximally. Then, we assign
16 a class label to a given test sample according to the distances of the sam-
17 ple to the estimated class regions. This approach [4] using convex hulls has
18 shown performance comparable with that of SVM in low-dimensional data.

19 However, it is computationally difficult to construct the exact convex hull in
20 high-dimensional data [5]. The algorithm by McBride *et al.* [6] also suffers
21 from the same type of dimensionality problem. In this paper, therefore, we
22 use a set of polyhedral convex sets that are constructed in a linear order of
23 dimension.

24 Zero training errors are achieved by using a sufficient number of convex
25 hulls in such a way that every training sample of a class is covered by at
26 least one convex hull and any other sample belonging to the other classes is
27 excluded, ensuring that no sample is shared by more than one class. Thus,
28 according to Occam's razor [7], we should choose the simplest classifier as
29 long as it attains the same degree of training error. In our case, we select
30 the smallest number of convex hulls with the smallest number of faces.

31 There are three problems to be solved. First, construction of the convex
32 hull of a given sample set is computationally difficult. The time and space
33 complexities are exponential in dimension in the worst case. Second, more
34 than one convex hull is generally needed to cover all training samples exhaus-
35 tively. Indeed, as is well known, if each class sample set is covered by a single
36 convex hull, then any pair of classes is linearly separable, and the reverse is
37 also true. Finally, when we use convex hulls for classification, the distance

38 between a point and the boundary of each convex hull must be measured.
39 However, the computational cost is quite high (e.g., see [8]).

40 In this paper, we first describe an algorithm for constructing approximate
41 convex hulls that can cope with these three problems in a reasonable way and
42 then we describe a model selection procedure for choosing simpler classifiers.
43 The algorithm is based on the prototype version introduced in [8].

44 A similar idea is realized in [9] in which the distance between a given point
45 and the convex hull of each class is used for class assignment. However, only
46 a single convex hull is assigned for each class, and thus a non-linear kernel
47 is necessary for solving non-linearly separable problems. Good selection of
48 a kernel and its parameters thus becomes problematic as well as the case of
49 SVM. The distance between a point and a convex hull is calculated by solving
50 an SVM optimization problem by assuming the point as a singleton set. Since
51 this calculation is made for each testing point, the time complexity is very
52 high when the training sample set is large. Cevikap *et al.* [10] discussed linear
53 manifolds spanned by nearest neighbors of a query sample and constructed
54 an affine hull (a convex hull is contained in it) for classification, but the
55 nonlinearization also relies on a kernel. In contrast to these studies, the
56 classifier developed here does not need a kernel.

2. Definitions of Convex Hull and Reflective Convex Hull

The convex hull $\text{conv}(S)$ of a given finite dataset $S = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is defined as the intersection of all convex sets containing S . Here, $\mathbf{x}_i \in R^m$ ($i = 1, \dots, n$) is a point in an m -dimensional Euclidean space. Since S is finite, $C = \text{conv}(S)$ is a polyhedron with at most n vertices.

By ∂C , we denote the boundary of C and divide it into q -faces according to the dimensions. For example, 0-faces are the vertices of C and $(m-1)$ -faces are the facets or hyper-planes. Let $V(C)$ be the set of vertices of C and let $F(C)$ be the set of facets of C . A convex hull of a finite set of S can be expressed by several ways. For example, the $\mathcal{V}$ -representation of C is given by $C = \{\mathbf{y} = \sum c_{\mathbf{x}} \mathbf{x} \mid \sum c_{\mathbf{x}} = 1, c_{\mathbf{x}} \geq 0, \mathbf{x} \in V(C)\}$. Another expression is the $\mathcal{H}$ -representation given by $C = \{\mathbf{y} \mid \langle \mathbf{w}, \mathbf{y} \rangle \leq c, \forall (\mathbf{w}, c) \in F(C)\}$, where $\langle \cdot, \cdot \rangle$ is the inner product and facet $(\mathbf{w}, c)$ is specified by a normal vector $\mathbf{w}$ ($\|\mathbf{w}\| = 1$) and a constant $c \in R$. We need both expressions to handle C efficiently in space complexity or in different goals. For example, an m -dimensional cube has $2m$ facets and 2^m vertices, and an m -dimensional simplex has $2m$ vertices and 2^m facets. For determining if a sample is included in C or not and for distance calculation to C , $\mathcal{H}$ -representation has an advantage of $\mathcal{V}$ -representation.

