Linear and Order Statistics Combiners for Pattern Classification

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Summary.

Several researchers have experimentally shown that substantial improvements can be obtained in difficult pattern recognition problems by combining or integrating the outputs of multiple classifiers. This chapter provides an analytical framework to *quantify* the improvements in classification results due to combining. The results apply to both linear combiners and order statistics combiners. We first show that to a first order approximation, the error rate obtained over and above the Bayes error rate, is directly proportional to the variance of the actual decision boundaries around the Bayes optimum boundary. Combining classifiers in output space reduces this variance, and hence reduces the "added" error. If N unbiased classifiers are combined by simple averaging, the added error rate can be reduced by a factor of N if the individual errors in approximating the decision boundaries are uncorrelated. Expressions are then derived for linear combiners which are biased or correlated, and the effect of output correlations on ensemble performance is quantified. For order statistics based non-linear combiners, we derive expressions that indicate how much the median, the maximum and in general the ith order statistic can improve classifier performance. The analysis presented here facilitates the understanding of the relationships among error rates, classifier boundary distributions, and combining in output space. Experimental results on several public domain data sets are provided to illustrate the benefits of combining and to support the analytical results.

0.1 Introduction

Training a parametric classifier involves the use of a *training* set of data with known labeling to estimate or "learn" the parameters of the chosen model. A *test* set, consisting of patterns not previously seen by the classifier, is then used to determine the classification performance. This ability to meaningfully respond to novel patterns, or generalize, is an important aspect of a classifier system and in essence, the true gauge of performance [38, 77]. Given infinite training data, consistent classifiers approximate the Bayesian decision boundaries to arbitrary precision, therefore providing similar generalizations [24]. However, often only a limited portion of the pattern space is available or observable [16, 22]. Given a finite and noisy data set, different classifiers typically provide different generalizations by realizing different decision boundaries [26]. For example, when classification is performed using a multilayered, feed-forward artificial neural network, different weight initializations, or different architectures (number of hidden units, hidden layers, node activation functions etc.) result in differences in performance. It is therefore beneficial to train an ensemble of classifiers when approaching a classification problem to ensure that a good model/parameter set is found.

Techniques such as cross-validation also lead to multiple trained classifiers. Selecting the "best" classifier is not necessarily the ideal choice, since potentially valuable information may be wasted by discarding the results of

less-successful classifiers. This observation motivates the concept of "combining" wherein the outputs of all the available classifiers are pooled before a decision is made. This approach is particularly useful for difficult problems, such as those that involve a large amount of noise, limited number of training data, or unusually high dimensional patterns. The concept of combining appeared in the neural network literature as early as 1965 [44], and has subsequently been studied in several forms, including *stacking* [78], *boosting* [15, 14, 19, 20] and *bagging* [9, 10]. Combining has also been studied in other fields such as econometrics, under the name "forecast combining" [28], or machine learning where it is called "evidence combination" [4, 23]. The overall architecture of the combiner form studied in this article is shown in Figure 0.1. The output of an individual classifier using a single feature set is given by f^{ind}. Multiple classifiers, possibly trained on different feature sets, provide the combined output f^{comb}.

Currently, the most popular way of combining multiple classifiers is via simple averaging of the corresponding output values [29, 39, 49, 69]. Weighted averaging has also been proposed, along with different methods of computing the proper classifier weights [7, 31, 39, 42]. Such linear combining techniques have been mathematically analyzed for both regression [31, 48] and classification [69] problems. Order statistics combiners that selectively pick a classifier on a per sample basis were introduced in [68, 72]. Other non-linear methods, such as rank-based combiners [1, 33], or voting schemes [5, 11, 30] have been investigated as well. Methods for combining beliefs in the Dempster-Shafer sense are also available [53, 55, 81, 82]. Combiners have been successfully applied a multitude of real world problems [6, 8, 27, 37, 61, 83].

Combining techniques such as majority voting can generally be applied to any type of classifier, while others rely on specific outputs, or specific interpretations of the output. For example, the confidence factors method found in machine learning literature relies on the interpretation of the outputs as the belief that a pattern belongs to a given class [32]. The rationale for averaging, on the other hand, is based on the result that the outputs of parametric classifiers that are trained to minimize a cross-entropy or mean square error (MSE) function, given "*one-of-L*" desired output patterns, approximate the *a posteriori* probability densities of the corresponding class [54, 57]. In particular, the MSE is shown to be equivalent to:

$$MSE = K_1 + \sum_i \int_x D_i(x) \left(p(C_i|x) - f_i(x)\right)^2 dx$$

where K_1 and $D_i(x)$ depend on the class distributions only, $f_i(x)$ is the output of the node representing class i given an output x, $p(C_i|x)$ denotes the posterior probability and the summation is over all classes [62]. Thus minimizing the MSE is equivalent to a weighted least squares fit of the network outputs to the corresponding posterior probabilities.

In this article we first analytically study the effect of linear and order statistics combining in output space with a focus on the relationship between

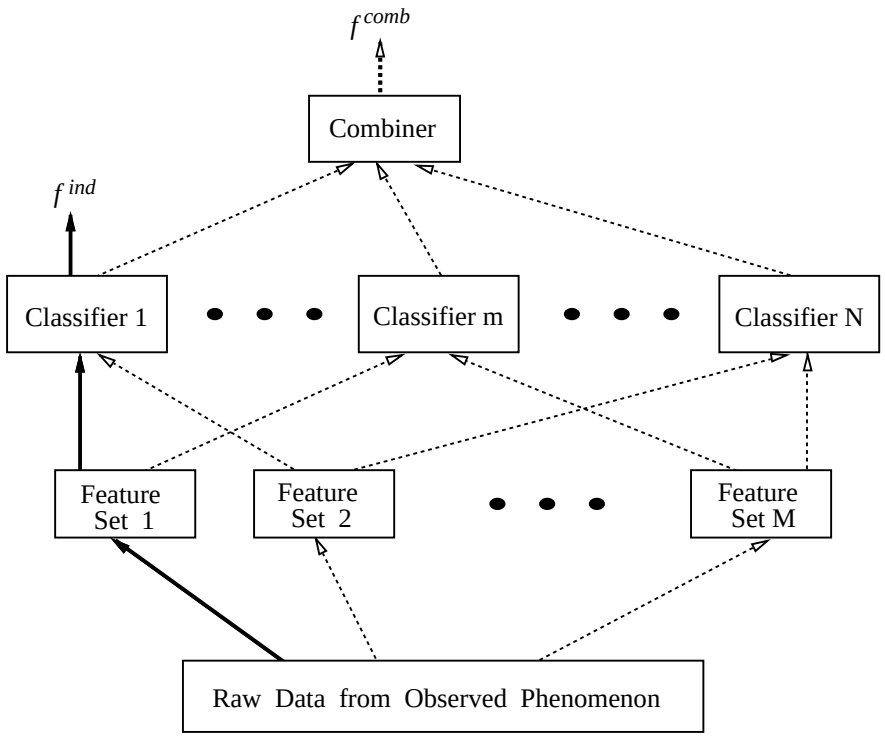

Fig. 0.1. Combining Strategy. The solid lines leading to f^{ind} represent the decision of a specific classifier, while the dashed lines lead to f^{comb}, the output of the combiner.

decision boundary distributions and error rates. Our objective is to provide an analysis that:

- encapsulates the most commonly used combining strategy, averaging in output space;
- is broad enough in scope to cover non-linear combiners; and
- relates the location of the decision boundary to the classifier error.

The rest of this article is organized as follows. Section 0.2 introduces the overall framework for estimating error rates and the effects of combining. In Section 0.3 we analyze linear combiners, and derive expressions for the error rates for both biased and unbiased classifiers. In Section 0.4, we examine order statistics combiners, and analyze the resulting classifier boundaries and error regions. In Section 0.5 we study linear combiners that make correlated errors, derive their error reduction rates, and discuss how to use this information to build better combiners. In Section 0.6, we present experimental results based

on real world problems, and we conclude with a discussion of the implications of the work presented in this article.

0.2 Class Boundary Analysis and Error Regions

Consider a single classifier whose outputs are expected to approximate the corresponding *a posteriori* class probabilities if it is reasonably well trained. The decision boundaries obtained by such a classifier are thus expected to be close to Bayesian decision boundaries. Moreover, these boundaries will tend to occur in regions where the number of training samples belonging to the two most locally dominant classes (say, classes i and j) are comparable.

We will focus our analysis on network performance around the decision boundaries. Consider the boundary between classes i and j for a single-dimensional input (the extension to multi-dimensional inputs is discussed in [73]). First, let us express the output response of the ith unit of a *one-of-L* classifier network to a given input x as[1]:

$$f_i(x) = p_i(x) + \epsilon_i(x) \,, \tag{0.1}$$

where $p_i(x)$ is the *a posteriori* probability distribution of the ith class given input x, and $\epsilon_i(x)$ is the error associated with the ith output[2].

