Bagging, Random Subspace Method and Biding

Satoshi Shirai, Mineichi Kudo, and Atsuyoshi Nakamura

Division of Computer Science
Graduate School of Information Science and Technology
Hokkaido University
Kita-14, Nishi-9, Kita-ku, Sapporo 060-0814, Japan
{satoshi,mine,atsu}@main.ist.hokudai.ac.jp
<http://prml.main.ist.hokudai.ac.jp>

Abstract. In recent years, many approaches for achieving high performance by combining some classifiers have been proposed. We exploit many random replicates of samples in the bagging, and randomly chosen feature subsets in the random subspace method. In this paper, we introduce a method for selecting both samples and features at the same time and demonstrate the effectiveness of the method. This method includes a parametric bagging and a parametric random subspace method as special cases. In some experiments, this method and the parametric random subspace method showed the best performance.

1 Introduction

Many classifiers have been proposed for pattern recognition, including plug-in Bayes classifiers, nearest neighbors, support vector machines, etc. It is well known that no classifier keeps the best position for every problem, so that we have to choose one of them depending on the problem at hand. When the number of training samples is small, an appropriate classifier with a complexity suitable for the problem size must be chosen. One attractive approach is to combine several classifiers to bring stability over them. This approach is called *classifier fusion* and has been widely studied [1,2,3,4,5]. Each such classifier is called a *component classifier*. This approach aims at decreasing the generalized error by producing many weak classifiers in one way or another from a provided training dataset and by consolidating them in majority voting (the case of classification) or averaging (the case of regressive prediction).

Two methods have been widely used: bagging [1] and random subspace method [4]. In bagging, many different training sets are generated by resampling and fed to a *base classifier* (a designing algorithm). On the other hand, in the random subspace method, many different feature subsets are randomly chosen for producing component classifiers. As a natural extension, simultaneous selection of sample and feature subsets has been studied [6] and has been shown to often outperform one-side selections.

The advantageous effect of classifier fusion has been analyzed in different ways. In the case of regressive prediction, it has been revealed that independent, hopefully negatively-correlated, component classifiers are effective. Even in the case of classification, with some different definitions of correlation, use of negatively-correlated component classifiers is known to be effective [6,7,8]. On the other hand, diversity of component classifiers [9,10,11] is often a useful measure to estimate the performance. Typically, higher diversity of component classifiers means better performance in fusion.

In this paper, we focus on resampling rates of bagging and the random subspace method. Examining possible resampling rates in a systematical way is useful for revealing the potential abilities of bagging and the random subspace method in detail. In addition, we propose simultaneous selection of sample and feature subsets with optimized resampling rates.

2 Formulation of Classifier Fusion

Producing different component classifiers from a single training sample set by resampling of samples or by reselection of features or both is typical in classifier fusion. Let us divide a training set into form and contents. Here, the form is denoted by

$$U_{N \times M} = T_N \times F_M,$$

where T_N is the index set of samples, $T_N = \{1, 2, \dots, N\}$, and F_M is the index set of features, $F_M = \{1, 2, \dots, M\}$. The contents are specified by a sampling (an observation) function $x : U_{N \times M} \rightarrow R$ with $(i, j) \mapsto x_{ij}$. Hereafter, U and the relatives are considered along with the contents $\{x_{ij}\}$ unless no confusion occurs.

2.1 Number of Distinct Elements by Resampling

In some cases, it is better to consider the set of distinct samples instead of the bootstrap sample T^* itself. Indeed, duplication of samples does not cause any change in the rule of nearest neighbors and support vector machines without a soft margin.

When $N\alpha$ ($0 \leq \alpha \leq 1$) elements are randomly and uniformly selected from N elements with replacement, the expected size $n = E\hat{n}$ of distinct elements is given by

$$n = (1 - (1 - \frac{1}{N})^{N\alpha})N \simeq (1 - e^{-\alpha})N.$$

Thus, $\theta = n/N = 0.63$ for $\alpha = 1$ (bagging case).

