

Ensemble Methods

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1 Introduction

The idea of *ensemble learning* is to employ multiple learners and combine their predictions. There is no definitive taxonomy. Jain, Duin and Mao (2000) list eighteen classifier combination schemes; Witten and Frank (2000) detail four methods of combining multiple models: bagging, boosting, stacking and error-correcting output codes whilst Alpaydin (2004) covers seven methods of combining multiple learners: voting, error-correcting output codes, bagging, boosting, mixtures of experts, stacked generalization and cascading. We focus on four methods, then review the literature in general, with, where possible, an emphasis on both theory and practical advice.

2 Bagging

Bagging (Breiman 1996), a name derived from “bootstrap aggregation”, was the first effective method of ensemble learning and is one of the simplest methods of arching¹. The meta-algorithm, which is a special case of the model averaging, was originally designed for classification and is usually applied to decision tree models, but it can be used with any type of model for classification or regression. The method uses multiple versions of a training set by using the bootstrap, i.e. sampling with replacement. Each of these data sets is used to train a different model. The outputs of the models are combined by averaging (in case of regression) or voting (in case of classification) to create a single output. Bagging is only effective when using unstable (i.e. a small change in the training set can cause a significant change in the model) nonlinear models.

3 Boosting (including AdaBoost)

Boosting (Schapire 1990) is a meta-algorithm which can be viewed as a model averaging method. It is the most widely used ensemble method and one of

¹Archiving (adaptive reweighting and combining) is a generic term that refers to reusing or selecting data in order to improve classification.

the most powerful learning ideas introduced in the last ten years. Originally designed for classification, it can also be profitably extended to regression. We first create a “weak” classifier, that is, it suffices that its accuracy on the training set is only slightly better than a random guessing. A succession of models are built iteratively, each one being trained on a data set in which points misclassified (or, with regression, those poorly predicted) by the previous model are given more weight. Finally, all of the successive models are weighted according to their success and then the outputs are combined using voting (for classification) or averaging (for regression), thus creating a final model. The original boosting algorithm combined three weak learners to generate a strong learner.

3.1 AdaBoost

AdaBoost (Freund and Schapire 1996), short for “adaptive boosting”, is the most popular boosting algorithm. It uses the same training set over and over again (thus it need not be large) and can also combine an arbitrary number of base-learners.

4 Stacked Generalization

Stacked generalization (or *stacking*) (Wolpert 1992) is a different way of combining multiple models, that introduces the concept of a meta learner. Although an attractive idea, it is less widely used than bagging and boosting. Unlike bagging and boosting, stacking may be (and normally is) used to combine models of different types. The procedure is as follows:

1. Split the training set into two disjoint sets.
2. Train several base learners on the first part.
3. Test the base learners on the second part.
4. Using the predictions from 3) as the inputs, and the correct responses as the outputs, train a higher level learner.

Note that steps 1) to 3) are the same as cross-validation, but instead of using a winner-takes-all approach, we combine the base learners, possibly nonlinearly.

5 Random Subspace Method

The *random subspace method* (RSM) (Ho 1998) is a relatively recent method of combining models. Learning machines are trained on randomly chosen subspaces of the original input space (i.e. the training set is sampled in the feature space). The outputs of the models are then combined, usually by a simple majority vote.

6 Literature Review

Wittner and Denker (1988) discussed strategies for teaching layered neural networks classification tasks.

Schapire (1990) introduced *boosting*. A theoretical paper by Kleinberg (1990) introduced a general method for separating points in multidimensional spaces through the use of stochastic processes called stochastic discrimination (SD). The method basically takes poor solutions as an input and creates good solutions. The paper introduced the promising ensemble method of stochastic discrimination, which led to the random subspace method. Hansen and Salamon (1990) showed the benefits of invoking ensembles of similar neural networks.

Wolpert (1992) introduced *stacked generalization*, a scheme for minimizing the generalization error rate of one or more generalizers. Xu, Krzyżak and Suen (1992) considered methods of combining multiple classifiers and their applications to handwriting recognition. They claim that according to the levels of output information by various classifiers, the problems of combining multiclassifiers can be divided into three types. They go on to compare three approaches from the first type: voting, Bayesian formalism and Dempster-Shafer formalism. They found that the performance of individual classifiers could be improved significantly and, if forced to pick one, they'd recommend the Dempster-Shafer formalism since it can obtain high recognition and reliability rates simultaneously and robustly.