76 Unfortunately, we know that the number of facets can be of order $n^{\lfloor \frac{m}{2} \rfloor}$ [5].
 77 Therefore, we propose to use an approximated convex hull that has a rea-
 78 sonable number of facets. To do this, we consider another expression of a
 79 convex hull. We use *support functions* [11] for the new expression, which is
 80 similar to $\mathcal{H}$ -representation but needs an infinite number of half-spaces. A
 81 *support function* of a unit vector $\mathbf{w}$ ($\|\mathbf{w}\| = 1$) is given by

$$H(S, \mathbf{w}) \triangleq \sup\{\langle \mathbf{x}, \mathbf{w} \rangle | \mathbf{x} \in S\},$$

82 where “sup” denotes the supremum. With the set W_0 of all possible unit
 83 vectors, the convex hull C is defined as

$$C = \text{conv}(S, W_0) \triangleq \bigcap_{\mathbf{w} \in W_0} \{\mathbf{y} | \langle \mathbf{y}, \mathbf{w} \rangle \leq H(S, \mathbf{w})\}.$$

84 Here, $h(S, \mathbf{w}) = \{\mathbf{y} | \langle \mathbf{y}, \mathbf{w} \rangle = H(S, \mathbf{w})\}$ is called a *support plane*. The convex
 85 hull is an area that is surrounded by support planes $h(S, \mathbf{w})$ for all $\mathbf{w} \in W_0$.
 86 An example of the convex hull constructed by support planes is shown in
 87 Fig. 1. As an example of the support plane, $h(S, \mathbf{w})$ with angle θ is also
 88 shown.

89 We notice that a finite subset $W \subset W_0$ gives an approximate convex hull
 90 $\text{conv}(S, W)$ and thus a good selection of W derives a good approximation. Of
 91 course, instead of W , we can use the vectors corresponding to $F(C)$. Then

Figure 1: (a) The convex hull of a set S , including points $v_1, v_2, \dots, v_4$, represented by support planes. Only one support plane $h(S, \mathbf{w})$ is shown for a directional vector $\mathbf{w}$ with angle θ . As the value of θ increases, starting from this angle about $\theta = 85^\circ$, support planes will find edge h_{12} first and then vertex v_2 , edge h_{23} , and so on. The behavior is shown in (b) as a graph of support function $d = H(S, \mathbf{w})$ with the changing angle θ of $\mathbf{w}$.

the exact convex hull is obtained. However, as described before, the number of facets can grow exponentially in dimension. Therefore, we use a constant number of facets by letting $K = |W|$ be constant.

Next, let us consider separating a finite set S from another finite set T by the convex hull of S when they are linearly or non-linearly separated. A support plane h of S might locate both S and T in the same side of the two half-spaces separated by it. Apparently, such support planes are useless for separating S from T . For separation of S from T , all we need is *reflective*

100 *support planes*, which are support planes separating S from T perfectly or
 101 partly. A *reflective convex hull*, $C_r = \text{conv}(S, W_r)$, is the polyhedral convex
 102 set specified by the (infinite) set W_r of all unit vectors generating reflective
 103 support planes. Then the reflective convex hull C_r is formally defined by

$$C_r = \text{conv}(S, W_r) = \bigcap_{\mathbf{w} \in W_r} \{\mathbf{y} | \langle \mathbf{y}, \mathbf{w} \rangle \leq H(S, \mathbf{w})\}.$$

104 From the definition, $C = \text{conv}(S, W_0) \subseteq C_r = \text{conv}(S, W_r)$ since $W_r \subseteq W_0$.
 105 Intuitively speaking, the reflective convex hull of S is the polyhedral convex
 106 set of S whose faces reflect rays emitted from points in T . An example of
 107 the reflective convex hull is shown in Fig. 2. Note that usually a reflective
 108 convex hull, unlike the convex hull that encloses the samples of a class, is
 109 open on the side opposite the decision boundary.

110 We can also define the *margin* $M(S, T, \mathbf{w})$ between S and T in direction
 111 $\mathbf{w}$ as

$$M(S, T, \mathbf{w}) \triangleq -H(T, -\mathbf{w}) - H(S, \mathbf{w}).$$

112 Note that when S and T are linearly separable, there exists a sup-
 113 port plane specified by a unit vector $\mathbf{w}$ with positive margin $M(S, T, \mathbf{w}) =$
 114 $M(T, S, -\mathbf{w})$. Now a reflective support plane can be defined formally as a

Figure 2: Reflective convex hull of the set of positive samples S against the set of negative samples T . A few reflective support planes are shown.