For the Bayes optimum decision, a vector x is assigned to class i if $p_i(x) > p_k(x)\ ,\ \forall k \neq i$. Therefore, the Bayes optimum boundary is the loci of all points x^* such that $p_i(x^*) = p_j(x^*)$ where $p_j(x^*) = \max_{k \neq i}\ p_k(x)$. Since our classifier provides $f_i(\cdot)$ instead of $p_i(\cdot)$, the decision boundary obtained, x_b, may vary from the optimum boundary (see Figure 0.2). Let b denote the amount by which the boundary of the classifier differs from the optimum boundary ($b = x_b - x^*$). We have:

$$f_i(x^* + b) = f_j(x^* + b),$$

by definition of the boundary. This implies:

$$p_i(x^* + b) + \epsilon_i(x_b) \ = \ p_j(x^* + b) + \epsilon_j(x_b) \,. \tag{0.2}$$

Within a suitably chosen region about the optimum boundary, the *a posteriori* probability of the correct class monotonically increases relative to the others as we move away from the boundary. This suggests a linear approximation of $p_k(x)$ around x^*:

$$p_k(x^* + b) \simeq p_k(x^*) \ + \ b\, p'_k(x^*) \ , \ \forall k \ , \tag{0.3}$$

[1] If two or more classifiers need to be distinguished, a superscript is added to $f_i(x)$ and $\epsilon_i(x)$ to indicate the classifier number.

[2] Here, $p_i(x)$ is used for simplicity to denote $p(C_i|x)$.

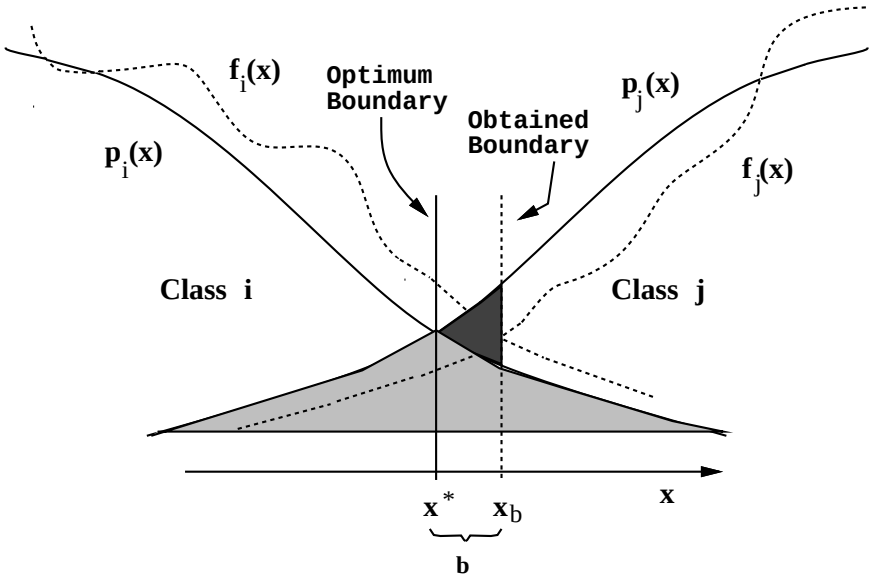

Fig. 0.2. Error regions associated with approximating the *a posteriori* probabilities. Lightly shaded region represents the Bayes error, while the darkly shaded area represents the additional error due to classifier f.

where $p'_k(\cdot)$ denotes the derivative of $p_k(\cdot)$. With this substitution, Equation 0.2 becomes:

$$p_i(x^*) + b\,p'_i(x^*) + \epsilon_i(x_b) = p_j(x^*) + b\,p'_j(x^*) + \epsilon_j(x_b). \tag{0.4}$$

Now, since $p_i(x^*) = p_j(x^*)$, we get:

$$b\,(p'_j(x^*) - p'_i(x^*)) = \epsilon_i(x_b) - \epsilon_j(x_b).$$

Finally we obtain:

$$b = \frac{\epsilon_i(x_b) - \epsilon_j(x_b)}{s}, \tag{0.5}$$

where:

$$s = p'_j(x^*) - p'_i(x^*). \tag{0.6}$$

Let the error $\epsilon_i(x_b)$ be broken into a bias and noise term ($\epsilon_i(x_b) = \beta_i + \eta_i(x_b)$). Note that the term "bias" and "noise" are only analogies, since the error is due to the classifier as well as the data. For the time being, the bias is assumed to be zero (i.e. $\beta_k = 0\ \forall k$). The case with nonzero bias will be discussed at the end of this section. Let $\sigma^2_{\eta_k}$ denote the variances of $\eta_k(x)$,

which are taken to be i.i.d. variables[3]. Then, the variance of the zero-mean variable b is given by (using Equation 0.5):

$$\sigma_b^2 \;=\; \frac{2\,\sigma_{\eta_k}^2}{s^2}. \tag{0.7}$$

Figure 0.2 shows the *a posteriori* probabilities obtained by a non-ideal classifier, and the associated added error region. The lightly shaded area provides the Bayesian error region. The darkly shaded area is the added error region associated with selecting a decision boundary that is offset by b, since patterns corresponding to the darkly shaded region are erroneously assigned to class i by the classifier, although ideally they should be assigned to class j.

The added error region, denoted by $A(b)$, is given by:

$$A(b) \;=\; \int_{x^*}^{x^*+b} (p_j(x) - p_i(x))\,dx. \tag{0.8}$$

Based on this area, the expected added error, E_{add}, is given by:

$$E_{add} = \int_{-\infty}^{\infty} A(b) f_b(b) db, \tag{0.9}$$

where f_b is the density function for b. More explicitly, the expected added error is:

$$E_{add} = \int_{-\infty}^{\infty}\int_{x^*}^{x^*+b} (p_j(x) - p_i(x))\;\; f_b(b)\,dxdb.$$

One can compute $A(b)$ directly by using the approximation in Equation 0.3 and solving Equation 0.8. The accuracy of this approximation depends on the proximity of the boundary to the ideal boundary. However, since in general, the boundary density decreases rapidly with increasing distance from the ideal boundary, the approximation is reasonable at least for the most likely (i.e. small) values of b. This leads to:

$$A(b) = \int_{x^*}^{x^*+b} \big((p_j(x^*) \;+\; (x-x^*)\,p_j'(x^*)) \;-\; (p_i(x^*) \;+\; (x-x^*)\,p_i'(x^*))\big)\,dx.$$

or:

$$A(b) = \frac{1}{2}\,b^2\,s, \tag{0.10}$$

where s is given by Equation 0.6.

[3] Each output of each network does approximate a smooth function, and therefore the noise for two nearby patterns on the same class (i.e. $\eta_k(x)$ and $\eta_k(x+\Delta x)$) is correlated. The independence assumption applies to inter-class noise (i.e. $\eta_i(x)$ and $\eta_j(x)$), not intra-class noise.

Equation 0.9 shows how the error can be obtained directly from the density function of the boundary offset. Although obtaining the exact form of the density function for b is possible (it is straightforward for linear combiners, but convoluted for order statistics combiners), it is not required. Since the area given in Equation 0.10 is a polynomial of the second degree, we can find its expected value using the first two moments of the distribution of b. Let us define the first and second moments of the the boundary offset:

$$M_1 = \int_{-\infty}^{\infty} x f_b(x) dx.$$

and:

$$M_2 = \int_{-\infty}^{\infty} x^2 f_b(x) dx.$$

Computing the expected error for a combiner reduces to solving:

$$E_{add} = \int_{-\infty}^{\infty} \frac{1}{2} b^2 s f_b(b) db,$$

in terms of M_1 and M_2, leading to:

$$E_{add} = \frac{s}{2} \int_{-\infty}^{\infty} b^2 f_b(b) db = \frac{sM_2}{2}. \tag{0.11}$$

The offset b of a single classifier without bias has $M_1 = 0$ and $M_2 = \sigma_b^2$, leading to:

$$E_{add} = \frac{s\sigma_b^2}{2}. \tag{0.12}$$

Of course, Equation 0.12 only provides the added error. The total error is the sum of the added error and the Bayes error, which is given by:

$$E_{tot} = E_{bay} + E_{add}. \tag{0.13}$$

Now, if the classifiers are biased, we need to proceed with the assumption that $\epsilon_k(x) = \beta_k + \eta_k(x)$ where $\beta_k \neq 0$. The boundary offset for a single classifier becomes:

$$b = \frac{\eta_i(x_b) - \eta_j(x_b)}{s} + \frac{\beta_i - \beta_j}{s}. \tag{0.14}$$

In this case, the variance of b is left unchanged (given by Equation 0.7), but the mean becomes $\beta = \frac{\beta_i - \beta_j}{s}$. In other words, we have $M_1 = \beta$ and $\sigma_b^2 = M_2 - {M_1}^2$, leading to the following added error:

$$E_{add}(\beta) = \frac{sM_2}{2} = \frac{s}{2}(\sigma_b^2 + \beta^2). \tag{0.15}$$

For analyzing the error regions after combining and comparing them to the single classifier case, one needs to determine how the first and second moment of the boundary distributions are affected by combining. The bulk of the work in the following sections focuses on obtaining those values.

