Geometrical Complexity of Classification Problems

Tin Kam Ho

Bell Laboratories, Lucent Technologies

Nov 20, 2003

Abstract

Despite encouraging recent progresses in ensemble approaches, classification methods seem to have reached a plateau in development. Further advances depend on a better understanding of geometrical and topological characteristics of point sets in high-dimensional spaces, the preservation of such characteristics under feature transformations and sampling processes, and their interaction with geometrical models used in classifiers. We discuss an attempt to measure such properties from data sets and relate them to classifier accuracies.

1 Introduction

Advances in ensemble learning have produced a significant rise in classification accuracy from those achieved when only monolithic classifiers are known. However, after the past decade of development, most methods seems to have reached maturity, so that no significant improvements are expected to result from incremental modifications. Often, for a certain benchmark problem, one can see many methods in close rivalry, producing more or less the same level of accuracy. Although continuous attempts are being made on interpreting existing techniques, testing known methods on new applications, or mix-matching different strategies, no revolutionary breakthrough appears to be in sight. It almost seems that a plateau has been reached in classification research, and questions like these begin to linger in our minds: 1) have we exhausted what can be learned from a given set of data? 2) have we reached the end of classifier development? and 3) what else can be done?

Obviously we have not solved all the classification problem in the world – new applications bring new challenges, many of which are still beyond reach. But do these require fundamental breakthroughs in classification research? Or are these "merely engineering problems" that will eventually be solved with more machine power, or more likely, more human power to find better feature extractors and fine tune the classifier parameters?

To answer these questions we need to know whether there exists a limit in the knowledge that can be derived from a dataset, and where this limit lies. That is, are the classes intrinsically distinguishable? And, to what extent are they distinguishable? These questions are about the intrinsic complexity of a classification problem, and the match between a classifier's capability to a problem's intrinsic complexity. We believe that an understanding of these is the only way to find out

about the current standing of classification research, and to obtain insights to guide further developments. In this lecture we describe our recent efforts along these lines.

2 Sources of difficulty in classification

We begin with an analysis of what makes classification difficult. Difficulties in classification can be traced to three sources: 1) class ambiguity, 2) boundary complexity, and 3) sample sparsity and feature space dimensionality.

Class ambiguity

Class ambiguity refers to the situation when there are cases in a classification problem whose classes cannot be distinguished using the given features by *any* classification algorithm. It is often a consequence of the problem formulation. Classes can be ambiguous for two reasons. It could be that the class concepts are poorly defined and intrinsically inseparable. An example for this is that the shapes of the lower case letter "l" and the numeral "1" are the same in many fonts (Figure 1(a)). Such ambiguity cannot be resolved at the classifier level, a solution has to involve the application context.

There is another situation where the classes are well defined, but the chosen features are not sufficient for indicating such differences (Figure 1(b)). Again, there is no remedy at the classifier level. The samples need to be represented by other features that are more informative about the classes. Class ambiguity can occur for only some input cases. Problems where the classes are ambiguous for at least some cases are said to have nonzero Bayes error, which sets a bound on the lowest achievable error rate.

(a) The shapes of the lower case letter "l" and the numeral "1" are the same in many fonts. They cannot be distinguished by shape alone. Which class a sample belongs to depends on context.

(b) There may be sufficient features for classifying the shells by shape, but not for classifying by the time of the day when they were collected, or by which hand they were picked up.

Fig. 1. Ambiguous classes due to (a) class definition; (b) insufficient features.

Boundary complexity

Among the three sources of difficulties, boundary complexity is closest to the notion of the intrinsic difficulty of a classification problem. Here we choose the class boundary to be the simplest (of minimum measure in the feature space) decision boundary that minimizes Bayes error. With a complete sample, the class boundary can be characterized by its Kolmogorov complexity [10] [12]. A class boundary is complex if it takes a long algorithm to describe, possibly including a listing of all the points together with their class labels. This aspect of difficulty is due to the nature of the problem and is unrelated to the sampling process. Also, even if the classes are well defined, their boundaries may still be complex (Figure 2). An example is a random labeling of a set of uniformly distributed points, where each point has a definite label, but points of the same label are scattered over the entire space with no obvious regularity. The only way to describe the classes may be an explicit listing of the positions of the points with the same label.
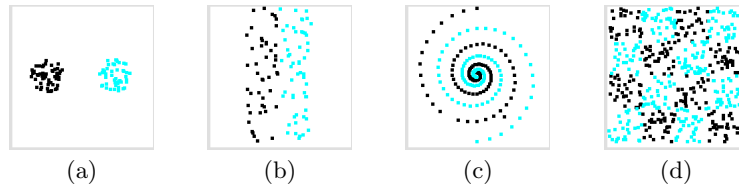