2.2 Bagging

In bagging, one resampling selects T_N^* of N samples from T_N of N samples, but some samples in T_N^* are duplicated. The average size n of distinct samples is

$n = 0.63N$. As a result, on average, we have the form $U_{n \times M} = T_n \times F_M$. The bagging method is a majority vote of predicted classes by $\phi(T_N^{*1}), \phi(T_N^{*2}), \dots, \phi(T_N^{*B})$, where ϕ is a base classifier and $T_N^{*1}, T_N^{*2}, \dots, T_N^{*B}$ are the B bootstrapped samples. The corresponding $T_{n_1}^1, T_{n_2}^2, \dots, T_{n_B}^B$ of distinct samples are different in size, but the basic performance for fixed $\theta_S^B = 0.63$ and $n = 0.63N$ can be analyzed.

2.3 Random Subspace Method

On the other hand, in the random subspace method [4], $F_{M/2}^*$ of $M/2$ distinct features are typically selected randomly from F_M of M features. As a result, we have the form $U_{N \times M/2}$ with $\theta_F^R = 0.5$ and $m = 0.5M$. Similarly to bagging, we use B bootstrapped features $F_{M/2}^1, F_{M/2}^2, \dots, F_{M/2}^B$ for designing component classifiers.

2.4 Parametric Bagging and Random Subspace Method

Let us analyze the performance of above two aggregating methods of component classifiers produced by random sampling with/without replacement. To make clear the difference in which direction sampling is made, we use θ_S for samples and θ_F for features. Then we have

$$\begin{aligned} U_{\theta_S N \times M} &= T_{\theta_S N} \times F_M : (\text{parametric}) \text{ bagging}, \\ U_{N \times \theta_F M} &= T_N \times F_{\theta_F M} : (\text{parametric}) \text{ random subspace method}. \end{aligned}$$

The question “what are the best values of θ_S and θ_F ?” naturally arises. To examine the relationship between θ_S (θ_F) and classification performance, we examined 10 real-world datasets. They are UCI datasets [12] that have more than 10 features and consist of continuous features only. The classification rate was estimated by 10-fold cross validation. In the following, the bagging is simulated by $\theta_S = 0.63$ and the random subspace method by $\theta_F = 0.5$. In this case, a certain subset of size $n(m)$ is chosen from a set of size $N(M)$ with a probability of $1/\binom{N}{n}$ ($1/\binom{M}{m}$). Here, $\theta_S(\theta_F)$ was changed in the range of 0.1 to 1.0 by step 0.1. The base classifier was the nearest-neighbor and $B = 100$. The results are shown in Table 1 and Table 2. In bagging, the parameter tuning did not greatly improve the performance. However, it did improve the performance when θ_S was low (for example, in **heart-statlog** and **waveform-5000**, the best value of θ_S is 10%). This is an astonishing result. This result implies the possibility of *sparse* sampling. Note that the nearest neighbor does not change its rule if $\theta_S > 0.5$, such as $\theta_S^B = 0.63$ for bagging, because the true nearest neighbor of a given sample appears over a half of $T_n^1, T_n^2, \dots, T_n^B$ with $n = \theta_S N$. The classification rates using the parametric random subspace method were improved at 3% on average from those using the original random subspace method. The optimal value of θ_F^* ranges from 0.2 to 0.7 but is mostly around 0.3. That is, the empirical selection $\theta_F = 0.5$ of a typical random subspace method is a little larger than the best choice.

Table 1. Recognition rates in bagging (Bag) with 1-NN. Here, θ_S^* is the sampling ratio bringing the best performance.

Dataname	#class	#sample	1-NN	Bag($\theta_S^B = 63\%$)	P-Bag($\theta_S^* \%$)	P-Bag/Bag
heart-statlog	2	270	59.62	59.62	68.14 (10)	1.148
ionosphere	2	351	86.92	86.92	87.76 (50)	1.009
optdigits	10	5620	98.75	98.75	98.84 (30)	1.001
page-blocks	5	5473	95.41	95.43	95.88 (30)	1.004
segment	7	2310	96.49	96.49	96.49 (60–100)	1.000
sonar	2	208	83.64	83.64	83.64 (60–100)	1.000
spambase	2	4601	82.41	82.37	82.78 (40)	1.004
vehicle	4	846	65.71	65.71	66.42 (50)	1.010
waveform-5000	3	5000	76.58	76.68	84.52 (10)	1.102
wine	3	178	74.73	74.73	75.26 (30)	1.007
Average			82.03	82.03	83.97 (41.0)	1.028