0.3 Linear Combining

0.3.1 Linear Combining of Unbiased Classifiers

Let us now divert our attention to the effects of linearly combining multiple classifiers. In what follows, the combiner denoted by *ave* performs an arithmetic average in output space. If N classifiers are available, the ith output of the *ave* combiner provides an approximation to $p_i(x)$ given by:

$$f_i^{ave}(x) = \frac{1}{N} \sum_{m=1}^{N} f_i^m(x), \tag{0.16}$$

or:

$$f_i^{ave}(x) = p_i(x) \; + \; \bar{\beta}_i \; + \; \bar{\eta}_i(x) \; ,$$

where:

$$\bar{\eta}_i(x) = \frac{1}{N} \sum_{m=1}^{N} \eta_i^m(x) \; ,$$

and

$$\bar{\beta}_i = \frac{1}{N} \sum_{m=1}^{N} \beta_i^m \; .$$

If the classifiers are unbiased, $\bar{\beta}_i = 0$. Moreover, if the errors of different classifiers are i.i.d., the variance of $\bar{\eta}_i$ is given by:

$$\sigma^2_{\bar{\eta}_i} = \frac{1}{N^2} \sum_{m=1}^{N} \sigma^2_{\eta_i^m} = \frac{1}{N} \sigma^2_{\eta_i} \; . \tag{0.17}$$

The boundary x^{ave} then has an offset b^{ave}, where:

$$f_i^{ave}(x^* + b^{ave}) = f_j^{ave}(x^* + b^{ave}),$$

and:

$$b^{ave} = \frac{\bar{\eta}_i(x_{b^{ave}}) - \bar{\eta}_j(x_{b^{ave}})}{s}. \tag{0.18}$$

The variance of b^{ave}, $\sigma^2_{b^{ave}}$, can be computed in a manner similar to σ^2_b, resulting in:

$$\sigma^2_{b^{ave}} = \frac{\sigma^2_{\bar{\eta}_i} + \sigma^2_{\bar{\eta}_j}}{s^2},$$

which, using Equation 0.17, leads to:

$$\sigma^2_{b^{ave}} = \frac{\sigma^2_{\eta_i} + \sigma^2_{\eta_j}}{N\, s^2},$$

or:

$$\sigma^2_{b^{ave}} = \frac{\sigma^2_b}{N}. \tag{0.19}$$

Qualitatively, this reduction in variance can be readily translated into a reduction in error rates, since a narrower boundary distribution means the likelihood that a boundary will be near the ideal one is increased. In effect, using the evidence of more than one classifier reduces the variance of the class boundary, thereby providing a "tighter" error-prone area. In order to establish the exact improvements in the classification rate, we need to compute the expected added error region, and explore the relationship between classifier boundary variance and error rates.

To that end, let us return to the added error region analysis. For the *ave* classifier, the first and second moments of the boundary offset, b^{ave}, are: $M_1^{ave} = 0$ and $M_2^{ave} = \sigma^2_{b^{ave}}$. Using Equation 0.19, we obtain $M_2^{ave} = \frac{\sigma^2_b}{N}$. The added error for the *ave* combiner becomes:

$$E^{ave}_{add} = \frac{sM_2^{ave}}{2} = \frac{s}{2}\,\sigma^2_{b^{ave}} = \frac{s}{2\,N}\,\sigma^2_b = \frac{E_{add}}{N}. \tag{0.20}$$

Equation 0.20 quantifies the improvements due to combining N classifiers. Under the assumptions discussed above, combining in output space reduces added error regions by a factor of N. Of course, the total error, which is the sum of Bayes error and the added error, will be reduced by a smaller amount, since Bayesian error will be non-zero for problems with overlapping classes. In fact, this result, coupled with the reduction factor obtained is Section 0.5.2, can be used to provide estimates for the Bayes error rate [67, 71].

0.3.2 Linear Combining of Biased Classifiers

In general, $\bar{\beta}_i$ is nonzero since at least one classifier is biased. In this case, the boundary offset b^{ave} becomes:

$$b^{ave} = \frac{\bar{\eta_i}(x_{b^{ave}}) - \bar{\eta_j}(x_{b^{ave}})}{s} + \frac{\bar{\beta}_i - \bar{\beta}_j}{s}. \tag{0.21}$$

The variance of $\bar{\eta}_i(x)$ is identical to that of the unbiased case, but the mean of b^{ave} is given by $\bar{\beta}$ where

$$\bar{\beta} = \frac{\bar{\beta}_i - \bar{\beta}_j}{s}. \tag{0.22}$$

The effect of combining is less clear in this case, since the average bias ($\bar{\beta}$) is not necessarily less than each of the individual biases. Let us determine

the first and second moments of b^{ave}. We have $M_1^{ave} = \bar{\beta}$, and $\sigma^2_{b^{ave}} = M_2^{ave} - (M_1^{ave})^2$, leading to:

$$E^{ave}_{add}(\bar{\beta}) \;=\; \frac{sM_2^{ave}}{2} \;=\; \frac{s}{2}\,(\sigma^2_{b^{ave}} + (\bar{\beta})^2)$$

which is:

$$E^{ave}_{add}(\bar{\beta}) \;=\; \frac{s}{2}\,\left(\frac{\sigma_b^2}{N} + \frac{\beta^2}{z^2}\right) \tag{0.23}$$

where $\bar{\beta} = \frac{\beta}{z}$, and $z \geq 1$. Now let us limit the study to the case where $z \leq \sqrt{N}$. Then[4]:

$$E^{ave}_{add}(\bar{\beta}) \;\leq\; \frac{s}{2}\,\left(\frac{\sigma_b^2 + \beta^2}{z^2}\right)$$

leading to:

$$E^{ave}_{add}(\bar{\beta}) \;\leq\; \frac{1}{z^2}\,E_{add}(\beta). \tag{0.24}$$

Equation 0.24 quantifies the error reduction in the presence of network bias. The improvements are more modest than those of the previous section, since both the bias and the variance of the noise need to be reduced. If both the variance and the bias contribute to the error, and their contributions are of similar magnitude, the actual reduction is given by $min(z^2, N)$. If the bias can be kept low (e.g. by purposefully using a larger network than required), then once again N becomes the reduction factor. These results highlight the basic strengths of combining, which not only provides improved error rates, but is also a method of controlling the bias and variance components of the error separately, thus providing an interesting solution to the bias/variance problem [24].

0.4 Order Statistics

0.4.1 Introduction

Approaches to pooling classifiers can be separated into two main categories: simple combiners, e.g., averaging, and computationally expensive combiners, e.g., stacking. The simple combining methods are best suited for problems where the individual classifiers perform the same task, and have comparable success. However, such combiners are susceptible to outliers and to unevenly performing classifiers. In the second category, "meta-learners," i.e., either sets of combining rules, or full fledged classifiers acting on the outputs of

[4] If $z \geq \sqrt{N}$, then the reduction of the variance becomes the limiting factor, and the reductions established in the previous section hold.

the individual classifiers, are constructed. This type of combining is more general, but suffers from all the problems associated with the extra learning (e.g., overparameterizing, lengthy training time).

Both these methods are in fact ill-suited for problems where *most* (but not all) classifiers perform within a well-specified range. In such cases the simplicity of averaging the classifier outputs is appealing, but the prospect of one poor classifier corrupting the combiner makes this a risky choice. Although, weighted averaging of classifier outputs appears to provide some flexibility, obtaining the optimal weights can be computationally expensive. Furthermore, the weights are generally assigned on a per classifier, rather than per sample or per class basis. If a classifier is accurate only in certain areas of the inputs space, this scheme fails to take advantage of the variable accuracy of the classifier in question. Using a meta learner that would have weights for each classifier on each pattern, would solve this problem, but at a considerable cost. The robust combiners presented in this section aim at bridging the gap between simplicity and generality by allowing the flexible selection of classifiers without the associated cost of training meta classifiers.

0.4.2 Background

In this section we will briefly discuss some basic concepts and properties of order statistics. Let X be a random variable with a probability density function $f_X(\cdot)$, and cumulative distribution function $F_X(\cdot)$. Let $(X_1, X_2, \cdots, X_N)$ be a random sample drawn from this distribution. Now, let us arrange them in non-decreasing order, providing:

$$X_{1:N} \leq X_{2:N} \leq \cdots \leq X_{N:N}.$$

The ith order statistic denoted by $X_{i:N}$, is the ith value in this progression. The cumulative distribution function for the smallest and largest order statistic can be obtained by noting that:

$$F_{X_{N:N}}(x) = P(X_{N:N} \leq x) = \Pi_{i=1}^{N} P(X_{i:N} \leq x) = [F_X(x)]^N$$

and:

$$\begin{aligned} F_{X_{1:N}}(x) &= P(X_{1:N} \leq x) = 1 - P(X_{1:N} \geq x) = 1 - \Pi_{i=1}^{N} P(X_{i:N} \geq x) \\ &= 1 - (1 - \Pi_{i=1}^{N} P(X_{i:N} \leq x) = 1 - [1 - F_X(x)]^N \end{aligned}$$

The corresponding probability density functions can be obtained from these equations. In general, for the ith order statistic, the cumulative distribution function gives the probability that exactly i of the chosen X's are less than or equal to x. The probability density function of $X_{i:N}$ is then given by [12]:

$$f_{X_{i:N}}(x) = \frac{N!}{(i-1)!\,(N-i)!} [F_X(x)]^{i-1} [1 - F_X(x)]^{N-i} f_X(x)\,. \qquad (0.25)$$

This general form however, cannot always be computed in closed form. Therefore, obtaining the expected value of a function of x using Equation 0.25 is not always possible. However, the first two moments of the density function are widely available for a variety of distributions [3]. These moments can be used to compute the expected values of certain specific functions, e.g. polynomials of order less than two.