(a)   (b)   (c)   (d)

Fig. 2. Classification problems of different geometrical complexity: (a) linearly separable problem with wide margins and compact classes; (b) linearly separable problem with narrow margins and extended classes; (c) problem with nonlinear class boundary; (d) heavily interleaved classes following a checker board layout.

Kolmogorov complexity describes the absolute amount of information in a dataset, and is known to be algorithmically incomputable [13]. Thus we resort to relative measures that depend on the chosen descriptors. Specifically, we can choose a number of geometrical descriptors that we believe to be relevant in the context of classification. We then describe the regularities and irregularities contained in the dataset in terms of the chosen geometrical primitives. We refer to these descriptors as measures of the *geometrical complexity* of a dataset. This would be sufficient for pattern recognition where most classifiers can also be characterized by geometrical descriptions of their decision regions.

Sample sparsity and feature space dimensionality

An incomplete or sparse sample adds another layer of difficulty to a discrimination problem, since how an unseen point should share the class labels of the training samples in its vicinity depends on specific generalization rules. Without sufficient samples to constrain a classifier's generalization mechanism, the decisions on the unseen samples can be largely arbitrary. The difficulty is especially

severe in high dimensional spaces where the classifier's decision region, or the generalization rule, can vary with a large degree of freedom. The difficulty of working with sparse samples in high dimensional spaces has been addressed by many other researchers [3] [15] [17].

In practical applications, often a problem becomes difficult because of a mixture of boundary complexity and sample sparsity effects. Sampling density is more critical for an intrinsically complex problem (e.g. one with many isolated subclasses) than an intrinsically simple problem (e.g. a linearly separable problem with wide margins), since longer boundaries need more samples to specify. If the sample is too sparse, an intrinsically complex problem may appear deceptively simple, like when representative samples are missing from many isolated subclasses. However, it can also happen that an intrinsically simple problem may appear deceptively complex. An example is a linearly separable problem that appears to have a nonlinear boundary when represented by a sparse training set. Thus, in lack of a complete sample, measures of problem complexity have to be qualified by the representativeness of the training set. We will refer to the boundary complexity computed from a fixed training set as *apparent* complexity.

With a given, fixed training set, there is little one can do to find out how close the apparent complexity is to the "true" complexity. But this does not prevent one to infer about the true complexity with some confidence, if some weak assumptions on the geometry of the class distributions can be made. Here we distinguish such assumptions from the more commonly adopted assumptions on the functional form of class distributions (e.g. Gaussians) which can be overly strong. By weak assumptions on class geometry, we mean those properties such as local compactness of the point sets, local continuity and piecewise linearity of the boundaries, all to be constrained by parameters specifying a small neighborhood.

We believe that even with very conservative assumptions on the geometrical regularity, better uses of limited training samples can be made, and more useful error estimates can be obtained than those derived from purely combinatorical arguments emphasizing the worst cases. One should be able do these without invoking strong assumptions on the functional form of the distributions.

3   Characterization of Geometrical Complexity

Among the different sources of classification difficulty, the geometrical complexity of class boundaries is probably most ready for detailed investigation. Thus in this lecture we focus on effective ways for characterizing the geometrical complexity of classification problems.

We assume that each problem is represented by a fixed set of training data consisting of points in a d-dimensional real space $\mathbf{R}^d$, and that each training point is associated with a class label. Furthermore, we assume that we have a sparse sample, i.e., there are unseen points from the same source that follow the same (unknown) probability distribution but are unavailable during classifier design. The finite and sparse sample limits our knowledge about the boundary complexity, thus we are addressing only the apparent geometrical complexity of

a problem based on a given training set. We discuss only two-class problems, because most of the measures we use are defined only for two-class discrimination. An n-class problem produces a matrix of two-class values for each chosen measure. To describe n-class problems, one needs a way to summarize such matrices. There are many ways to do so, possibly involving cost matrices. We acknowledge that the summary by itself is a nontrivial problem.