Perrone and Cooper (1993) presented a general theoretical framework for ensemble methods of constructing significantly improved regression estimates. Jordan and Jacobs (1993) presented a hierarchical mixtures of experts model.

Ho, Hull and Srihari (1994) suggest a multiple classifier system based on rankings. In the field of handwritten digit recognition, Battiti and Colla (1994) found that the use of a small number of neural nets (two to three) with a sufficiently large uncorrelation in their mistakes reaches a combined performance that is significantly higher than the best obtainable from the individual nets.

Cho and Kim (1995) combined the results from multiple neural networks using fuzzy logic which resulted in more accurate classification. Bishop (1995) covers the theoretical aspects of committees of neural networks. If L networks produce errors which have zero mean and are uncorrelated, then the sum-of-squares error can be reduced by a factor of L simply by averaging the predictions of the L networks. Although in practice the errors are likely to be highly correlated. However, by making use of Cauchy's inequality, he also shows that the committee averaging process cannot produce an increase in the expected error. It is important to note that because the reduction in error can be viewed as arising from reduced variance due to the averaging over many solutions, when we select individual members, the optimal trade-off between bias and variance should have relatively smaller bias, since the extra variance can be removed by averaging. If we give greater weight to the committee members that make the better predictions, we can reduce the error further. The benefits of committee averaging are not limited to sum-of-squares error, but apply to any error function which is convex. Bishop also shows that the concept of a committee arises

naturally in a Bayesian framework. Krogh and Vedelsby (1995) showed that there is a lot to be gained from using unlabeled data when training ensembles. Lam and Suen (1995) studied the performance of four combination methods: the majority vote, two Bayesian formulations and a weighted majority vote (with weights obtained through a genetic algorithm). They conclude: “in the absence of a truly representative training set, simple majority vote remains the easiest and most reliable solution among the ones studied here.”

Tumer and Ghosh (1996) showed that combining neural networks linearly in output space reduces the variance of the actual decision region boundaries around the optimum boundary. Of great practical importance, Sollich and Krogh (1996) found that in large ensembles, it is advantageous to use under-regularized students, which actually over-fit the training data. This allows one to maximize the benefits of the variance-reducing effects of ensemble learning. Freund and Schapire (1996) introduced AdaBoost. Breiman (1996) introduced bagging.

Raftery, Madigan and Hoeting (1997) consider the problem of accounting for model uncertainty in linear regression models and offer two extensions to Bayesian model averaging: Occam’s window and Markov chain Monte Carlo. Woods, Kegelmeyer and Bowyer (1997) presented a method for combining classifiers that uses estimates of each individual classifier’s local accuracy in small regions of feature space surrounding an unknown test sample. An empirical evaluation showed that their local accuracy approach was more effective than the Classifier Rank algorithm, the Modified Classifier Rank algorithm and the Behavior-Knowledge Space (BKS) algorithm (which performed worst). In fact, on average, the Classifier Rank algorithm and the BKS algorithm both failed to outperform the single best classifier. The authors believe that the combining classifiers works best with large data sets with data distributions that are too complex for most individual classifiers. Larkey and Croft (1997) found that combining classifiers in text categorization improved performance. Lam and Suen (1997) analyzed the application of majority voting to pattern recognition.

Kittler (1998) developed a theoretical framework for combining classifiers in the two main fusion scenarios: fusion of opinions based on identical and on distinct representations. For the shared representation they showed that here the aim of fusion was to obtain a better estimation of the appropriate a posteriori class probabilities. For distinct representations they pointed out that the techniques based on the benevolent sum-rule fusion are more resilient to errors than those derived from the severe product rule. In both cases (distinct and shared representations), the expert fusion involves the computation of a linear or nonlinear function of the a posteriori class probabilities estimated by the individual experts. Kittler, *et al.* (1998) developed a common theoretical framework for classifier combination. An experimental comparison between the product rule, sum rule, min rule, max rule, median rule and majority voting found that the sum rule outperformed other classifier combinations schemes, and sensitivity analysis showed that the sum rule is most resilient to estimation errors (which may be as a plausible explanation for its superior performance). Ho (1998) introduces the random subspace method for constructing decision forests.