Table 2. Recognition rates in the random subspace method (RS) with 1-NN. Here, θ_F^* is the sampling ratio bringing the best performance

Dataname	#feature	SVM	RS($\theta_F^R = 50\%$)	P-RS($\theta_F^* \%$)	P-RS/RS
heart-statlog	13	59.62	66.67	73.33 (40)	1.100
ionosphere	34	86.92	90.61	94.02 (20)	1.037
optdigits	64	98.75	99.02	99.05 (70)	1.000
page-blocks	10	95.41	95.52	95.70 (60)	1.002
segment	19	96.49	97.74	97.74 (50)	1.000
sonar	60	83.64	85.07	89.90 (20)	1.056
spambase	57	82.41	91.72	93.21 (30)	1.016
vehicle	18	65.71	69.14	71.14 (20)	1.029
waveform-5000	40	76.58	84.60	84.82 (30)	1.002
wine	13	74.73	88.20	96.07 (30)	1.089
Average		82.03	86.83	89.50 (37.0)	1.033

2.5 Biding

Choice of the best pair $(\theta_S, \theta_F)^*$ is clearly more effective than a single choice of best θ_S^* or θ_F^* . Therefore, we consider simultaneous selection of (θ_S, θ_F) and call the aggregating method using the selected parameter pair “Biding” (abbreviation of BIDirectional aggregatING). In biding, a component classifier has a form

$$U_{\theta_S N \times \theta_F M} = T_{\theta_S N} \times F_{\theta_F M} : \textit{biding}.$$

Parametric bagging (P-Bag) corresponds to the case of $(\theta_S, 1.0)$ and the parametric random subspace method (P-RS) corresponds to the case of $(1.0, \theta_F)$. The functional relation between performance and (θ_S, θ_F) is shown in Fig.1 concretely for **heart-statlog** and **segment** datasets. From Fig.1, we see the effectiveness of simultaneous selection. We conducted the same experiment with (θ_S, θ_F) . The performance is shown in Table 3. Biding is naturally the best among all three

Fig. 1. Recognition rate over (θ_S, θ_F) : (a) the best pair $(\theta_S, \theta_F)^* = (40, 30)$ in heart-statlog, (b) the best pair $(\theta_S, \theta_F)^* = (60, 50)$ in segment

Table 3. Comparison of parametric bagging (P-Bag), parametric random subspace (P-RS) method and bidding

Dataname	P-Bag(θ_S^* %)	P-RS(θ_F^* %)	Biding($\theta_S\%, \theta_F\%$) [*]	Biding/P-Bag	Biding/P-RS
heart-statlog	68.14 (10)	73.33 (40)	78.51 (40,30)	1.152	1.070
ionosphere	87.76 (50)	94.02 (20)	94.02 (100,20)	1.071	1.000
optdigits	98.84 (30)	99.05 (70)	99.06 (60,80)	1.002	1.000
page-blocks	95.88 (30)	95.70 (60)	96.08 (40,90)	1.002	1.004
segment	96.49 (60–100)	97.74 (50)	97.92 (60,50)	1.015	1.002
sonar	83.64 (60–100)	89.90 (20)	89.92 (90,20)	1.075	1.000
spambase	82.78 (40)	93.21 (30)	93.21 (100,30)	1.125	1.000
vehicle	66.42 (50)	71.14 (20)	71.50 (60,30)	1.076	1.005
waveform-5000	84.52 (10)	84.82 (30)	85.84 (20,60)	1.015	1.012
wine	75.26 (30)	96.07 (30)	97.18 (40,20)	1.291	1.011
Average	83.97	89.50	90.32	1.082	1.010

variants including itself. The improvement ratios to the parametric bagging and parametric random subspace method with the optimal parameters were 1.08 and 1.01, respectively.