One natural measure of a problem's difficulty is the error rate of a chosen classifier. However, since our eventual goal is to study behavior of different classifiers, we want to find other measures that are less dependent on classifier choices. Moreover, measures other than classifier error rates may give hints on how the errors arise, which could lead to improvements in classifier design, and give guidance on collection of additional samples.

Early in our investigations it became clear that there are multiple aspects of a problem's complexity that cannot be easily described by a single known measure. Furthermore, while it is easy to construct different measures for various characteristics of a dataset, an arbitrary measure may not necessarily correlate well with any complexity scale of a reasonable notion. Such considerations led us to an evaluation of many different types of measures under a control study, where each measure is computed for a wide range of problems of known levels of difficulty.

We constructed a feature (measurement) space for classification problems, where each feature dimension is a specific complexity measure, and each problem, defined by a labeled training set, is represented by a point in this space. Most of the individual measures came from the literature of both supervised and unsupervised learning, with a few others defined by us. All measures are normalized as far as possible for comparability across problems. The measures we investigated can be divided into several categories:

1. **Measures of overlaps in feaure values from different classes.** These measures focus on the effectiveness of a single feature dimension in separating the classes, or the composite effects of a number of dimensions. They examine the range and spread of values in the dataset w.r.t. each feature, and check for overlaps among different classes (Table 1).
2. **Measures of separability of classes.** These measures evaluate to what extent two classes are separable by examining the existence and shape of the class boundary. The contributions of different feature dimensions are summarized in a distance metric rather than evaluated individually (Table 2).
3. **Measures of geometry, topology, and density of manifolds.** These measures give indirect characterizations of class separability. They assume that a point class is made up of single or multiple manifolds which form the support of the probability distribution of the given class. The shape, position, and interconnectedness of these manifolds give hints on how well two classes are separated, but they do not describe separability by design (Table 3).

F1	maximum Fisher's discriminant ratio	
	Fisher's discriminant ratio for one feature dimension is defined as: $$f = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2}$$ where μ_1, μ_2, σ_1^2, σ_2^2 are the means and variances of the two classes respectively, in that feature dimension. We compute f for each feature and take the maximum as measure F1.	For a multi-dimensional problem, not necessarily all features have to contribute to class discrimination. As long as there exists one discriminating feature, the problem is easy. Therefore the maximum f over all feature dimensions is the one most relevant to class separability.
F2	volume of overlap region	
	Let the maximum and minimum values of each feature f_i in class c_j be $max(f_i, c_j)$ and $min(f_i, c_j)$, then the overlap measure F2 is defined to be $$F2 = \prod_i \frac{\text{MINMAX}_i - \text{MAXMIN}_i}{\text{MAXMAX}_i - \text{MINMIN}_i}$$ where $i = 1, ..., d$ for a d-dimensional problem, and $\text{MINMAX}_i = \text{MIN}(max(f_i, c_1), max(f_i, c_2))$ $\text{MAXMIN}_i = \text{MAX}(min(f_i, c_1), min(f_i, c_2))$ $\text{MAXMAX}_i = \text{MAX}(max(f_i, c_1), max(f_i, c_2))$ $\text{MINMIN}_i = \text{MIN}(min(f_i, c_1), min(f_i, c_2))$	F2 measures the amount of overlap of the bounding boxes of two classes. It is a product of the per-feature ratio of the size of the overlapping region over the size of total occupied region by the two classes. The volume is zero as long as there is at least one dimension in which the value ranges of the two classes are distinct.
F3	maximum (individual) feature efficiency	
	In a procedure that progressively removes unambiguous points falling outside the overlapping region in each chosen dimension [4], the *efficiency* of each feature is defined as the fraction of all remaining points separable by that feature. To represent the contribution of the feature most useful in this sense, we use the *maximum feature efficiency* (largest fraction of points distinguishable with only one feature) as a measure (F3).	This measure considers only separating hyperplanes perpendicular to the feature axes. Therefore, even for a linearly separable problem, F3 may be less than 1 if the optimal separating hyperplane happens to be oblique.