The method worked well in practice and was shown to perform best when the dataset has a large number of features and not too few samples. Schapire, *et al.* (1998) offer an explanation for the effectiveness of voting methods. They show that this phenomenon is related to the distribution of margins of the training examples with respect to the generated voting classification rule, where the margin of an example is simply the difference between the number of correct votes and the maximum number of votes received by any incorrect label.

Schapire (1999) introduces the boosting algorithm AdaBoost, and explains the underlying theory of boosting. Opitz and Maclin (1999) compared Bagging and two Boosting methods: Ada-Boosting and Arching. They found that in a low noise regime, Boosting outperforms Bagging, which outperforms a single classifier, whilst as a general technique Bagging is the most appropriate. Opitz (1999) consider feature selection for ensembles. Miller and Yan (1999) developed a critic-driven ensemble for classification. Hoeting, *et al.* (1999) provide a tutorial on Bayesian model averaging (BMA). Liu and Yao (1999) presented negative correlation learning for neural network ensembles.

Jain, Duin and Mao (2000) include a section on classifier combination. They list reasons for combining multiple classifiers: we may have different feature sets, different training sets, different classification methods or different training sessions, all resulting in a set of classifiers whose results may be combined with the hope of improved overall classification accuracy. They provide a taxonomy, see table. In terms of experimental work, they train twelve classifiers on six feature sets from a digit dataset and use four methods of classifier combination—median, product, nearest mean and 1-NN—across both the different feature sets and the different classifiers. Measuring performance against the best single result, our own conclusions from their results are that 1) there is no benefit in just combining different classifiers across the same feature set and 2) there is substantial benefit in combining the results of one classifier across different feature sets (1-NN worked best, but voting failed). However, when the classifiers are first combined on one feature set at a time, and then these results are combined, then using the nearest mean method for both stages of model combination gave the best overall result. This was also the best result of the entire experiment. Kleinberg (2000) bridged the gap between the theoretical promise shown by stochastic discrimination and a practical solution by providing the algorithmic implementation. He also showed that SD outperformed both boosting and bagging in the majority of benchmark problems that it was tested on. Kuncheva, *et al.* (2000) consider whether independence is good for combining classifiers. Their results support the intuition that negatively related classifiers are better than independent classifiers, and they also show that this relationship is ambivalent. Dietterich (2000) compared the effectiveness of randomization, bagging and boosting for improving the performance of the decision-tree algorithm C4.5. Their experiments showed that in situations with little or no classification noise, randomization is competitive with (and perhaps slightly superior to) bagging but not as accurate as boosting. In situations with substantial classification noise, bagging is much better than boosting, and sometimes better than randomization. Kuncheva and Jain (2000) designed two

classifier fusion systems using genetic algorithms and found that selection of classifiers and (possibly overlapping) feature subsets worked well, but selection of disjoint feature subsets did not. Tax, *et al.* (2000) sought to answer the question of whether to combine multiple classifiers by averaging or multiplying. They concluded that averaging-estimated posterior probabilities is to be preferred in the case when posterior probabilities are not well estimated. Only in the case of problems involving multiple classes with good estimates of posterior class probabilities did the product combination rule outperform the mean combination rule. Liu, Yao and Higuchi (2000) presented evolutionary ensembles with negative correlation learning (EENCL). Allwein, Schapire and Singer (2000) proved a general empirical multiclass loss bound given the empirical loss of the individual binary learning algorithms.

In a PhD thesis, Skurichina (2001) tackled the problem of stabilizing weak classifiers and compares bagging, boosting and the RSM. Bagging is useful for weak and unstable classifiers with a non-decreasing learning curve and critical training sample sizes. Boosting is beneficial only for weak, simple classifiers, with a non-decreasing learning curve, constructed on large training sample sizes. The RSM is advantageous for weak and unstable classifiers that have a decreasing learning curve and are constructed on small and critical training sample sizes.

Kuncheva (2002b) give formulas for the classification error for the following fusion methods: average, minimum, maximum, median, majority vote, and oracle. For a uniformly distributed posterior probability, the minimum/maximum method performed the best; whilst for normally distributed errors, the fusion methods all gave a very similar performance. Kuncheva (2002a) presented a combination of classifier selection and fusion by using statistical inference to switch between the two. In their experiments, there was no clear preference of one combination approach over the rest, the only consistent pattern being that the improvement over the best individual classifier was negligible. Shipp and Kuncheva (2002) studied the relationships between different methods of classifier combination and measures of diversity in combining classifiers. The only positive correlation was that the Double-Fault measure of diversity and the measure of difficulty both showed reasonable correlation with Majority Vote and Naive Bayes combinations (a not unexpected result). The ambiguous relationship between diversity and accuracy discourages optimising the diversity. Skurichina and Duin (2002) applied and compared bagging, boosting and the random subspace method to linear discriminant analysis. They discovered that boosting is useful for large training sample sizes, whilst bagging and the random subspace method are useful for critical training sample sizes. In a very good paper, Valentini and Masulli (2002) present an overview of ensemble methods. Dietterich (2002) published a review of ensemble learning.