0.4.3 Combining Unbiased Classifiers through OS

Now, let us turn our attention to order statistic combiners. For a given input x, let the network outputs of each of the N classifiers for each class i be ordered in the following manner:

$$f_i^{1:N}(x) \leq f_i^{2:N}(x) \leq \cdots \leq f_i^{N:N}(x).$$

Then, the *max*, *med* and *min* combiners are defined as follows [12]:

$$f_i^{max}(x) = f_i^{N:N}(x), \tag{0.26}$$

$$f_i^{med}(x) = \begin{cases} \frac{f_i^{\frac{N}{2}:N}(x) + f_i^{\frac{N}{2}+1:N}(x)}{2} & \text{if } N \text{ is even} \\ f_i^{\frac{N+1}{2}:N}(x) & \text{if } N \text{ is odd,} \end{cases} \tag{0.27}$$

$$f_i^{min}(x) = f_i^{1:N}(x). \tag{0.28}$$

These three combiners are chosen because they represent important qualitative interpretations of the output space. Selecting the maximum combiner is equivalent to selecting the class with the highest posterior. Indeed, since the network outputs approximate the class *a posteriori* distributions, selecting the maximum reduces to selecting the classifier with the highest confidence in its decision. The drawback of this method however is that it can be compromised by a single classifier that repeatedly provides high values. The selection of the minimum combiner follows a similar logic, but focuses on classes that are unlikely to be correct, rather than on the correct class. Thus, this combiner eliminates less likely classes by basing the decision on the lowest value for a given class. This combiner suffers from the same ills as the *max* combiner, although it is less dependent on a single error, since it performs a min-max operation, rather than a max-max[5]. The median classifier on the other hand considers the most "typical" representation of each class. For highly noisy data, this combiner is more desirable than either the *min* or *max* combiners since the decision is not compromised as much by a single large error.

The analysis of the properties of these combiners does not depend on the order statistic chosen. Therefore we will denote all three by $f_i^{os}(x)$ and derive the error regions. The network output provided by $f_i^{os}(x)$ is given by:

[5] Recall that the pattern is ultimately assigned to the class with the highest combined output.

$$f_i^{os}(x) = p_i(x) + \epsilon_i^{os}(x)\ , \tag{0.29}$$

Let us first investigate the zero-bias case ($\beta_k = 0\ \forall k$). We get $\epsilon_k^{os}(x) = \eta_k^{os}(x)\ \forall k$, since the variations in the kth output of the classifiers are solely due to noise. Proceeding as before, the boundary b^{os} is shown to be:

$$b^{os} \ = \ \frac{\eta_i^{os}(x_b) - \eta_j^{os}(x_b)}{s}. \tag{0.30}$$

Since η_k's are i.i.d, and η_k^{os} is the same order statistic for each class, the moments will be identical for each class. Moreover, taking the order statistic will shift the mean of both η_i^{os} and η_j^{os} by the same amount, leaving the mean of the difference unaffected. Therefore, b^{os} will have zero mean, and variance:

$$\sigma_{b^{os}}^2 \ = \ \frac{2\,\sigma_{\eta_k^{os}}^2}{s^2} \ = \ \frac{2\,\alpha\sigma_{\eta_k}^2}{s^2} \ = \ \alpha\sigma_b^2, \tag{0.31}$$

where α is a reduction factor that depends on the order statistic and on the distribution of b. For most distributions, α can be found in tabulated form [3]. For example, Table 0.1 provides α values for all three *os* combiners, up to 15 classifiers, for a Gaussian distribution [3, 58].

Returning to the error calculation, we have: $M_1^{os} = 0$, and $M_2^{os} = \sigma_{b^{os}}^2$, providing:

$$E_{add}^{os} = \frac{sM_2^{os}}{2} = \frac{s\sigma_{b^{os}}^2}{2} = \frac{s\alpha\sigma_b^2}{2} = \alpha\ E_{add}. \tag{0.32}$$

Table 0.1. Reduction factors α for the *min, max* and *med* combiners.

N	OS Combiners	
	minimum/maximum	median
1	1.00	1.00
2	.682	.682
3	.560	.449
4	.492	.361
5	.448	.287
6	.416	.246
7	.392	.210
8	.373	.187
9	.357	.166
10	.344	.151
11	.333	.137
12	.327	.127
13	.315	.117
14	.308	.109
15	.301	.102

Equation 0.32 shows that the reduction in the error region is directly related to the reduction in the variance of the boundary offset b. Since the means and variances of order statistics for a variety of distributions are widely available in tabular form, the reductions can be readily quantified.

0.4.4 Combining Biased Classifiers through OS

In this section, we analyze the error regions in the presence of bias. Let us study b^{os} in detail when multiple classifiers are combined using order statistics. First note that the bias and noise cannot be separated, since in general $(a+b)^{os} \neq a^{os} + b^{os}$. We will therefore need to specify the mean and variance of the result of each operation[6]. Equation 0.30 becomes:

$$b^{os} = \frac{(\beta_i + \eta_i(x_b))^{os} - (\beta_j + \eta_j(x_b))^{os}}{s}. \tag{0.33}$$

Now, β_k has mean $\bar{\beta}_k$, given by $\frac{1}{N}\sum_{m=1}^{N}\beta_k^m$, where m denotes the different classifiers. Since the noise is zero-mean, $\beta_k + \eta_k(x_b)$ has first moment $\bar{\beta}_k$ and variance $\sigma^2_{\eta_k} + \sigma^2_{\beta_k}$, where $\sigma^2_{\beta_k} = \frac{1}{N-1}\sum_{m=1}^{N}(\beta_k^m - \bar{\beta}_k)^2$.

Taking a specific order statistic of this expression will modify both moments. The first moment is given by $\bar{\beta}_k + \mu^{os}$, where μ^{os} is a shift which depends on the order statistic chosen, but not on the class. The first moment of b^{os} then, is given by:

$$\frac{(\bar{\beta}_i + \mu^{os}) - (\bar{\beta}_j + \mu^{os})}{s} = \frac{\bar{\beta}_i - \bar{\beta}_j}{s} = \bar{\beta}. \tag{0.34}$$

Note that the bias term represents an "average bias" since the contributions due to the order statistic are removed. Therefore, reductions in bias cannot be obtained from a table similar to Table 0.1.

Now, let us turn our attention to the variance. Since $\beta_k + \eta_k(x_b)$ has variance $\sigma^2_{\eta_k} + \sigma^2_{\beta_k}$, it follows that $(\beta_k + \eta_k(x_b))^{os}$ has variance $\sigma^2_{\eta_k^{os}} = \alpha(\sigma^2_{\eta_k} + \sigma^2_{\beta_k})$, where α is the factor discussed in Section 0.4.3. Since b^{os} is a linear combination of error terms, its variance is given by:

$$\sigma^2_{b^{os}} = \frac{\sigma^2_{\eta_i^{os}} + \sigma^2_{\eta_j^{os}}}{s^2} = \frac{2\,\alpha\sigma^2_{\eta_i}}{s^2} + \frac{\alpha(\sigma^2_{\beta_i} + \sigma^2_{\beta_j})}{s^2} \tag{0.35}$$

$$= \alpha(\sigma_b^2 + \sigma_\beta^2), \tag{0.36}$$

where $\sigma_\beta^2 = \frac{\sigma^2_{\beta_i} + \sigma^2_{\beta_j}}{s^2}$ is the variance introduced by the biases of different classifiers. The result of bias then manifests itself both in the mean and the variance of the boundary offset b^{os}.

We have now obtained the first and second moments of b^{os}, and can compute the added error region. Namely, we have $M_1^{os} = \bar{\beta}$ and $\sigma^2_{b^{os}} = M_2^{os} - (M_1^{os})^2$ leading to:

$$E^{os}_{add}(\beta) = \frac{s}{2}\,M_2^{os} = \frac{s}{2}\,(\sigma^2_{b^{os}} + \bar{\beta}^2) \tag{0.37}$$

$$= \frac{s}{2}\,(\alpha(\sigma_b^2 + \sigma_\beta^2) + \bar{\beta}^2). \tag{0.38}$$

[6] Since the exact distribution parameters of b^{os} are not known, we use the sample mean and the sample variance.