Table 1. Measures of overlaps in feaure values from different classes.

Many of these measures have been used before, in isolation, to characterize classification problems. But there have been little serious studies on their effectiveness. Some are known to be good only for certain types of datasets. For instance, Fisher's discriminant ratio is good for indicating the separation between two classes each following a Gaussian distribution, but not for two classes forming non-overlapping concentric rings one inside the other. It is our hope that more measures used in combination will provide a more complete picture about class separation, which determines the difficulty of classification.

L1	minimized sum of error distance by linear programming (LP)	
	Linear classifiers can be obtained by a linear programming formulation proposed by Smith [16] that minimizes the sum of distances of error points to the separating hyperplane (subtracting a constant margin): $$\text{minimize} \quad \mathbf{a}^t\mathbf{t}$$ $$\text{subject to} \ \mathbf{Z}^t\mathbf{w} + \mathbf{t} \geq \mathbf{b}$$ $$\mathbf{t} \geq \mathbf{0}$$ where $\mathbf{a}$, $\mathbf{b}$ are arbitrary constant vectors (both chosen to be $\mathbf{1}$), $\mathbf{w}$ is the weight vector, $\mathbf{t}$ is an error vector, and $\mathbf{Z}$ is a matrix where each column $\mathbf{z}$ is defined on an input vector $\mathbf{x}$ (augmented by adding one dimension with a constant value 1) and its class c (with value c_1 or c_2) as follows: $$\begin{cases} \mathbf{z} = +\mathbf{x} \text{ if } c = c_1 \\ \mathbf{z} = -\mathbf{x} \text{ if } c = c_2. \end{cases}$$ The value of the objective function in this formulation is used as a measure (L1).	The measure is zero for a linearly separable problem. Notice that this measure can be heavily affected by outliers that happen to be on the wrong side of the optimal hyperplane. We normalize this measure by the number of points in the problem and also by the length of the diagonal of the hyperrectangular region enclosing all training points in the feature space.
L2	error rate of linear classifier by LP	
	This measure is the error rate of the linear classifier defined for L1, measured with the training set.	With a small training set this may be a severe underestimate of the true error rate.
N1	fraction of points on boundary (MST method)	
	This method constructs a class-blind MST over the entire dataset, and counts the number of points incident to an edge going across the opposite classes. The fraction of such points over all points in the dataset is used as a measure.	For two heavily interleaved classes, a majority of points are located next to the class boundary. However, the same can be true for a linearly separable problem with margins narrower than the distances between points of the same class.
N2	ratio of average intra/inter class NN distance	
	We first compute the Euclidean distance from each point to its nearest neighbor within the class, and also to its nearest neighbor outside the class. We then take the average (over all points) of all the distances to intra-class nearest neighbors, and the average of all the distances to inter-class nearest neighbors. The ratio of the two averages is used as a measure.	This compares the within-class spread to the size of the gap between classes. It is sensitive to the classes of the closest neighbors to a point, and also to the difference in magnitude of the between-class distances and that of the with-class distances.
N3	error rate of 1NN classifier	
	This is simply the error rate of a nearest-neighbor classifier measured with the training set.	The error rate is estimated by the leave-one-out method.

Table 2. Measures of class separability.