Kittler and Alkoot (2003) investigated the Sum versus majority Vote in multiple classifier systems. They showed that for Gaussian estimation error distributions, Sum always outperforms Vote; whilst for heavy tail distributions, Vote may outperform Sum. This is of especial interest to the financial domain with the presence of leptokurtosis in market returns. Kuncheva, *et al.* (2003)

derived upper and lower limits on the majority vote accuracy for individual classifiers. They deduce that negative pairwise dependence between classifiers is best, and ideally all pairs of classifiers in the pool should have the same negative dependence. They also deduce that diversity is not always beneficial. Kuncheva and Whitaker (2003) considered measures of diversity in classifier ensembles and their relationship with the ensemble accuracy. Their results raise some doubts about the usefulness of diversity measures in building classifier ensembles in real-life pattern recognition problems. Topchy, Jain and Punch (2003) investigate clustering ensembles.

In a relevant and interesting paper, Evgeniou, Pontil and Elisseeff (2004) studied the leave-one-out and generalization errors of ensembles of kernel machines such as SVMs. They found that the best SVM and the best ensembles had about the same test performance: “with appropriate tuning of the parameters of the machines, combining SVMs does not lead to performance improvement compared to a single SVM.” However, ensembles of kernel machines are more stable learning algorithms than the equivalent single kernel machine, i.e. bagging increases the stability of unstable learning machines. In a directly relevant paper, Valentini and Dietterich (2004) analyzed bias-variance in SVMs for the development of SVM-based ensemble methods. They suggest two promising approaches for designing ensembles of SVMs. One approach is to employ low-bias SVMs as base learners in a bagged ensemble, whilst the other approach is to apply bias-variance analysis to construct a heterogeneous, diverse set of accurate and low-bias classifiers.

7 Taxonomy

Table 1: Ensemble Methods

Scheme	Architecture	Trainable	Adaptive	Info-level	Comments
Voting	Parallel	No	No	Abstract	Assumes independent classifiers
Sum, mean median	Parallel	No	No	Confidence	Robust; assumes independent confidence estimators
Product, min, max	Parallel	No	No	Confidence	Assumes independent features
Generalized ensemble	Parallel	Yes	No	Confidence	Considers error correlation

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Scheme	Architecture	Trainable	Adaptive	Info-level	Comments
Adaptive weighting	Parallel	Yes	Yes	Confidence	Explores local expertise
Stacking	Parallel	Yes	No	Confidence	Good utilization of training data
Borda count	Parallel	Yes	No	Rank	Converts ranks into confidences
Logistic regression	Parallel	Yes	No	Rank confidence	Converts ranks into confidences
Class set reduction	Parallel cascading	Yes / No	No	Rank confidence	Efficient
Dempster-Shafer	Parallel	Yes	No	Rank confidence	Fuses non-probabilistic confidences
Fuzzy integrals	Parallel	Yes	No	Confidence	Fuses non-probabilistic confidences
Mixture of local experts (MLE)	Gated parallel	Yes	Yes	Confidence	Explores local expertise; joint optimization
Hierarchical MLE	Gated parallel hierarchical	Yes	Yes	Confidence	Same as MLE; hierarchical
Associative switch	Parallel	Yes	Yes	Abstract	Same as MLE, but no joint optimization
Bagging	Parallel	Yes	No	Confidence	Needs many comparable classifiers

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Scheme	Architecture	Trainable	Adaptive	Info-level	Comments
Boosting	Parallel hierarchical	Yes	No	Abstract	Improves margins; unlikely to overtrain, sensitive to mislabels; needs many comparable classifiers
Random subspace	Parallel	Yes	No	Confidence	Needs many comparable classifiers
Neural trees	Hierarchical	Yes	No	Confidence	Handles large numbers of classes

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