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# Probability Estimation in Random Forests

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Probability Estimation in Random Forests

by

Chunyang Li

A thesis submitted in partial fulfillment  
of the requirements for the degree

of

MASTER OF SCIENCE

in

Statistics

Approved:

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Logan, Utah

2013

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## ABSTRACT

Probability Estimation in Random Forests

by

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Utah State University, 2013

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Random Forests is a useful ensemble approach that provides accurate predictions for classification, regression and many different machine learning problems. Classification has been a very useful and popular application for Random Forests. However, it is preferable to have the probability of a membership rather than the simple knowledge that one belongs to whichever group. Votes and the regression method are current probability estimation methods that have been developed in Random Forests. In this thesis, we introduce two new methods, proximity weighting and the out-of-bag method, trying to improve the current methods. Several different simulations are designed to evaluate the new methods and compare them with the old ones. Finally, we use real data sets from UCI machine learning repository to further evaluate and compare those methods.

I dedicated this to my parents, who love me deeply and give me greatest support.

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Chunyang Li

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## CHAPTER 1

### INTRODUCTION

#### 1.1 Classification

Classification is the problem of predicting which class a new observation belongs to, given a training set of data from  $K$  known classes. One way to think about classification is that it's like regression but we have a categorical response variable instead of a continuous response.

Assume we have a sample  $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$  of independent and identically distributed observations, where  $\mathbf{x}_i = (x_{i1}, \dots, x_{iM})^T \in \mathcal{X} \subseteq \mathbb{R}^M$  and  $y_i \in \{1, \dots, K\}$  for  $i = 1, \dots, N$ . The values of  $y_i$  refer to the *classes* and the problem is to classify a new observation  $\mathbf{x}_{\text{new}}$  into one of the  $K$  classes, i.e. to estimate  $\hat{y}_{\text{new}}$ . No formal distributional assumptions are made, although there are implicit assumptions that “nearby” values of  $\mathbf{x}$  provide information about  $y$ .

#### 1.2 Probability Estimation

Most machine learning approaches only provide a classification result. However, it is not enough and probabilities are essential in some cases like predicting diseases. It is important to estimate the probability of belonging to each of the groups rather than making a simple statement that a patient is in one group or another. Therefore, our research problem is using Random Forests to get the most accurate probability estimates.

More formally, let  $f_k(\mathbf{x})$  denote the density function for observations in class  $k$ . Then

$$f(\mathbf{x}) = \sum_{k=1}^K \pi_k f_k(\mathbf{x})$$

where  $0 \leq \pi_k \leq 1$  and  $\sum_{k=1}^K \pi_k = 1$ . We can view the data  $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$  as realizations of random variables  $(\mathbf{x}, y)$ , where

$$P(y = k) = \pi_k$$

and

$$f(\mathbf{x}|y = k) = f_k(\mathbf{x})$$

so

$$f(\mathbf{x}) = \sum_k \pi_k f_k(\mathbf{x})$$

As well as predicting  $y$  when  $\mathbf{X} = \mathbf{x}_{new}$ , we would like to estimate

$$\begin{aligned} p_k &= P(y = k | \mathbf{X} = \mathbf{x}_{new}) \\ &= \frac{\pi_k f_k(\mathbf{x}_{new})}{f(\mathbf{x})} \end{aligned}$$

### 1.3 Trees

A classification tree is usually grown by firstly considering a “root” node containing all the observations. Observations in the node are sent to the descendant nodes, using a “split” on a single predictor variable. The initial (“root”) node contains the data of interest and nodes that can’t be split are called “terminal” nodes. At any stage of the tree-growing process, a node contains observations in some or all of the classes  $\{1, \dots, K\}$  and the  $y$ -values in the node can be summarized by a vector  $\mathbf{n} = (n_1, \dots, n_K)^T$  where  $n_k$  is the number of observations of class  $k$  in the node.

Considering every possible split on every predictor variable, a particular split of a node is chosen. The predictor and split combination giving the “best” value according to some criterion, such as Gini index, entropy, etc., is used to partition the node. In this report, we use the Gini Index.