The reduction in the error is more difficult to assess in this case. By writing the error as:

$$E_{add}^{os}(\beta) \;=\; \alpha(\frac{s}{2}\,(\sigma_b^2+\beta^2)) \;+\; \frac{s}{2}\,(\alpha\sigma_\beta^2+\bar{\beta}^2-\alpha\beta^2),$$

we get:

$$E_{add}^{os}(\beta) \;=\; \alpha\,E_{add}(\beta)+\frac{s}{2}\,(\alpha\sigma_\beta^2+\bar{\beta}^2-\alpha\beta^2). \tag{0.39}$$

Analyzing the error reduction in the general case requires knowledge about the bias introduced by each classifier. However, it is possible to analyze the extreme cases. If each classifier has the same bias for example, σ_β^2 is reduced to zero and $\bar{\beta}=\beta$. In this case the error reduction can be expressed as:

$$E_{add}^{os}(\beta) \;=\; \frac{s}{2}\,(\alpha\sigma_b^2+\beta^2),$$

where only the error contribution due to the variance of b is reduced. In this case it is important to reduce classifier bias before combining (e.g. by using an overparametrized model). If on the other hand, the biases produce a zero mean variable, i.e. they cancel each other out, we obtain $\bar{\beta}=0$. In this case, the added error becomes:

$$E_{add}^{os}(\beta) \;=\; \alpha\,E_{add}(\beta)+\frac{s\,\alpha}{2}\,(\sigma_\beta^2-\beta^2)$$

and the error reduction will be significant as long as $\sigma_\beta^2 \leq \beta^2$.

0.5 Correlated Classifier Combining

0.5.1 Introduction

The discussion so far focused on finding the types of combiners that improve performance. Yet, it is important to note that if the classifiers to be combined repeatedly provide the same (either erroneous or correct) classification decisions, there is little to be gained from combining, regardless of the chosen scheme. Therefore, the selection and training of the classifiers that will be combined is as critical an issue as the selection of the combining method. Indeed, classifier/data selection is directly tied to the amount of correlation among the various classifiers, which in turn affects the amount of error reduction that can be achieved.

The tie between error correlation and classifier performance was directly or indirectly observed by many researchers. For regression problems, Perrone and Cooper show that their combining results are weakened if the networks are not independent [49]. Ali and Pazzani discuss the relationship between error correlations and error reductions in the context of decision trees [2]. Meir discusses the effect of independence on combiner performance [41], and

Jacobs reports that $N' \leq N$ independent classifiers are worth as much as N dependent classifiers [34]. The influence of the amount of training on ensemble performance is studied in [64]. For classification problems, the effect of the correlation among the classifier errors on combiner performance was quantified by the authors [70].

0.5.2 Combining Unbiased Correlated Classifiers

In this section we derive the explicit relationship between the correlation among classifier errors and the error reduction due to combining. Let us focus on the linear combination of unbiased classifiers. Without the independence assumption, the variance of $\bar{\eta}_i$ is given by:

$$\begin{aligned}\sigma^2_{\bar{\eta}_i} &= \frac{1}{N^2}\sum_{l=1}^{N}\sum_{m=1}^{N} cov(\eta_i^m(x), \eta_i^l(x)) \\ &= \frac{1}{N^2}\sum_{m=1}^{N}\sigma^2_{\eta_i^m(x)} + \frac{1}{N^2}\sum_{m=1}^{N}\sum_{l\neq m} cov(\eta_i^m(x), \eta_i^l(x))\end{aligned}$$

where $cov(\cdot,\cdot)$ represents the covariance. Expressing the covariances in term of the correlations ($cov(x,y) = corr(x,y)\,\sigma_x\,\sigma_y$), leads to:

$$\sigma^2_{\bar{\eta}_i} = \frac{1}{N^2}\sum_{m=1}^{N}\sigma^2_{\eta_i^m(x)} + \frac{1}{N^2}\sum_{m=1}^{N}\sum_{l\neq m} corr(\eta_i^m(x), \eta_i^l(x))\sigma_{\eta_i^m(x)}\sigma_{\eta_i^l(x)}. \quad (0.40)$$

In situations where the variance of a given output is comparable across the different classifiers, Equation 0.40 is significantly simplified by using the common variance σ_{η_i}, thus becoming:

$$\sigma^2_{\bar{\eta}_i} = \frac{1}{N}\sigma^2_{\eta_i(x)} + \frac{1}{N^2}\sum_{m=1}^{N}\sum_{l\neq m} corr(\eta_i^m(x), \eta_i^l(x))\sigma^2_{\eta_i(x)}\ .$$

Let δ_i be the correlation factor among all classifiers for the ith output:

$$\delta_i = \frac{1}{N\,(N-1)}\sum_{m=1}^{N}\sum_{m\neq l} corr(\eta_i^m(x), \eta_i^l(x)).$$

The variance of $\bar{\eta}_i$ becomes:

$$\sigma^2_{\bar{\eta}_i} = \frac{1}{N}\sigma^2_{\eta_i(x)} + \frac{N-1}{N}\,\delta_i\,\sigma^2_{\eta_i(x)}\ .$$

Now, let us return to the boundary x^{ave}, and its offset b^{ave}, where:

$$f_i^{ave}(x^* + b^{ave}) = f_j^{ave}(x^* + b^{ave}).$$

In Section 0.3.1, the variance of b^{ave} was shown to be:

$$\sigma^2_{b^{ave}} \;=\; \frac{\sigma^2_{\bar{\eta}_i} + \sigma^2_{\bar{\eta}_j}}{s^2}.$$

Therefore:

$$\sigma^2_{b^{ave}} \;=\; \frac{1}{s^2}\left(\frac{1}{N}\sigma^2_{\eta_i(x)}(1+(N-1)\delta_i) \;+\; \frac{1}{N}\sigma^2_{\eta_j(x)}(1+(N-1)\delta_j)\right)$$

which leads to:

$$\sigma^2_{b^{ave}} \;=\; \frac{1}{s^2 N}\left(\sigma^2_{\eta_i(x)} \;+\; \sigma^2_{\eta_j(x)} \;+\; (N-1)\,(\delta_i\,\sigma^2_{\eta_i(x)} \;+\; \delta_j\,\sigma^2_{\eta_j(x)})\right),$$

or:

$$\sigma^2_{b^{ave}} \;=\; \frac{\sigma^2_{\eta_i(x)} \;+\; \sigma^2_{\eta_j(x)}}{Ns^2} \;+\; \frac{N-1}{Ns^2}(\delta_i\sigma^2_{\eta_i(x)} + \delta_j\sigma^2_{\eta_j(x)}). \tag{0.41}$$

Recalling that the noise between classes are i.i.d. leads to[7]:

$$\begin{aligned}\sigma^2_{b^{ave}} &= \frac{1}{N}\sigma^2_b \;+\; (\frac{N-1}{N})\frac{2\sigma^2_{\eta_j(x)}}{s^2}\frac{\delta_i+\delta_j}{2}\\ &= \frac{\sigma^2_b}{N}\left(1 \;+\; (N-1)\frac{\delta_i+\delta_j}{2}\right).\end{aligned}$$

This expression only considers the error that occur between classes i and j. In order to extend this expression to include all the boundaries, we introduce an overall correlation term δ. Then, the added error is computed in terms of δ. The correlation among classifiers is calculated using the following expression:

$$\delta = \sum_{i=1}^{L} P_i\,\delta_i \tag{0.42}$$

where P_i is the prior probability of class i. The correlation contribution of each class to the overall correlation, is proportional to the prior probability of that class.

Let us now return to the error region analysis. With this formulation the first and second moments of b^{ave} yield: $M_1^{ave} = 0$, and $M_2^{ave} = \sigma^2_{b^{ave}}$. The derivation is identical to that of Section 0.3.1 and the only change is in the relation between σ^2_b and $\sigma^2_{b^{ave}}$. We then get:

$$\begin{aligned}E^{ave}_{add} &= \frac{sM_2^{ave}}{2} \;=\; \frac{s}{2}\,\sigma^2_{b^{ave}}\\ &= \frac{s}{2}\,\sigma^2_b\left(\frac{1+\delta(N-1)}{N}\right)\\ &= E_{add}\left(\frac{1+\delta(N-1)}{N}\right).\end{aligned} \tag{0.43}$$

[7] The errors between classifiers are correlated, not the errors between classes.

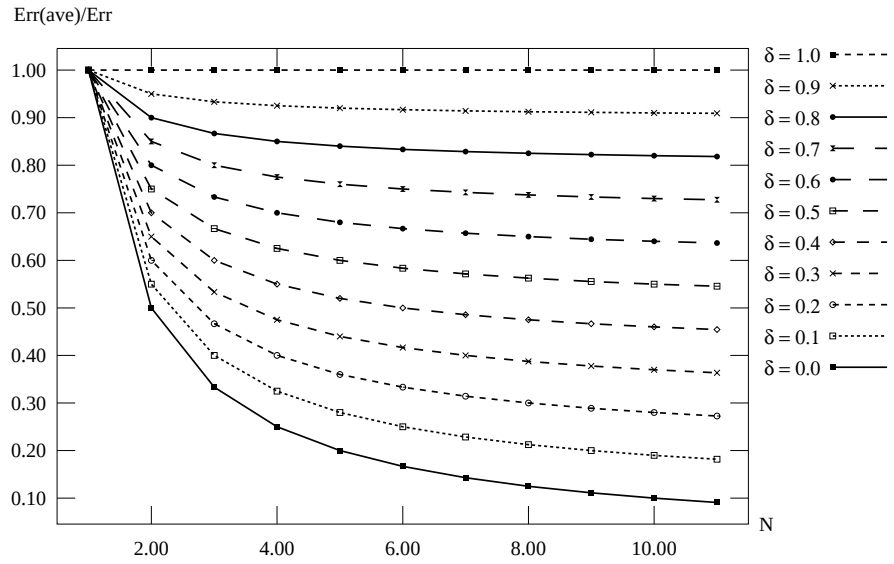

Fig. 0.3. Error reduction ($\frac{E^{ave}_{add}}{E_{add}}$) for different classifier error correlations.