Table 3 also shows the difference between $(\theta_S, \theta_F)^*$ and (θ_S^*, θ_F^*) . From Fig.2, we see that $(\theta_S, \theta_F)^*$ tends to be located at the right-hand or upper-right of (θ_S^*, θ_F^*) . This is natural because either θ_S or θ_F is fixed to one when θ_S^* or θ_F^* is calculated. Combining results shown in Table 1, Table 2, and Table 3, bidding improved the original (but simulated) bagging at ratio 0.3 – 31.7% and the random subspace method at ratio 0.2 – 2.3%.

3 Estimation of $(\theta_S, \theta_F)^*$ by Optimization

For practical usage, we have to estimate the optimal parameters in bidding and its two variants. It is natural to use a validation dataset cut from the training set. The problem is the cost of calculation. It costs the number of (θ_S, θ_F) pairs to be

Fig. 2. Point diagram of (θ_S^*, θ_F^*) and $(\theta_S, \theta_F)^*$. An ellipsoid encloses the same dataset.

Fig. 3. Quadratic approximation by nine points

examined multiplied by the cost of one-time validation test and by the number B of bootstrapping. It is therefore crucial to reduce the size of the candidate set of (θ_S, θ_F) 's.

To do this, assuming smoothness of the target function (see Fig.1), we approximate it by a quadratic function that is estimated surrounding eight points and the center point (Fig.3). Then we narrow the search region by a factor of $1/4$ for once. By three times of narrowing, we find an estimation of $(\theta_S, \theta_F)^*$ with 27 values of the target function on $[0.2, 1.0] \times [0.2, 1.0]$. For P-Bag and P-RS, we use 20 points in $[0.05, 1.0]$ on each axis.

4 Experiments

We conducted some experiments to demonstrate the effectiveness of P-Bag, P-RS and bidding. The base classifier is either of the nearest neighbor and the support vector machine (SVM) with a radial basis kernel, and $B = 100$. The result of

Table 4. Recognition rate by SVM method

Data	SVM	Bag	RS	P-Bag(θ_S^* %)	P-RS(θ_F^* %)	Biding($((\theta_S, \theta_F)^*)$)
heart-statlog	62.22	62.22	73.70	59.63 (72.0)	80.37 (28.5)	81.11 (33.2, 21.0)
ionosphere	93.46	92.60	94.04	92.31 (83.5)	92.90 (64.5)	92.61 (58.2, 49.6)
optdigits	96.49	96.21	99.04	96.37 (65.5)	99.04 (50.0)	98.81 (58.3, 38.8)
page-blocks	92.42	92.51	94.06	92.44 (80.5)	94.46 (33.5)	93.88 (57.2, 30.0)
segment	92.51	92.38	96.74	92.55 (93.5)	96.71 (43.0)	97.10 (64.8, 35.9)
sonar	81.17	80.69	80.69	80.21 (72.0)	81.69 (55.5)	76.68 (51.0, 44.7)
spambase	86.61	86.79	93.74	86.55 (65.0)	93.68 (43.0)	93.33 (51.8, 41.9)
vehicle	57.20	56.85	69.84	55.55 (62.0)	73.87 (29.0)	72.21 (34.8, 21.9)
waveform-5000	83.08	85.08	85.78	86.52 (21.0)	85.60 (45.5)	86.44 (25.0, 60.2)
wine	70.72	69.64	89.87	69.64 (61.5)	96.57 (32.5)	97.71 (34.5, 24.2)
Average	81.59	81.50	87.75	81.18 (65.7)	89.49 (42.5)	88.98 (46.9, 36.8)

SVM is shown in Table 4. We also obtained the result of 1-NN, but it is not shown here for economizing the space, but the tendency was similar. We have tried to use SVM in the experiments of the previous section, but gave up due to its high computation cost.

In both 1-NN and SVM, P-RS was best for many cases and bidding followed. This is mainly because the number 27 of search points in bidding was insufficient for 2-dimensional search space, compared to 20 for 1-dimensional search space in the other two variants. Indeed, it is noted that when (θ_S, θ_F) is chosen close to the optimal value in Table 3, the bidding attained the best performance.