Figure 3: Distances $D(\mathbf{x}, \partial conv(S, W))$ from $\mathbf{x}$ to an approximated convex hull $conv(S, W)$ with W are shown by solid lines and the exact distances $D(\mathbf{x}, \partial conv(S))$ to the exact convex hull are shown by dashed lines.

support plane $h_r(S, \mathbf{w})$ with $\mathbf{w}$ satisfying

$$H(T, \mathbf{w}) - H(S, \mathbf{w}) > 0.$$

The (signed) distance between a point $\mathbf{x}$ and the nearest boundary of a convex hull $conv(S, W_0)$ is given by

$$D(\mathbf{x}, \partial conv(S, W_0)) = \sup_{\mathbf{w} \in W_0} \{M(S, \{\mathbf{x}\}, \mathbf{w})\}.$$

Here D takes a positive value for $\mathbf{x}$ outside $conv(S, W_0)$ and a negative value for $\mathbf{x}$ strictly inside $conv(S, W_0)$. The closer $\mathbf{x}$ is to $\partial conv(S, W_0)$,

120 the smaller the absolute value is. Note that the general calculation problem
 121 of $D(\mathbf{x}, \partial conv(S, W_0))$ is known to be NP-hard [12, 13]. In our case, since we
 122 will use a finite set $W \subset W_r$, we can calculate the distance $D(\mathbf{x}, \partial conv(S, W))$
 123 in a linear order of $|W|$ as

$$D(\mathbf{x}, \partial conv(S, W)) = \max_{\mathbf{w} \in W} \{M(S, \{\mathbf{x}\}, \mathbf{w})\}. \quad (1)$$

124 An example is shown in Fig. 3. The method for calculating the distance
 125 $D(\mathbf{x}, \partial conv(S, W))$, where $conv(S, W)$ is the approximate convex hull speci-
 126 fied by W , is shown in Fig. 3. When $\mathbf{x}$ is outside $conv(S, W)$ such as $\mathbf{x}_1$ and
 127 $\mathbf{x}_2$, then the distance takes a positive value; otherwise, e.g., $\mathbf{x}_3$, the distance
 128 takes a negative value. It is noted that the distance calculation can be made
 129 by Eq.(1) regardless of whether the point is inside or outside $conv(S, W)$.
 130 The difference from the true distance becomes smaller if we use a large set
 131 of W . For example, the nearest point of $\mathbf{x}_1$ on $\partial conv(S, W)$ is $\mathbf{p}$, but the
 132 distance calculated by (1) is the distance to the support plane h_1 .

133 3. Approximation of a class region by reflective convex hulls

134 In this section, we introduce an algorithm to find a set of approximated
 135 reflective convex hulls for a class.

136 3.1. Algorithm

137 The following algorithm is applied class by class.

- 138 1. Let S be the positive sample set of a target class and T be the negative
139 sample set of other classes. Let $\mathcal{C} = W = \emptyset$. Let L be an upper bound
140 of the number of convex hulls and K be the number of normal vectors,
141 that is, the number of facets of a convex hull.
- 142 2. Find random K pairs of $\mathbf{x}$ ($\in S$) and $\mathbf{y}$ ($\in T$) and put $\mathbf{w} = \frac{\mathbf{y}-\mathbf{x}}{\|\mathbf{y}-\mathbf{x}\|}$ in
143 set W .
- 144 3. Repeat L times the following steps 4–5.
- 145 4. Let $U = \emptyset$. According to a random presentation order of positive
146 samples, add positive samples $\mathbf{x}$ to U as long as $\text{conv}(U \cup \{\mathbf{x}\}, W) \cap T =$
147 $\emptyset$.
- 148 5. Add the obtained $\text{conv}(U, W)$ into $\mathcal{C}$, unless it is already in $\mathcal{C}$.
- 149 6. Select a subset of $\mathcal{C}$ by a greedy set cover procedure for all positive
150 samples. That is, the largest member of $\mathcal{C}$ is chosen first and then the
151 member including the largest number of uncovered samples is chosen,
152 and so on.

153 By this procedure, we have at most L approximated convex hulls that
154 include samples of one class only. It should be noted that each convex hull

155 includes the positive samples maximally in Step 4.