The effect of the correlation between the errors of each classifier is readily apparent from Equation 0.43. If the errors are independent, then the second part of the reduction term vanishes and the combined error is reduced by N. If on the other hand, the error of each classifier has correlation 1, then the error of the combiner is equal to the initial errors and there is no improvement due to combining. Figure 0.3 shows how the variance reduction is affected by N and δ (using Equation 0.43).

In general, the correlation values lie between these two extremes, and some reduction is achieved. It is important to understand the interaction between N and δ in order to maximize the reduction. As more and more classifiers are used (increasing N), it becomes increasingly difficult to find uncorrelated classifiers. Figure 0.3 can be used to determine the number of classifiers needed for attaining satisfactory combining performance.

0.5.3 Combining Biased Correlated Classifiers

Let us now return to the analysis of biased classifiers. As discussed in Section 0.3, the boundary offset of a single classifier is given by:

$$b \;=\; \frac{\eta_i(x_b) - \eta_j(x_b)}{s} + \beta \;, \tag{0.44}$$

where $\beta = \frac{\beta_i - \beta_j}{s}$, leading to the following added error term:

$$E_{add}(\beta) = \frac{s}{2}\,(\sigma_b^2 + \beta^2). \tag{0.45}$$

Let us now focus on the effects of the *ave* combiner on the boundary. The combiner output is now given by:

$$f_i^{ave}(x) = p_i(x) \;+\; \bar{\beta}_i \;+\; \bar{\eta}_i(x)\;,$$

where $\bar{\eta}_i(x)$ and $\bar{\beta}_i$ are given in Section 0.3. The boundary offset, b^{ave} is:

$$b^{ave} \;=\; \frac{\bar{\eta}_i(x_b) - \bar{\eta_j}(x_b)}{s} + \bar{\beta}, \tag{0.46}$$

where $\bar{\beta}$ is given by Equation 0.22. The variance of b^{ave} is not affected by the biases, and the derivation of Section 0.5.2 applies to this case as well.

The first and second moments of b^{ave}, the boundary offset obtained using the *ave* combiner, for biased, correlated classifiers, are given by: $M_1^{ave} = \bar{\beta}$ and $M_2^{ave} = \sigma_{b^{ave}}^2 - (\bar{\beta})^2$. The corresponding added error region is:

$$E_{add}^{ave}(\bar{\beta}) \;=\; \frac{sM_2^{ave}}{2} \;=\; \frac{s}{2}\,(\sigma_{b^{ave}}^2 + (\bar{\beta})^2)\,.$$

Using the overall correlation term obtained in the previous section, we can represent this expression in terms of the boundary parameters of the single classifier, and the bias reduction factor z introduced in Section 0.3.2:

$$E_{add}^{ave}(\bar{\beta}) \;=\; \frac{s}{2}\,\left(\sigma_b^2\left(\frac{1+\delta(N-1)}{N}\right) + \frac{\beta^2}{z^2}\right)\,. \tag{0.47}$$

In order to obtain the error reduction rates, let us introduce τ, the factor that will determine the final reduction:

$$\tau^2 = min\left(z^2, \left(\frac{1+\delta(N-1)}{N}\right)\right). \tag{0.48}$$

Now, Equation 0.47 leads to:

$$E_{add}^{ave}(\bar{\beta}) \;\leq\; \frac{1}{\tau}\,E_{add}(\beta)\,. \tag{0.49}$$

Equation 0.49 shows the error reduction for correlated, biased classifiers. As long as the biases of individual classifiers are reduced by a larger amount than the correlated variances, the reduction will be similar to those in Section 0.5.2. However, if the biases are not reduced, the improvement gains will not be as significant. These results are conceptually identical to those obtained in Section 0.3, but vary in how the bias reduction z relates to N. In effect, the requirements on reducing z are lower than they were previously, since in the presence of bias, the error reduction is less than $\frac{1}{N}$. The practical implication of this observation is that, even in the presence of bias, the correlation dependent variance reduction term (given in Equation 0.43) will often be the limiting factor, and dictate the error reductions.

0.5.4 Discussion

In this section we established the importance of the correlation among the errors of individual classifiers in a combiner system. One can exploit this relationship explicitly by reducing the correlation among classifiers that will be combined. Several methods have been proposed for this purpose and many researchers are actively exploring this area [60].

Cross-validation, a statistical method aimed at estimating the "true' error [21, 65, 75], can also be used to control the amount of correlation among classifiers. By only training individual classifiers on overlapping subsets of the data, the correlation can be reduced. The various boosting algorithms exploit the relationship between corrlation and error rate by training subsequent classifiers on training patterns that have been "selected" by earlier classifiers [15, 13, 19, 59] thus reducing the correlation among them. Krogh and Vedelsky discuss how cross-validation can be used to improve ensemble performance [36]. Bootstrapping, or generating different training sets for each classifier by resampling the original set [17, 18, 35, 75], provides another method for correlation reduction [47]. Breiman also addresses this issue, and discusses methods aimed at reducing the correlation among estimators [9, 10]. Twomey and Smith discuss combining and resampling in the context of a 1-d regression problem [74]. The use of principal component regression to handle multi-collinearity while combining outputs of multiple regressors, was suggested in [42]. Another approach to reducing the correlation of classifiers can be found in input decimation, or in purposefully withholding some parts of each pattern from a given classifier [70]. Modifying the training of individual classifiers in order to obtain less correlated classifiers was also explored [56], and the selection of individual classifier through a genetic algorithm is suggested in [46].

In theory, reducing the correlation among classifiers that are combined increases the ensemble classification rates. In practice however, since each classifier uses a subset of the training data, individual classifier performance can deteriorate, thus offsetting any potential gains at the ensemble level [70]. It is therefore crucial to reduce the correlations without increasing the individual classifiers' error rates.

0.6 Experimental Combining Results

In order to provide in depth analysis and to demonstrate the result on public domain data sets, we have divided this section into two parts. First we will provide detailed experimental results on one difficult data set, outlining all the relevant design steps/parameters. Then we will summarize results on several public domain data sets taken from the UCI depository/Proben1 benchmarks [50].

0.6.1 Oceanic Data Set

The experimental data set used in this section is derived from underwater SONAR signals. From the original SONAR signals of four different underwater objects, two feature sets are extracted [25, 27]. The first one (FS1), a 25-dimensional set, consists of Gabor wavelet coefficients, temporal descriptors and spectral measurements. The second feature set (FS2), a 24-dimensional set, consists of reflection coefficients based on both short and long time windows, and temporal descriptors. Each set consists of 496 training and 823 test patterns. The data is available at URL *http://www.lans.ece.utexas.edu.*

Combining Results. In this section we present detailed results obtained from the Oceanic data described above. Two types of feed forward networks, namely a multi-layered perceptron (MLP) with a single hidden layer with 50 units and a radial basis function (RBF) network with 50 kernels, are used to classify the patterns. Table 0.2 provides the test set results for individual classifier/feature set pairs. The reported error percentages are averaged over 20 runs. Tables 0.3 and 0.4 show the combining results for each feature set. Combining consists of utilizing the outputs of multiple MLPs, RBFs or an MLP/RBF mix, and performing the operations described in Equations 0.16, 0.26, 0.27 and 0.28. When combining an odd number of classifiers, the classifier with the better performance is selected once more than the less successful one. For example, when combining the MLP and RBF results on FS1 for $N = 5$, three RBF networks and two MLPs are used. Table 0.5 shows the improvements that are obtained if more than one feature set is available[8].

Table 0.2. Individual Classifier Performance on Test Set.

Classifier/ Feature Set	Error Rate	st. dev.
FS1/MLP	7.47	0.44
FS1/RBF	6.79	0.41
FS2/MLP	9.95	0.74
FS2/RBF	10.94	0.93

The performance of the *ave* combiner is better than that of the *os* combiners, especially for the second feature set (FS2). While combining information from two different feature sets, the linear combiner performed best with the RBF classifiers, while the *max* combiner performed best with the MLP classifiers. Furthermore, using different types of classifiers does not change the performance of the linear combiner when qualitatively different feature sets are used. However, for the *os* combiners, the results do improve when both different classifier types and different feature sets are used.

[8] All the combining results provide improvements that are statistically significant over the individual classifiers, or more precisely, the hypothesis that the two means are equal (t–test) is rejected for $\alpha = .05$.