L3	nonlinearity of linear classifier by LP	
	Hoekstra and Duin [9] proposed a measure for the *nonlinearity* of a classifier w.r.t. to a given dataset. Given a training set, the method first creates a test set by linear interpolation (with random coefficients) between randomly drawn pairs of points from the same class. Then the error rate of the classifier (trained by the given training set) on this test set is measured. Here we use such a nonlinearity measure for the linear classifier defined for L1.	This measure is sensitive to the smoothness of the classifier's decision boundary as well as the overlap of the convex hulls of the classes. For linear classifiers and linearly separable problems, it measures the alignment of the decision surface with the class boundary. It carries the effects of the training procedure in addition to those of the class separation.
N4	nonlinearity of 1NN classifier	
	This is the nonlinearity measure, as defined for L3, calculated for a nearest neighbor classifier.	This measure is for the alignment of the nearest-neighbor boundary with the shape of the gap or overlap between the convex hulls of the classes.
T1	fraction of points with associated adherence subsets retained	
	This measure originated from a work on describing shapes of class manifolds based on a notion of *adherence subsets* in pretopology [11]. Simply speaking, it counts the number of balls needed to cover each class, where each ball is centered at a training point and grown to the maximal size before it touches another class. Redundant balls lying completely in the interior of other balls are removed. We normalize the count by the total number of points.	A list of such balls is a composite description of the shape of the classes. The number and size of the balls indicate how much the points tend to cluster in hyperspheres or spread into elongated structures. In a problem where each point is closer to points of the other class than points of its own class, each point is covered by a distinctive ball of a small size, resulting in a high value of the measure.
T2	average number of points per dimension	
	This is a simple ratio of the number of points in the dataset over the number of feature dimensions.	This measure is included mostly for connection with prior studies on sample sizes. Since the volume of a region scales exponentially with the number of dimensions, a linear ratio between the two is not a good measure of sampling density.

Table 3. Measures of geometry, topology, and density of manifolds.

4 Datasets for Validating Complexity Measures

We evaluated the effectiveness of the complexity measures with two collections of classification problems. The first collection includes all pairwise discrimination problems from 14 datasets in the UC-Irvine Machine Learning Depository [2]. The datasets are those that contain at least 500 points with no missing values: *abalone, car, german, kr-vs-kp, letter, lrs, nursery, pima, segmentation, splice, tic-tac-toe, vehicle, wdbc, and yeast.* Categorical features in some datasets are numerically coded. There are altogether 844 two-class discrimination problems, with training set sizes varying from 2 to 4648, and feature space dimensionality varying from 8 to 480. Using the linear programming procedure by Smith [16] (as given in the description of the L1 measure in Table 2), 452 out of the 844 problems are found to be linearly separable. The class boundary in each of these problems, as far as the training set is concerned, can be described entirely by the weight vector of the separating hyperplane, so by Kolmogorov's notion these are simple problems. Thus a valid complexity measure should place these problems at one end of its scale.

The second collection consists of 100 artificial two-class problems each having 1000 points per class. Problem 1 has one feature dimension, problem 2 has two, so forth and the last problem contains 100 features. Each feature is a uniformly distributed pseudorandom number in $[0, 1]$. The points are randomly labeled, with equal probability, as one of two classes. Therefore, these are intrinsically complex problems, and they are expected to locate at the other end of any complexity scale.

We studied the complexity measures on the distribution of these three groups of problems, namely, (1) UCI linearly separable, (2) UCI linearly nonseparable, and (3) random labelings. A single measure is considered useful for describing problem complexity if the three groups of problems are separable on its scale, and a set of measures are considered useful if the groups of problems are separable in the space spanned by the set.

5 Key Observations

The distribution of the three groups of classification problems in this 12-dimensional complexity space displays many interesting characteristics. A detailed description of the observations in this study can be found in [6]. Here we summarize the main findings.

5.1 Continuum of problem locations in complexity space

The first remarkable observation in this study is that the datasets fall on a continuum of positions along many dimensions of the complexity space. Even though there have been no special selection criteria imposed on these naturally arising datasets, we find that the problems cover a large range of values in almost all the chosen complexity scales. This reminds us of the challenges in the

practice of pattern recognition: to pursue a good match of methods to problems, we must make sure that the classifier methodology we choose is robust to variations in these problem characteristics, or we must understand the nature of the dependence of classifier behavior on such variations. Without accomplishing either, applications of classifiers to problems are nothing but a blind match, and there is little hope of ensuring highest success.

A more encouraging observation is that many of the real-world (UCI) datasets are located far away from the random labelings, suggesting that these practical problems do indeed contain some intrinsic, learnable structure.

Interestingly, there is substantial spread among the random labelings of different dimensionality. While there is no obvious explanation for how dimensionality affects their intrinsic difficulties, closer examination of the differences suggests that this is more an effect of differences in apparent complexity due to different sampling densities, since these datasets all have the same size while the volume of the space increases exponentially with dimensionality.