5 Analysis of Classifier Fusion in Classification

So far, many studies have been invoked to reveal when classifier fusion works best [1,3,4,5]. The standard ways to connect the generalized error possibly reduced by classifier fusion with the characteristics of component classifiers can be divided into three: 1) bias and variance decomposition, 2) dependency analysis, that is, what degree the component classifiers are correlated to each other, and 3) diversity measures among component classifiers.

Let us first use a disagreement measure. The disagreement measure $Dis_{b,b'}$ between component classifiers ϕ_b and $\phi_{b'}$ is calculated by N samples with N_1 outputs of both correct or both incorrect and N_0 outputs of one-sided correct such as

$$Dis_{b,b'} = \frac{N_0}{N_0 + N_1}, \quad Dis = \frac{1}{B(B-1)} \sum_b \sum_{b' \neq b} Dis_{b,b'}. \quad (1)$$

The relationship between improvement rate and diversity is shown in Fig.4. In Fig.4, we notice that there is a positive correlation between them, and bidding and random subspace method brought the largest diversity. Note that $Dis_{b,b'}$ is a post-event evaluation, that is, this value is available only with true labels. On the other hand, we can use this measure without such true labels if the number of classes is two.

Next, we state the relationship among above 1), 2) and 3) in a theoretical way. Let us assume that a classifier (strictly speaking, a design algorithm) ϕ produces an estimate $\hat{\eta}(x)$, with a training sample set, for the posterior density $\eta(x) = P(Y = 1|X = x)$ in a two-class problem ($Y \in \{1, 0\}$). Then the assignment by $\hat{\eta}$ is given by $\hat{y}(x) = \text{sign}(\hat{\eta}(x) - 1/2)$. Let $y_B(x)$ be the assignment by the Bayes classifier as $y_B(x) = \text{sign}(\eta(x) - 1/2)$.

According to Friedman [13], the bias-variance decomposition at a certain point x for classification is given by a multiplicative form, unlike an additive form for regression, as

$$P(\hat{y}(x) \neq Y) - P(y_B(x) \neq Y) = |2\eta(x) - 1| \text{Erf} \left(\frac{-b(\eta(x), E \hat{\eta}(x))}{\sqrt{\text{Var} \hat{\eta}(x)}} \right), \quad (2)$$

where $\text{Erf}(x)$ is the error function defined by $\text{Erf}(x) = 1/\sqrt{2\pi} \int_x^\infty e^{-u^2/2} du$ and the boundary bias b is given by

$$b(\eta(x), E \hat{\eta}(x)) = \text{sign}(\eta(x) - 1/2) (1/2 - E \hat{\eta}(x)). \quad (3)$$

Fig. 4. Relationship between improvement rate and diversity

That is, the generalized error $P(\hat{y}(x) \neq Y)$ at x is expressed by the Bayes error plus a multiplicative decomposition of the boundary bias $b(\eta(x), E \hat{\eta}(x))$ and the square-rooted variance $\sqrt{\text{Var } \hat{\eta}(x)}$. Here, the distribution of $\hat{\eta}(x)$ is assumed to be a Gaussian to exploit the error function.

Eq. (2) implies that if the boundary bias is negative, hence the assignment is agreed between the Bayes classifier and ϕ , then a smaller variance is effective for improving the performance, and, if not, a larger variance is effective for making $\text{Erf}(x)$ approach 1/2.

From (2), we have the total generalized error $\text{Err}(\phi)$ as

$$0 \leq \text{Err}(\phi) - \text{Err}_{\text{Bayes}} = \int |2\eta(x) - 1| \text{Erf} \left(\frac{-b(\eta(x), E \hat{\eta}(x))}{\sqrt{\text{Var } \hat{\eta}(x)}} \right) p(x) dx. \quad (4)$$