156 Let us analyze the time complexity first. The dominant step is Step
157 4 in which we add a positive sample $\mathbf{x} \in S$ to the current subset U in
158 order to expand the previous convex hull to $\text{conv}(U \cup \{\mathbf{x}\}, W)$. This needs
159 $O(K)$ steps. Then we check if this convex hull is still exclusive, that is, if it
160 does not include any negative sample $\mathbf{y} \in T$. To do this, we need $O(Kn^-)$
161 steps for n^- negative samples ($n^- = |T|$). Since we need to scan every
162 positive sample, $O(Kn^+n^-)$ is necessary in Step 4 to obtain one exclusive
163 and maximal convex hull for n^+ positive samples ($n^+ = |S|$). In Step 3,
164 we repeat these procedures L times, so that the total order is $O(LKn^+n^-)$.
165 Here the time complexity with respect to dimensionality m is omitted, but
166 it is linear because we can obtain all necessary values by the inner product
167 between two vectors in an m -dimensional space. Regarding L as a constant
168 and regarding n^+ and n^- as the same complexity as the total sample number
169 n , we have $O(Kn^2m)$. It is also noted that the complexity to measure the
170 distance of a query sample to one convex hull with K facets is $O(Km)$. In
171 summary, this algorithm needs $O(Kn^2m)$ for training and $O(Km)$ for testing.
172 Since the worst-case complexity of SVM procedure with p support vectors is
173 $O(n^3m)$ ($O(nmp)$ with SMO solver) for training and $O(mp)$ for testing [14],

174 the proposed method is comparable with SVM.

175 The space complexity is the memory amount required to hold all the
176 convex hulls. It is $O(LK + mK)$, because one convex hull is expressed by
177 K values to specify the distances from the origin in K directions, and each
178 direction is specified by an m -dimensional vector.

179 A controllable nature of complexity is a characteristic of the proposed
180 algorithm. By decreasing the value of K we can reduce the time and space
181 complexities at the expense of approximation precision to the exact convex
182 hull. As will be discussed later, approaching to the exact convex hull is
183 not necessarily recommended. We need to choose the best model in sample-
184 limited situations.

185 One problem may arise when noisy samples are included in the training
186 data. It is easily understood that only one negative sample greatly breaks
187 down a convex hull covering many positive samples if it appears inside the
188 convex hull. Any kind of region-based algorithm shares the same problem. In
189 the proposed method, we cope with this problem by a simple technique. We
190 carry out the above algorithm twice over all classes. The first one is carried
191 out in order to find noisy samples and the second one is carried out in order
192 to find class regions. After the first round, we regard the samples that are

193 included in only small convex hulls as *noisy samples* and remove them for the
 194 second round. The second round is carried out without such noisy samples.
 195 To distinguish noisy samples from normal samples, we use a threshold α . If
 196 a convex hull is smaller than α in the *size*, that is, if the ratio of the number
 197 of samples included in the convex hull to the number of positive samples is
 198 less than α ($= 1\%$ in the following experiments), all samples included in it
 199 are judged as noisy.

200 To emphasize the number of facets, we call an approximated reflective
 201 convex hull with K directional unit vectors a *K-directional approximated*
 202 *reflective convex hull* (in short, *K-ARCH*). A convex hull might have less
 203 than K facets, but we use this terminology whenever $|W| = K$. The number
 204 of vectors K is controllable, so the (time) complexity can be decreased if
 205 we use *K-ARCHs* instead of the exact (reflective) convex hulls. Roughly
 206 speaking, as K increases, the corresponding *K-ARCH* approaches the true
 207 reflective convex hull. Class assignment of an unknown sample is carried out
 208 on the basis of distance to the nearest boundary of *K-ARCHs*.

209 Extension to multi-class classification is straightforward. Changing the
 210 role of positive samples and negative samples class by class, we obtain c sets
 211 of L *K-ARCHs* for c classes. Since the classification of a query sample is

Figure 4: Approximated class regions by K -directional reflective convex hulls ($K = 50$). The dataset is 3-class 2-dimensional K-L expanded *iris* dataset. The decision boundary is also shown.

Figure 5: Effective vertices necessary for LOO upper bound. The circled vertices are not necessary.

212 made by the closest convex hull, the time complexity is $O(cLKm)$.

213 An example is shown in Fig. 4. Figure 4 shows the approximate class
 214 regions for 2-dimensional *iris* data consisting of two principal components.
 215 The original data is taken from a database [15]. The value of K is 50. There
 216 are five K -ARCHs covering all samples. In Fig. 4, we can confirm that 1) the
 217 approximated convex hulls are larger than the corresponding exact convex
 218 hulls, 2) the convex hulls are often unbounded, and 3) the decision boundary
 219 is taken to keep the maximum margin locally.