5.2 Effectiveness of individual measures in separating problems of known levels of difficulty

The concentrations of the three groups of datasets (UCI linearly separable, UCI linearly nonseparable, and random labelings) in different regions in the complexity space suggest that many of the measures can reveal their differences. As a stand-alone scale of complexity, several measures (F1,F2,F3,L2,L3) are especially effective in separating at least two of the three groups, with the easiest set (UCI linearly separable) and the most difficult set (random labelings) occupying two opposite ends of the scale. However, none of the measures can completely separate the three groups with no overlaps. Some measures, such as N4 and T2, are especially weak when used in isolation.

5.3 Distorted nearest neighbor error rates of sparse datasets

The nearest-neighbor related measures (N1,N2,N3) have almost the same discriminating power for the three groups, except for a few peculiar cases where the training set consists of only 2 or 3 points. For those extremely sparse datasets, although the class boundary (for the training set) is linear, the nearest neighbors are almost always in a wrong class, thus the nearest-neighbor error rate becomes very high. This is an artifact of the leave-one-out estimate. However, it also suggests that a single error rate, even that of a simple and well-understood classifier, may tell a distorted story about the data complexity.

5.4 Pairwise Correlations between complexity measures

Bivariate plots of the distributions show that some pairs of measures, such as L2 and L3, or N1 and N3, are strongly correlated, while little correlation is seen between many other pairs (Table 4). The existence of many uncorrelated pairs

suggests that there are more than one independent factors affecting a problem's complexity.

An examination of the correlation between L2 (linear classifier error rate) and N3 (nearest neighbor error rate) and between each of these two measures and others suggests that these error rates are not perfectly correlated, nor are they always predictable by an arbitrary measure. This reconfirms the risk of relying on simple classifier error rates for complexity measurement. These two classifiers, operating on very different principles (linearity versus proximity), have difficulties caused by different characteristics of a problem (Figure 3).

Some measures, while on their own are very weak in separating all three groups of problems, can reveal the group differences when used in combination with other measures (Figure 4). This demonstrates the importance of examining the multiple aspects of a problem's complexity jointly.

The measure T1, while on its own being a strong separator of the three groups, characterizes a very different aspect of complexity from others as evidenced by its weak correlation with others. Inspection of the plots involving T1 and others suggests that while the shapes of the classes can vary a lot across different problems, it is less relevant to classification accuracy than the shapes of the class boundaries.

	F1	F2	F3	L1	L2	L3	N1	N2	N3	N4	T1	T2
F1	1.00	-0.02	0.06	-0.01	-0.02	-0.02	0.07	0.01	0.14	-0.02	0.03	-0.03
F2		1.00	-0.53	0.07	0.91	0.91	0.69	0.71	0.61	0.17	0.28	0.19
F3			1.00	-0.24	-0.65	-0.62	-0.39	-0.69	-0.29	-0.40	-0.68	-0.28
L1				1.00	0.33	0.32	0.37	0.37	0.28	0.53	0.18	-0.10
L2					1.00	1.00	0.78	0.81	0.67	0.47	0.37	0.16
L3						1.00	0.78	0.81	0.67	0.46	0.35	0.16
N1							1.00	0.76	0.96	0.49	0.39	-0.02
N2								1.00	0.68	0.51	0.55	0.12
N3									1.00	0.38	0.38	-0.04
N4										1.00	0.28	0.30
T1											1.00	0.17
T2												1.00

Table 4. Correlation coefficients between each pair of measures.