Table 0.3. Combining Results for FS1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	7.19	0.29	7.25	0.21	7.38	0.37	7.19	0.37
	5	7.13	0.27	7.30	0.29	7.32	0.41	7.20	0.37
	7	7.11	0.23	7.27	0.29	7.27	0.37	7.35	0.30
RBF	3	6.15	0.30	6.42	0.29	6.22	0.34	6.30	0.40
	5	6.05	0.20	6.23	0.18	6.12	0.34	6.06	0.39
	7	5.97	0.22	6.25	0.20	6.03	0.35	5.92	0.31
BOTH	3	6.11	0.34	6.02	0.33	6.48	0.43	6.89	0.29
	5	6.11	0.31	5.76	0.29	6.59	0.40	6.89	0.24
	7	6.08	0.32	5.67	0.27	6.68	0.41	6.90	0.26

Table 0.4. Combining Results for FS2.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	9.32	0.35	9.47	0.47	9.64	0.47	9.39	0.34
	5	9.20	0.30	9.22	0.30	9.73	0.44	9.27	0.30
	7	9.07	0.36	9.11	0.29	9.80	0.48	9.25	0.36
RBF	3	10.55	0.45	10.49	0.42	10.59	0.57	10.74	0.34
	5	10.43	0.30	10.51	0.34	10.55	0.40	10.65	0.37
	7	10.44	0.32	10.46	0.31	10.58	0.43	10.66	0.39
BOTH	3	8.46	0.57	9.20	0.49	8.65	0.47	9.56	0.53
	5	8.17	0.41	8.97	0.54	8.71	0.36	9.50	0.45
	7	8.14	0.28	8.85	0.45	8.79	0.40	9.40	0.39

Correlation Factors. Let us now estimate the correlation factors among the different classifiers in order to determine the compatibility of the various classifier/feature set pairs. The data presented in Section 0.6.1 will be used in this section. Table 0.6 shows the estimated average error correlations between:

- different runs of a single classifier on a single feature set (first four rows);
- different classifiers trained with a single feature set (fifth and sixth rows);
- single classifier trained on two different feature sets (seventh and eighth rows).

There is a striking similarity between these correlation results and the improvements obtained through combining. When different runs of a single classifier are combined using only one feature set, the combining improvements are very modest. These are also the cases where the classifier correlation coefficients are the highest. Mixing different classifiers reduces the correlation, and in most cases, improves the combining results. The most drastic improvements are obtained when two qualitatively different feature sets are used, which are also the cases with the lowest classifier correlations.

Table 0.5. Combining Results when Both Feature Sets are Used.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	5.21	0.33	6.25	0.36	4.37	0.41	4.72	0.28
	5	4.63	0.35	5.64	0.32	4.22	0.41	4.58	0.17
	7	4.20	0.40	5.29	0.28	4.13	0.34	4.51	0.20
RBF	3	3.70	0.33	5.78	0.32	4.76	0.37	3.93	0.50
	5	3.40	0.21	5.38	0.38	4.73	0.35	3.83	0.43
	7	3.42	0.21	5.15	0.31	4.70	0.36	3.76	0.33
BOTH	3	3.94	0.24	4.52	0.29	4.34	0.42	4.51	0.30
	5	3.42	0.23	4.35	0.32	4.13	0.49	4.48	0.29
	7	3.40	0.26	4.05	0.29	4.10	0.36	4.39	0.24

Table 0.6. Experimental Correlation Factors Between Classifier Errors.

Feature Set/Classifier Pairs	Estimated Correlation
Two runs of FS1/MLP	0.89
Two runs of FS1/RBF	0.79
Two runs of FS2/MLP	0.79
Two runs of FS2/RBF	0.77
FS1/MLP and FS1/RBF	0.38
FS2/MLP and FS2/RBF	0.21
FS1/MLP and FS2/MLP	-0.06
FS1/RBF and FS2/RBF	-0.21

0.6.2 Proben1 Benchmarks

In this section, examples from the Proben1 benchmark set[9] are used to study the benefits of combining [50]. Table 0.7 shows the test set error rate for both the MLP and the RBF classifiers on six different data sets taken from the Proben1 benchmarks[10].

Table 0.7. Performance of Individual Classifiers on the Test Set.

	MLP		RBF		Proben1-A		Proben1-B	
	Error	σ	Error	σ	Error	σ	Error	σ
CANCER1	0.69	0.23	1.49	0.79	1.47	0.64	1.38	0.49
CARD1	13.87	0.76	13.98	0.95	13.64	0.85	14.05	1.03
DIABETES1	23.52	0.72	24.87	1.51	24.57	3.53	24.10	1.91
GENE1	13.47	0.44	14.62	0.42	15.05	0.89	16.67	3.75
GLASS1	32.26	0.57	31.79	3.49	39.03	8.14	32.70	5.34
SOYBEAN1	7.35	0.90	7.88	0.75	9.06	0.80	29.40	2.50

[9] Available from: *ftp://ftp.ira.uka.de/pub/papers/techreports/1994/1994-21.ps.Z.*

[10] These Proben1 results correspond to the "pivot" and "no-shortcut" architectures (A and B respectively), reported in [50]. The large error in the Proben1 no-shortcut architecture for the SOYBEAN1 problem is not explained.

Table 0.8. Combining Results for CANCER1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	0.60	0.13	0.63	0.17	0.66	0.21	0.66	0.21
	5	0.60	0.13	0.58	0.00	0.63	0.17	0.63	0.17
	7	0.60	0.13	0.58	0.00	0.60	0.13	0.60	0.13
RBF	3	1.29	0.48	1.12	0.53	1.90	0.52	0.95	0.42
	5	1.26	0.47	1.12	0.47	1.81	0.58	0.98	0.37
	7	1.32	0.41	1.18	0.43	1.81	0.53	0.89	0.34
BOTH	3	0.86	0.39	0.63	0.18	1.03	0.53	0.95	0.42
	5	0.72	0.25	0.72	0.25	1.38	0.43	0.83	0.29
	7	0.86	0.39	0.58	0.00	1.49	0.39	0.83	0.34

Table 0.9. Combining Results for CARD1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	13.37	0.45	13.61	0.56	13.43	0.44	13.40	0.47
	5	13.23	0.36	13.40	0.39	13.37	0.45	13.31	0.40
	7	13.20	0.26	13.29	0.33	13.26	0.35	13.20	0.32
RBF	3	13.40	0.70	13.58	0.76	14.01	0.66	13.08	1.05
	5	13.11	0.60	13.29	0.67	13.95	0.66	12.88	0.98
	7	13.02	0.33	12.99	0.33	13.75	0.76	12.82	0.67
BOTH	3	13.75	0.69	13.69	0.70	13.49	0.62	13.66	0.70
	5	13.78	0.55	13.66	0.67	13.66	0.65	13.75	0.64
	7	13.84	0.51	13.52	0.58	13.66	0.60	13.72	0.70

The six data sets used here are CANCER1, DIABETES1, CARD1, GENE1, GLASS1 and SOYBEAN1. The name and number combinations correspond to a specific training/validation/test set split[11]. In all cases, training was stopped when the test set error reached a plateau. We report error percentages on the test set, and the standard deviation on those values based on 20 runs.

CANCER1 is based on breast cancer data, obtained from the University of Wisconsin Hospitals, from Dr. William H. Wolberg [40, 76]. This set has 9 inputs, 2 outputs and 699 patterns, of which 350 is used for training. An MLP with one hidden layer of 10 units, and an RBF network with 8 kernels is used with this data.

The CARD1 data set consists of credit approval decisions [51, 52]. 51 inputs are used to determine whether or not to approve the credit card application of a customer. There are 690 examples in this set, and 345 are used for training. The MLP has one hidden layer with 20 units, and the RBF network has 20 kernels.

The DIABETES1 data set is based on personal data of the Pima Indians obtained from the National Institute of Diabetes and Digestive and Kidney Diseases [63]. The binary output determines whether or not the subjects

[11] We are using the same notation as in the Proben1 benchmarks.

Table 0.10. Combining Results for DIABETES1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	23.15	0.60	23.20	0.53	23.15	0.67	23.15	0.67
	5	23.02	0.59	23.13	0.53	22.81	0.78	22.76	0.79
	7	22.79	0.57	23.07	0.52	22.89	0.86	22.79	0.88
RBF	3	24.69	1.15	24.77	1.28	24.82	1.07	24.77	1.09
	5	24.32	0.86	24.35	0.72	24.66	0.81	24.56	0.90
	7	24.22	0.39	24.32	0.62	24.79	0.80	24.35	0.73
BOTH	3	24.32	1.14	23.52	0.60	24.35	1.21	24.51	1.07
	5	24.53	0.97	23.49	0.59	24.51	1.16	24.66	1.02
	7	24.43	0.93	23.85	0.63	23.85	0.93	24.53	0.86

show signs of diabetes according to the World Health Organization. The input consists of 8 attributes, and there are 768 examples in this set, half of which are used for training. MLPs with one hidden layer with 10 units, and RBF networks with 10 kernels are selected for this data set.

The GENE1 is based on intron/exon boundary detection, or the detection of splice junctions in DNA sequences [45, 66]. 120 inputs are used to determine whether a DNA section is a donor, an acceptor or neither. There are 3175 examples, of which 1588 are used for training. The MLP architecture consists of a single hidden layer network with 20 hidden units. The RBF network has 10 kernels.