220 4. Model Selection

221 In reference [8], we used a fixed value of K for each dataset. It is expected
222 to raise the performance of the proposed K -ARCH algorithm by choosing the
223 optimal value of K . Unfortunately, it is not so easy to solve this optimiza-
224 tion problem because the performance evaluation is theoretically difficult.
225 Therefore, in this paper we propose a model selection procedure to find a
226 suboptimal value of K . In the following, we will show the efficacy of this
227 model selection procedure in the process speed and in the classification per-
228 formance of the resultant classifier.

229 4.1. Estimation of generalization error

230 As a measure of testing error, we use the LOO (Leave-One-Out) error
231 rate. Leaving one sample out, we construct a classifier from the remaining
232 samples to test the left-out sample, and continue this procedure to estimate
233 the classification performance. As is well known, the LOO rate is almost
234 unbiased (Luntz and Brailovsky Theorem [16]), but it requires the building
235 of n classifiers for n samples. Hence, we consider an upper bound of LOO
236 that can be easily obtained without reconstruction of classifiers. Let ϵ_{LOO}
237 be the LOO error rate, V be the set of vertices of all convex hulls and Z be

238 the set of samples that are outside all convex hulls. If a single convex hull is
 239 taken in each class, ϵ_{LOO} is bounded by the sum of $|V|$ and $|Z|$ divided by n ,
 240 because removal of samples inside a convex hull does not affect the classifier
 241 design. However, in the case of more than one convex hull being taken in a
 242 class, a vertex of one convex hull can be covered by another. Figure 5 shows
 243 such a case. Such vertices can be safely ignored when counting for possible
 244 errors. We call vertices “*effective vertices*” if they are not covered by the
 245 other convex hulls. Let V_e be the set of effective vertices on the boundary
 246 of the approximated class region as the union of the convex hulls. Then we
 247 have an upper bound by

$$\epsilon_{LOO} \leq \frac{|V_e| + |Z|}{n}. \quad (2)$$

248 Here, in the numerator we count the number of samples that can change the
 249 classifier if one of them is left out of training.

250 We use the value on the right-hand side of (2). Obviously, there is a trade-
 251 off between $|V_e|$ and $|Z|$. The greater is the number of convex hulls, the larger
 252 is the size of $|V_e|$, while the smaller is the number of samples that are not
 253 included in any convex hull, the smaller is the size of $|Z|$. In addition, a large
 254 number of K increases the number of approximate convex hulls because a
 255 more acute angle is allowed in a convex hull with a large variety of direction

Table 1: The statistics of datasets.

Dataset	#classes	#attributes	#samples
balance-scale	3	4	625
diabetes	2	8	768
ecoli	8	8	336
glass	6	10	214
heart-statlog	2	13	270
ionosphere	2	34	351
iris	3	4	150
sonar	2	60	208
wine	3	13	178

256 vectors. We therefore use the right-hand side term of (2) as our criterion.

257 4.2. Experiments

258 To construct W of unit vectors, we used n_p positive samples and $n_p(c-1)$
259 negative samples, so that $K = n_p^2(c-1)$ unit vectors were chosen randomly,
260 where c is the number of classes. In the following, we changed the value of
261 n_p in $[1, 50]$, thus, K in $[c-1, 2500(c-1)]$.

262 We used 9 datasets taken from the UCI machine learning repository [15].
 263 In Table 1, the number of classes, the number of attributes (the dimension-
 264 ality of the feature space), and the number of samples are shown. It is noted
 265 that in some of them the dimensionality m is too large (34 in `ionosphere`
 266 and 60 in `sonar`) to find the exact convex hull of these sizes of the train-
 267 ing sample set. We increased the value of K until K reached the maximum
 268 value. For each value of K , we repeated the algorithm 10 times to reduce
 269 the effect of other random factors. Among 10 trials with a fixed value of K ,
 270 we chose the best case in which the LOO estimate (2) took the minimum
 271 value. The recognition rate was estimated by 10-fold cross validation. The
 272 loop number L of the algorithm (Steps 4 and 5) was set to $L = 20$. That is,
 273 the number of convex hulls was limited to 20 in each class. The K-ARCH
 274 algorithm was implemented in `C++` and SVMTorch algorithm [17] was used
 275 for SVMs. Both algorithms were executed on a PC with Intel Core 2 Quad
 276 Q8200 2.33GHz CPU and 3GB RAM.