5.5 Principal components of the complexity space

A principal component analysis using the distribution of the problems in the 12-dimensional space shows that there are six significant components each explaining more than 5% of the variance. Among these, the first component explains over 50% of the variance, and comprises even contributions from F2,L2,L3,N1,N2, and N3. It is a combination of effects of linearity of class boundaries and proximity
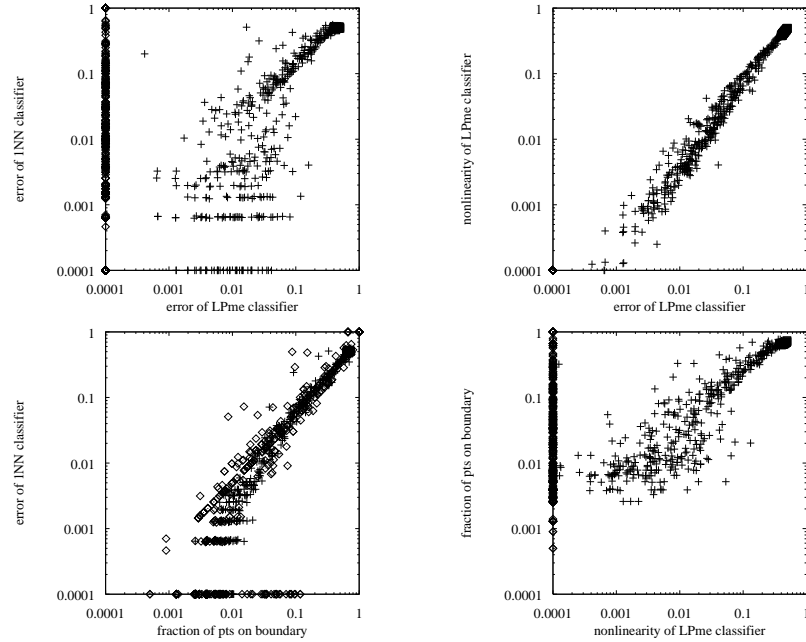
Fig. 3. Error rates of linear and nearest-neighbor classifiers, and the measures they are most strongly correlated with. (⋄: UCI linearly separable problems; +: UCI linearly nonseparable problems; □: random labelings)

between opposite class neighbors. The next 3 components explain 12%, 11% and 9% of the variance respectively, and can be interpreted as (PC2:) a balance of within-class and between-class scatter, (PC3:) the concentration and orientation of class overlaps, and (PC4:) within-class scatter. For a more detailed discussion of these components, as well as for the trajectory traced in the PC projection by an example series of problems with controlled class separation, we again refer readers to [6].

6 Studies of Problems and Classifiers Using Complexity Measures

A complexity measurement space like this has many potentially interesting uses. For a particular application domain, the scales of complexity can help determine the existence of any learnable structure, which can be used to set expectations on automatic learning algorithms. They can also be used to determine if a particular dataset is suitable for evaluating different learning algorithms.

The measures can be used to compare different problem formulations, including class definitions, choice of features, and potential feature transformations. They can be used to guide the selection of classifiers and classifier combination
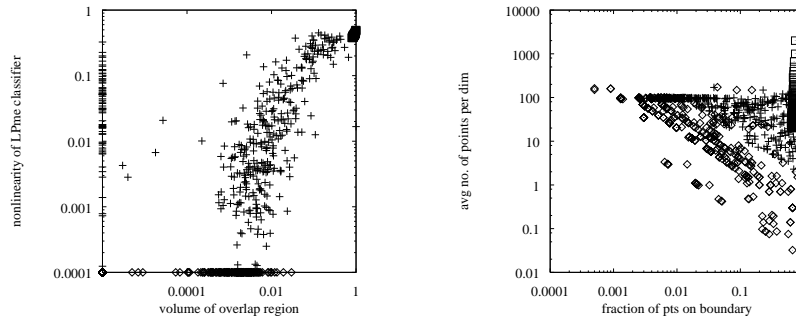
Fig. 4. Groups of problems that overlap heavily on an individual complexity scale may show clear separation in the interaction of the effects. (⋄: UCI linearly separable problems; +: UCI linearly nonseparable problems; □: random labelings)

schemes, or control the process of classifier training. A use of these measures for comparing two methods for decision forest construction is reported in [7].

Regions occupied by datasets on which classifiers display homogeneous performances can be used to outline the domain of competences of those classifiers, with the expectation that performances on new datasets falling in the same region can be predicted accordingly. Regions where no classifiers can do well may be characterized in detail by the complexity measures, which could lead to new classifier designs covering those blind spots. In [14] we report a study of the domain of competence of XCS, a genetic algorithm based classifier.