When aggregation is applied to B component classifiers with

$$\hat{y}_1, \hat{y}_2, \dots, \hat{y}_b, \dots, \hat{y}_B, \quad \forall b, E \hat{y}_b = E \hat{y},$$

we have an aggregated estimate and assignment as

$$\hat{\eta}_A = \frac{1}{B} \sum_b \hat{y}_b, \quad \hat{y}_A = \text{sign}(\hat{\eta}_A - 1/2).$$

Then,

$$\begin{aligned} E \hat{\eta}_A &= E \hat{y}, \quad \text{Var } \hat{\eta}_A = E \left\{ \left(\frac{1}{B} \sum_b \hat{y}_b - E \hat{y} \right)^2 \right\} \\ &= \frac{1}{B} \text{Var } \hat{y} + \frac{1}{B^2} \sum_b \sum_{b' \neq b} \text{Cov}(\hat{y}_b, \hat{y}_{b'}), \end{aligned} \quad (5)$$

where

$$\text{Var } \hat{y} = E \hat{y}(1 - E \hat{y}), \quad \text{Cov}(\hat{y}_b, \hat{y}_{b'}) = E(\hat{y}_b - E \hat{y})(\hat{y}_{b'} - E \hat{y}). \quad (6)$$

That is, by aggregating, the variance is reduced by $1/B$ and a positive (negative) correlation increases (decreases) the variance.

Here, we notice that

$$\begin{aligned} E(\hat{y}_b - 1/2)(\hat{y}_{b'} - 1/2) &= E(\hat{y}_b - E\hat{y})(\hat{y}_{b'} - E\hat{y}) + (E\hat{y} - 1/2)^2 \\ &= \text{Cov}(\hat{y}_b, \hat{y}_{b'}) + (E\hat{y} - 1/2)^2. \end{aligned}$$

Then, we can evaluate Eq. (5) as

$$\begin{aligned} \text{Var } \hat{\eta}_A &= \frac{1}{B} \text{Var } \hat{y} - \frac{1}{B^2} \sum_b \sum_{b' \neq b} E(\hat{y}_b - 1/2)(1/2 - \hat{y}_{b'}) \\ &\quad - (1 - \frac{1}{B})(E\hat{y} - 1/2)^2. \end{aligned} \quad (7)$$

That is, the variance is reduced if the degree of disagreement between b and b' is (positively) high or if $E\hat{y}$ is far from $1/2$, or both.

On the other hand, the *disagreement* measure Dis (1) is evaluated over $\{x_i\}$ as

$$\begin{aligned} Dis &= \frac{1}{B(B-1)} \sum_b \sum_{b' \neq b} \frac{1}{N} \sum_{i=1}^N \{2(\hat{y}_b(x_i) - 1/2)(1/2 - \hat{y}_{b'}(x_i)) + \frac{1}{2}\} \\ &\rightarrow \frac{2}{B(B-1)} \sum_b \sum_{b' \neq b} \int (\hat{y}_b(x) - 1/2)(1/2 - \hat{y}_{b'}(x))p(x)dx + \frac{1}{2} \\ &\quad \text{as } N \rightarrow \infty. \end{aligned} \quad (8)$$

Comparing Eqs. (7) and (8), we notice that Dis (1) shows to what degree the variance of the aggregated classifier is reduced on average as a sample estimation. The difference is that the expectation is taken for the training sets in (7) and is taken for $\{x\}$ in (8).

In total, (5), (7) and (8) reveal the relationship among the variance of an aggregating classifier, the correlation between component classifiers, and the disagreement between component classifiers. When the disagreement is high, then the correlation becomes negative and thus the variance of aggregation is reduced.

6 Conclusion

We have proposed a parametric bagging, a parametric random subspace method, and biding as a parent of them for classifier fusion. We confirmed that the parametric random subspace method and biding are both effective in most cases. We also found that 1) sparse sampling (a parametric bagging with a small sampling rate) may be useful for large datasets, 2) traditional random subspace method is reasonable but a little larger in the sampling rate, and 3) simultaneous random selection of samples and features is promising.

Among them, biding is the most powerful in theory. The main drawback of biding is the cost of estimating optimal parameters. In the experiments, a very

simple technique for optimization was employed with only 27 function values. A more sophisticated optimization technique would be considered for improving the performance of bidding.

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