277 4.3. Results

278 We compared the proposed K -ARCH algorithm with an SVM in which an
 279 RBF (Radial Basis Function) kernel with the default values of parameters
 280 (standard deviation $\sigma = 10.0$ and soft margin parameter $\gamma = 100.0$) was

Table 2: Recognition rates of SVM and K^* -ARCH where K^* is optimal in our model selection criterion and $|V_e|$ is the number of effective vertices.

Dataset	Classifier		#SV or $ V_e $	
	SVM	K^* -ARCH (K^*)	SVM	K^* -ARCH
balance-scale	93.2	90.3 (98)	255.0	200.1
diabetes	64.1	75.0 (2401)	1310.0	483.3
ecoli	79.8	83.0 (252)	385.7	144.6
glass	66.3	63.6 (180)	336.9	138.0
heart-statlog	59.3	63.7 (2401)	479.4	201.8
ionosphere	94.0	90.9 (196)	132.5	331.2
iris	98.0	95.3 (18)	54.0	20.2
sonar	77.4	80.4 (121)	214.0	429.3
wine	72.5	87.0 (3200)	447.2	67.7
average	78.3	81.0	401.6	224.0

(a) balance-scale

(b) ecoli

(c) ionosphere

(d) sonar

Figure 6: Error rate of K -ARCH as the number K of facets increases on four datasets. The three curves show the estimated LOO error (right-hand term of Ineq. (2)), the training error and testing error. The circled testing-error corresponds to the optimal value of K chosen by the minimum LOO error.

281 used [17]. For the K -ARCH algorithm, we used K^* -ARCHs for classification,
 282 where K^* is the value of K attaining the minimum LOO upper bound of (2).
 283 The results are shown in Table 2.

284 In Table 2, it is noted that K^* -ARCH outperforms SVM in more than
 285 half of the cases (5/9). Note that three problems of the remaining 4/9 cases
 286 are all easier or well-separated class problems. Indeed, in these three prob-
 287 lems (**balance-scale**, **iris** and **ionosphere**), the recognition rates are over
 288 90%. This might mean that K -ARCH tends to generate a slightly more com-
 289 plicated decision boundary compared with that of SVM. Note that a large
 290 number K^* is chosen for more difficult problems. This implies that K -ARCH
 291 formed a complex boundary. Note also that the number of (effective) vertices
 292 is often less than the number of support vectors. This means that K^* -ARCH
 293 often has higher sparsity than SVM.

294 We can see the details in some datasets in Fig. 6. From Fig. 6, we see that
 295 after reaching the optimal value K^* , the testing error is no longer significantly
 296 reduced. In general, a model selection criterion is expected to form a valley
 297 to simulate the testing error, but this is not the case. This implies that
 298 K -ARCH does not change its decision boundary even if the model becomes
 299 more complicated than necessary. We can interpret this phenomenon as

300 follows. Even if the facets increase more than necessary, they are limited in
 301 the location opposite to the decision boundary. Such a situation is shown
 302 in Fig 7. As can be seen in Fig 7, such a redundant non-reflective support
 303 plane can be generated by some noisy samples. In this sense, we have to be
 304 careful about the value of α used for the judgment of noisy samples. The
 305 curve of the testing error fluctuates a little as K increases. This is because
 306 small convex hulls with very acute angles can be generated when K is large.

Figure 7: Redundant faces generated by noisy vectors.

307

308 5. Comparison with SVM

309 It is worth comparing the proposed K -ARCH algorithm with SVM to
 310 make clear the advantages and disadvantages of K -ARCH algorithm. They
 311 are summarized in Table 3.

Table 3: Comparison between the proposed K -ARCH and SVM. In below, n is the number of training samples and m is the dimensionality.

Evaluation item	Classifier	
	SVM	K -ARCH
Maximization of margin	in the kernel space	in the original space
Adaptation to nonlinearity	kernel	multiple K -ARCHs
Extension to multi-class	one-against-other	natural
Classification performance	high	high
Training time	medium ($O(nm) - O(n^3m)$)	slow ($O(n^2m)$)
Testing time	fast ($O(m)$)	fast ($O(m)$)

312 The largest difference is the space where the margin is taken. An SVM
 313 uses a kernel to solve non-linearly separable problems. It is guaranteed to
 314 keep the maximum (linear) margin in the mapped space with the kernel, but
 315 the (non-linear) margin in the original feature space is not always maximized.
 316 On the other hand, the K -ARCH algorithm keeps (locally linear) maximum
 317 margins in the original space, though the margins are measured between
 318 closest pairs of K -ARCHs of two different classes. As a result, in some cases,
 319 the latter finds a better decision boundary than the former as shown in Fig. 8.
 320 Note that the margin is not maximized by SVM in Fig. 8.