One may wish to study the distribution of all classification problems in this space. An empirical approach will be to seek a representation of the distribution by a much larger collection of practical problems. A theoretical approach will be more challenging; it involves reasoning about regions in this space that are possible or impossible for any dataset to occupy. The identification of such regions will require a better understanding of constraints in high-dimensional data geometry and topology. The intrinsic dimensionality of the problem distribution will give more conclusive evidence on how many independent factors contribute to a problem's difficulty.

7 Conclusions

We describe some early investigation into the complexity of a classification problem, with emphasis on the geometrical characteristics that can be measured directly from a training set. We took some well known measures from the pattern recognition literature, and studied their descriptive power using a collection of problems of known levels of difficulty. We found some interesting spread among the different types of problems, and evidence of existence of independent factors affecting a problem's difficulty. We believe that such descriptors of complexity are useful for identifying and comparing different classes of problems, character-

izing the domain of competence of classifier or ensemble methods, and in many ways guiding the development of a solution to a pattern recognition problem.

These are our first steps towards developing elements of a language with which we can talk more precisely about properties of high dimensional datasets, especially those aspects affecting classifier performances. We believe this is necessary for classification research to advance beyond the current plateau. Finally, we believe that such abstract studies are best coupled with tools for interactive visualization of a dataset, so that an intuitive understanding may be obtained on how the complexity arises from a particular problem [8].

References

1. M. Basu, T.K. Ho, The learning behavior of single neuron classifiers on linearly separable or nonseparable input, *Proceedings of the 1999 International Joint Conference on Neural Networks*, Washington, DC, July 1999.
2. C.L. Blake, C.J. Merz, UCI Repository of machine learning databases, http://www.ics.uci.edu~mlearn/MLRepository.html, University of California, Department of Information and Computer Science, Irvine, CA, 1998.
3. L. Devroye, Automatic pattern recognition: A study of the probability of error, IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 10, no. 4, 1988, 530-543.
4. T.K. Ho, H.S. Baird, Pattern classification with compact distribution maps, *Computer Vision and Image Understanding*, **70**, 1, April 1998, 101-110.
5. T.K. Ho, Multiple classifier combination: Lessons and next steps, in A. Kandel, H. Bunke, (eds.), *Hybrid Methods in Pattern Recognition*, World Scientific, 2002.
6. T.K. Ho, M. Basu, Complexity Measures of Supervised Classification Problems, IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 24, no. 3, 2002, 289-300.
7. T.K. Ho, A Data Complexity Analysis of Comparative Advantages of Decision Forest Constructors, Pattern Analysis and Applications, vol. 5, 2002, 102-112.
8. T.K. Ho, Exploratory Analysis of Point Proximity in Subspaces, *Proceedings of the 16th International Conference on Pattern Recognition*, Quebec City, Canada, August 11-15, 2002.
9. A. Hoekstra, R.P.W. Duin, On the nonlinearity of pattern classifiers, *Proc. of the 13th ICPR*, Vienna, August 1996, **D**271-275.
10. A.N. Kolmogorov, Three approaches to the quantitative definition of information, *Problems of Information Transmission*, **1**, 1965, 4-7.
11. F. Lebourgeois, H. Emptoz, Pretopological approach for supervised learning, *Proceedings of the 13th International Conference on Pattern Recognition*, Vienna, 1996, 256-260.
12. M. Li, P. Vitanyi, *An Introduction to Kolmogorov Complexity and Its Applications*, Springer-Verlag, 1993.
13. J.M. Maciejowski, Model discrimination using an algorithmic information criterion, *Automatica*, **15**, 1979, 579-593.
14. E.B. Mansilla, T.K. Ho, Domain of Competence of XCS Classifier System in Complexity Measurement Space, in revision for *IEEE Transactions on Evolutionary Computation*, 2003.

15. S. Raudys, A.K. Jain, Small sample size effects in statistical pattern recognition: Recommendations for practitioners, *IEEE Trans. PAMI*, **13**, 3, 1991, 252-264.
16. F.W. Smith, Pattern classifier design by linear programming, *IEEE Transactions on Computers*, **C-17**, 4, April 1968, 367-372.
17. V. Vapnik, *Statistical Learning Theory*, John Wiley & Sons, 1998.