The GLASS1 data set is based on the chemical analysis of glass splinters. The 9 inputs are used to classify 6 different types of glass. There are 214 examples in this set, and 107 of them are used for training. MLPs with a single hidden layer of 15 units, and RBF networks with 20 kernels are selected for this data set.

The SOYBEAN1 data set consists of 19 classes of soybean, which have to be classified using 82 input features [43]. There are 683 patterns in this set, of which 342 are used for training. MLPs with one hidden layer with 40 units, and RBF networks with 40 kernels are selected.

Table 0.11. Combining Results for GENE1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	12.30	0.42	12.46	0.40	12.73	0.55	12.62	0.56
	5	12.23	0.40	12.40	0.40	12.67	0.41	12.33	0.57
	7	12.08	0.23	12.27	0.35	12.57	0.31	12.18	0.43
RBF	3	14.48	0.37	14.52	0.30	14.53	0.40	14.42	0.33
	5	14.35	0.33	14.43	0.29	14.38	0.24	14.36	0.35
	7	14.33	0.35	14.40	0.24	14.28	0.18	14.33	0.32
BOTH	3	12.43	0.48	12.67	0.32	12.87	0.65	12.77	0.51
	5	12.28	0.40	12.54	0.35	12.80	0.54	12.47	0.65
	7	12.17	0.36	12.69	0.35	12.70	0.46	12.25	0.66

Table 0.12. Combining Results for GLASS1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	7	32.07	0.00	32.07	0.00	32.07	0.00	32.07	0.00
	5	32.07	0.00	32.07	0.00	32.07	0.00	32.07	0.00
	7	32.07	0.00	32.07	0.00	32.07	0.00	32.07	0.00
RBF	3	29.81	2.28	30.76	2.74	30.28	2.02	29.43	2.89
	5	29.25	1.84	30.19	1.69	30.85	2.00	28.30	2.46
	7	29.06	1.51	30.00	1.88	31.89	1.78	27.55	1.83
BOTH	3	30.66	2.52	29.06	2.02	33.87	1.74	29.91	2.25
	5	32.36	1.82	28.30	1.46	33.68	1.82	29.72	1.78
	7	32.45	0.96	27.93	1.75	34.15	1.68	29.91	1.61

Table 0.13. Combining Results for SOYBEAN1.

Classifier(s)		Ave		Med		Max		Min	
	N	Error	σ	Error	σ	Error	σ	Error	σ
MLP	3	7.06	0.00	7.09	0.13	7.06	0.00	7.85	1.42
	5	7.06	0.00	7.06	0.00	7.06	0.00	8.38	1.63
	7	7.06	0.00	7.06	0.00	7.06	0.00	8.88	1.68
RBF	3	7.74	0.47	7.65	0.42	7.85	0.47	7.77	0.44
	5	7.62	0.23	7.68	0.30	7.77	0.30	7.65	0.42
	7	7.68	0.23	7.82	0.33	7.68	0.29	7.59	0.45
BOTH	3	7.18	0.23	7.12	0.17	7.56	0.28	7.85	1.27
	5	7.18	0.23	7.12	0.17	7.50	0.25	8.06	1.22
	7	7.18	0.24	7.18	0.23	7.50	0.25	8.09	1.05

Tables 0.8 - 0.13 show the performance of the *ave* and *os* combiners. From these results, we see that improvements are modest in general. However, recall that the reduction factors obtained in the previous sections are on the *added* errors, not the overall error. For the Proben1 problems, individual classifiers are performing well (as well or better than the results reported in [50] in most cases) and it is therefore difficult to improve the results drastically. However, even in those cases, combining provides an advantage: although the classification rates are not dramatically better, they are more reliable. Indeed, a lower standard deviation means the results are less dependent on outside factors such as initial conditions and training regime. In some cases all 20 instances of the combiner provide the same result, and the standard deviation is reduced to zero. This can be seen in both the CANCER1 and SOYBEAN1 data sets.

One important observation that emerges from these experiments is that combining two different types of classifiers does not necessarily improve upon (or in some cases, even reach) the error rates obtained by combining multiple runs of the better classifier. This apparent inconsistency is caused by two factors. First, as described in section 0.3.2 the reduction factor is limited by

the bias reduction in most cases. If the combined bias is not lowered, the combiner will not outperform the better classifier. Second, as discussed in section 0.5.2, the correlation plays a major role in the final reduction factor. There are no guarantees that using different types of classifiers will reduce the correlation factors. Therefore, the combining of different types of classifiers, especially when their respective performances are significantly different (the error rate for the RBF network on the CANCER1 data set is over twice the error rate for MLPs) has to be treated with caution.

Determining which combiner (e.g. *ave* or *med*), or which classifier selection (e.g. multiple MLPs or MLPs and RBFs) will perform best in a given situation is not generally an easy task. However, some information can be extracted from the experimental results. The linear combiner, for example, appears more compatible with the MLP classifiers than with the RBF networks. When combining two types of network, the *med* combiner often performs better than other combiners. One reason for this is that the outputs that will be combined come from different sources, and selecting the largest or smallest value can favor one type of network over another. These results emphasize the need for closely coupling the problem at hand with a classifier/combiner. There does not seem to be a single type of network or combiner that can be labeled "best" under all circumstances.

0.7 Discussion

Combining the outputs of several classifiers before making the classification decision, has led to improved performance in many applications [27, 81, 83]. This article presents a mathematical framework that underlines the reasons for expecting such improvements and quantifies the gains achieved. We show that combining classifiers in output space reduces the variance in boundary locations about the optimum (Bayes) boundary decision. Moreover, the added error regions associated with different classifiers are directly computed and given in terms of the boundary distribution parameters. In the absence of classifier bias, the reduction in the added error is directly proportional to the reduction in the variance. For linear combiners, if the errors of individual classifiers are zero-mean i.i.d., the reduction in boundary variance is shown to be N, the number of classifiers that are combined. When the classifiers are biased, and/or have correlated outputs, the reductions are less than N.

Order statistics combiners are discussed as an alternative to linear methods, and are motivated by their ability to extract the "right" amount of information. We study this family of combiners analytically, and we present experimental results showing that *os* combiners improve upon the performance of individual classifiers. During the derivation of the main result, the decision boundary is treated as a random variable without specific distribution assumptions. However, in order to obtain the table of reduction factors for the order statistics combiners, a specific error model needed to be adopted.

Since there may be a multitude of factors contributing to the errors, we have chosen the Gaussian model. Reductions for several other noise models can be obtained from similar tables available in order statistics textbooks [3, 12]. The expected error given in Equation 0.9 is in general form, and any density function can be used to reflect changes in the distribution function.

Although most of our analysis focuses on two classes, it is readily applicable to multi-class problems. In general, around a boundary decision, the error is governed by the two (locally) dominant classes. Therefore, even in a multi-class problem, one only needs to consider the two classes with the highest activation values (i.e., highest posterior) in a given localized region.

Another important feature that arises from this study provides a new look to the classic bias/variance dilemma. Combining provides a method for decoupling the two components of the error to a degree, allowing a reduction in the overall error. Bias in the individual classifiers can be reduced by using larger classifiers than required, and the increased variance due to the larger classifiers can be reduced during the combining stage. Studying the effects of this coupling between different errors and distinguishing situations that lead to the highest error reduction rates are the driving motivations behind this work. That goal is attained by clarifying the relationship between output space combining and classification performance.

Several practical issues that relate to this analysis can now be addressed. First, let us note that since in general each individual classifier will have some amount of bias, the actual improvements will be less radical than those obtained in Section 0.3.1. It is therefore important to determine how to keep the individual biases minimally correlated. One method is to use classifiers with paradigms/architectures based on different principles. For example, using multi-layered perceptrons and radial basis function networks provides both global and local information processing, shows less correlation than if classifiers of only one type were used. Other methods such as resampling, cross-validation or actively promoting diversity among classifiers can also be used, as long as they do not adversely affect the individual classification results.

The amount of training that is required before classifiers are combined is also an interesting question. If a combiner can overcome overtraining or undertraining, new training regimes could be used for classifiers that will be combined. We have observed that combiners do compensate for overtraining, but not undertraining (except in cases where the undertraining is very mild). This corroborates well with the theoretical framework which shows combining to be more effective at variance reduction than bias reduction.

The classification rates obtained by the order statistics combiners in section 0.6 are in general, comparable to those obtained by averaging. The advantage of OS approaches should be more evident in situations where there is substantial variability in the performance of individual classifiers, and the thus robust properties of OS combining can be brought to bear upon. Such

variability in individual performance may be due to, for example, the classifiers being geographically distributed and working only on locally available data of highly varying quality. Current work by the authors indicate that this is indeed the case, but the issue needs to be examined in greater detail.

One final note that needs to be considered is the behavior of combiners for a large number of classifiers (N). Clearly, the errors cannot be arbitrarily reduced by increasing N indefinitely. This observation however, does not contradict the results presented in this analysis. For large N, the assumption that the errors were i.i.d. breaks down, reducing the improvements due to each extra classifier. The number of classifiers that yield the best results depends on a number of factors, including the number of feature sets extracted from the data, their dimensionality, and the selection of the network architectures.

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