Table 4: Execution time of K-ARCH and SVM in training and testing phases. The time (seconds) is the results of 10 trials of the same task.

Dataset	K-ARCH		SVM	
	Training	Testing	Training	Testing
balance	30.40	0.04	1.59	0.07
diabetes	25.03	0.02	1.71	0.22
ecoli	29.36	0.20	0.84	0.11
glass	7.83	0.06	0.95	0.05
heart	3.07	0.01	0.44	0.10
ionos	6.36	0.02	0.44	0.11
iris	1.38	0.00	0.41	0.05
sonar	2.73	0.01	0.50	0.10
wine	2.32	0.02	0.56	0.06

Figure 8: Decision boundaries by SVM with RBF and K -ARCH algorithms. Samples of class 1 are denoted by circles and samples of class 2 by crosses.

321 The K -ARCH algorithm is also advantageous to SVM in extension to
322 multi-class problems. Typically one-against-other strategy is adopted to use
323 two-class SVM for multi-class problems, though some multi-class SVMs have
324 been studied (e.g., see [18]). It is known, however, that such an extension
325 does not work in some cases [19]. On the contrary, K -ARCH algorithm can
326 naturally deal with multi-class problems because it finds a set of K -ARCHs
327 in each class and classify a sample to the class of the closest K -ARCH.

328 Note that we can see the example of Fig. 8 as a 3-class problem by re-
329 garding two clusters of one class (denoted by circles) as two different classes.
330 Then the problem of inappropriate decision boundary of SVM still remains
331 because of the one-against-other strategy.

332 In the usage of SVMs, the choice of a kernel and its parameters can be
333 problematic. In this respect, K -ARCH is advantageous because the critical
334 parameter is only the number K of facets.

335 In time complexity, SVM is superior to K -ARCH algorithm, especially
336 in the training phase. In the testing phase, they are almost the same. The
337 execution time on the nine datasets is shown in Table 4, from which we can
338 confirm that K -ARCH is comparable to SVM and sometimes even faster than
339 SVM in the testing time. It is also noted that parallelization of K -ARCH
340 algorithm is easy due to its simple procedure.

341 6. Discussion

342 It is well known, in the case of two-class problems, that the hyper-plane
343 of linear SVM is equivalent to the bisector between the closest points on
344 the boundaries of the convex hulls, each of which encloses the training sam-
345 ples of one class, if the training sample sets are linearly separable [2]. Re-
346 cently a similar relationship was reported even for soft-margin SVM using
347 *reduced convex hulls* [20, 21]. Our classifier is almost identical to SVM when
348 two classes are linearly separable (e.g., see Fig 4) in which one convex hull
349 is sufficient for one class. An advantage of our approach is the capability of

350 handling non-linearly separable cases in which more than one convex hull is
 351 required for one class. Even in such cases, our K -ARCH algorithm maximizes
 352 the margin locally with a relatively smooth decision boundary (see Fig. 8).
 353 In this respect, our classifier is one of the maximum margin classifiers.

354 One drawback of the proposed algorithm is that it includes many ran-
 355 dom factors producing different classifiers. The direction vectors in W are
 356 randomly chosen and the set of K -ARCHs has a randomness because of the
 357 random algorithm. This randomness does not affect much to the resultant
 358 classifier, but needs an appropriate control to reduce its bad effect.

359 7. Conclusion

360 In this paper, a model selection procedure for a family of polyhedron clas-
 361 sifiers has been proposed. The family is based on polyhedral class regions
 362 close to the convex hulls of some parts of training samples. In the polyhedron
 363 family here, complexity mainly comes from the number of facets and vertices
 364 of each polyhedral region. The selection procedure employs an upper bound
 365 of the LOO error for time reduction and showed satisfactory results in se-
 366 lecting a good model. However, more sophisticated, hopefully theoretically
 367 established, procedure to choose the optimal value of K is desired. Another

direction of study is to find another criterion instead of margin maximization.
Once nonlinear margins are taken into consideration, it is not easy even to
define the nonlinear margins appropriately. As long as considering the ge-
ometric margin between training samples of two classes, the largest margin
is kept by the nearest neighbor rule. However, it is not the best classifier
when only a limited number of samples is given for training. The authors
are currently considering a way to widen the margin taken by the proposed
algorithm. The result would be helpful for seeking a better criterion.

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References

- [1] V. N. Vapnik, The nature of statistical learning theory, Springer, 1996.
- [2] D. Zhou, B. Xiao, H. Zhou, R. Dai, Global geometry of svm classifiers,
Institute of Automation, Chinese Academy of Sciences, Technical report,
AI Lab.

- 384 [3] B. V. Dasarathy, Nearest neighbor(NN) norms: NN pattern classifica-
385 tion techniques, IEEE Computer Society Press, Los Alamitos, 1991.
- 386 [4] M. Kudo, M. Shimbo, Approximation of class region by convex hulls,
387 Technical report of IEICE. PRMU 100 (507) (2000) 1–6, (In Japanese).
- 388 [5] E. Jeff, New lower bounds for convex hull problems in odd dimensions,
389 SIAM Journal of Computing 28 (4) (1999) 1198–1214.
- 390 [6] B. McBride, G. L. Peterson, Blind data classification using hyper-
391 dimensional convex polytopes, in: Proceedings of the 17th International
392 FLAIRS Conference, 2004, pp. 520–525.
- 393 [7] A. Blumer, A. Ehrenfeucht, D. Haussler, W. M.K., Occam’s razor, Read-
394 ings in machine learning (1990) 201–204.
- 395 [8] M. Kudo, I. Takigawa, A. Nakamura, Classification by reflective con-
396 vex hulls, Proceedings of the 19th International Conference on Pattern
397 Recognition (ICPR2008), Tampa, Florida, USA.
- 398 [9] G. I. Nalbantov, P. J. F. Groenen, J. C. Bioch, Nearest convex hull
399 classification, Econometric Institute Report.
- 400 [10] H. Cevikalp, D. Larlus, M. Neamtu, B. Triggs, F. Jurie, Manifold based

- 401 local classifiers: Linear and nonlinear approaches, *Journal of Signal Pro-*
 402 *cessing Systems* (2008) 1–13.
- 403 [11] P. K. Ghosh, K. V. Kumar, Support function representation of convex
 404 bodies, its application in geometric computing, and some related rep-
 405 resentations, *Computer Vision and Image Understanding* 72 (3) (1998)
 406 379–403.
- 407 [12] O. L. Mangasarian, Polyhedral boundary projection, *SIAM Journal on*
 408 *Optimization*, 9 (4) (1999) 1128–1134.
- 409 [13] P. Gritzmann, V. Klee, Computational complexity of inner and outer
 410 j -radii of polytopes in finite-dimensional normed spaces, *Mathematical*
 411 *Programming* 59 (1) (1993) 163–213.
- 412 [14] D. Decoste, B. Schölkopf, Training invariant support vector machines,
 413 *Machine Learning* 46 (1) (2002) 161–190.
- 414 [15] A. Asuncion, D. Newman, *UCI machine learning repository* (2007).
- 415 [16] A. Luntz, V. Brailovsky, On estimation of characters obtained in statis-
 416 tical procedure of recognition, *Technicheskaya Kibernetika* 3 (6).

- 417 [17] R. Collobert, S. Bengio, SVMTorch: support vector machines for large-
418 scale regression problems, *Journal of Machine Learning Research* 1
419 (2001) 143–160.
- 420 [18] K. Crammer, Y. Singer, On the algorithmic implementation of multi-
421 class kernel-based vector machines, *The Journal of Machine Learning*
422 *Research* 2 (2002) 265–292.
- 423 [19] Y. Lee, Y. Lin, G. Wahba, Multicategory support vector machines, the-
424 ory, and application to the classification of microarray data and satellite
425 radiance data, *Journal of the American Statistical Association* 99 (2004)
426 67–81.
- 427 [20] S. Theodoridis, M. Mavroforakis, Reduced convex hulls: A geometric
428 approach to support vector machines, *IEEE Signal Processing Magazine*
429 24 (3) (2007) 119–122.
- 430 [21] B. Goodrich, D. Albrecht, P. Tischer, Algorithms for the computation of
431 reduced convex hulls, *AI 2009: Advances in Artificial Intelligence* (2009)
432 230–239.