For continuous predictors, each split is of the form  $x_j < c$  for some  $c$  and  $j \in \{1, \dots, M\}$ , where  $x_j$  denotes the value of variable  $j$ . Observations that have  $x_j < c$  go to the left descendant node, and the others go to the right. The values of  $j$  and  $c$  for each node are found by minimizing a measure of the “badness” of the split based on the Gini index. For a node whose  $y$ -values are summarized by  $\mathbf{n} = (n_1, \dots, n_K)^T$  of size  $S = \sum_{k=1}^K n_k$ , the Gini index is

$$G(\mathbf{n}) = \sum_{k \neq k'} \left( \frac{n_k}{N} \right) \left( \frac{n_{k'}}{N} \right).$$

A particular choice of  $c$  and  $j$  will give left and right nodes summarized by  $\mathbf{n}_L = \mathbf{n}_L(c, j)$

and  $\mathbf{n}_R = \mathbf{n}_R(c, j)$  with size  $S_L$  and  $S_R$  where  $S_L + S_R = S$ . The values of  $c$  and  $j$  are chosen to minimize

$$S_L G(\mathbf{n}_L) + S_R G(\mathbf{n}_R).$$

Denoting the sorted sample values of variable  $j$  in the node by  $x_{(1)j}, \dots, x_{(S)j}$ , the minimization is performed over

$$c \in \{(x_{(i)j} + x_{(i+1)j})/2, i = 1, \dots, S - 1\}.$$

For stand-alone trees, the minimization is performed over  $j \in \{1, \dots, M\}$ . In random forests, the minimization is performed over  $j$  in a random subset of  $\{1, \dots, M\}$ , chosen independently at each node. Typically, the size of the subset is close to  $\sqrt{M}$ .

The minimization over both  $j$  and  $c$  is performed using an exhaustive search over all combinations of  $c$  and  $j$  as described above. For a given variable  $j$ , the Gini index is updated as we move through the possible values of  $c$  from smallest to largest.

The trees are usually grown until a stopping criterion is met, or the nodes contain a small enough number of cases.

To predict the class of  $\mathbf{x}_{\text{new}}$ , we start from the root node and move down the tree. At a node, if the  $j$ th component of  $\mathbf{x}_{\text{new}}$  satisfies the appropriate condition, it goes to the left, otherwise it goes to the right. In this way,  $\mathbf{x}_{\text{new}}$  ends up in a terminal node. The predicted class at the terminal node is the most popular class among the training data at the node with ties broken at random.

#### 1.4 Random Forests

The Random Forest method was introduced by Leo Breiman in 2001 [1] and is a very useful tool for machine learning. It is a combination of tree predictors such that each tree depends on the information of a bootstrap sample from the original data (training set). It can be used for classification and regression. Here, we are only considering Classification Random Forests.

Trees like those described in sections 1.3 are used in Random Forests as described in the following. The parameters  $ntree$  and  $m$  (the number of must be chosen. The value of  $ntree$ , the number of trees in the forest, can be chosen as large as desired. There is no penalty, in terms of fit, for choosing  $ntree$  too large, but the fit may be poor if it is too small. The default value of  $ntree$  in the R implementation is 500. The value of  $m$ , which controls the number of randomly chosen predictors at each node (as described in Section 1.3), is usually taken to be an integer close to  $\sqrt{M}$ .

To construct the forest, suppose we have a training set  $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$  and let  $A = \{1, \dots, N\}$ . Then for  $t$  in  $1, \dots, ntree$ :

1. Take a bootstrap sample from the data (sample  $N$  times, at random, with replacement).
2. Denote the set of observations appearing in the bootstrap sample by  $B_t \subset A$ .
3. Denote the set of observations *not* appearing in the bootstrap sample by  $B_t^c = A \setminus B_t$ .
4. Fit a classification tree (Section 1.3) to the bootstrap sample, splitting until all the observations in each terminal node come from the same class (“pure”).
5. Find the predicted class at each terminal node (the class of members of  $B_t$  in the node).
6. For each member of  $B_t^c$ , pass it down the tree.
7. Let  $q_t(i)$  denote the terminal nodes for all  $i \in A$ .

The predicted class for observations in the training set is the most frequent class in the trees for which the observation is a member of  $B_t^c$ . This process is often described as “voting” the trees. For new observations, all the trees in the forest are used in the voting. The observations in  $B_t^c$  are said to be “out-of-bag” for tree  $t$ . The “out-of-bag” error rate is the

error rate of the Random Forest predictions for the training set. These predictions are also used to give the “out-of-bag” confusion matrix.

Let the proximity between the  $i$ th and  $j$ th observations be the proportion of the time observations  $i$  and  $j$  are in the same terminal node, where the proportion is taken over trees for which  $i$  and  $j$  are in  $B_t^c$  (i.e. both out-of-bag):

$$prox(i, j) = \frac{\sum_{t=1}^{ntree} I(i \in B_t^c) I(j \in B_t^c) I(q_t(i) = q_t(j))}{\sum_{t=1}^{ntree} I(i \in B_t^c) I(j \in B_t^c)}$$

where  $I$  denotes the indicator function. To find the proximity between an observation from the training set, and one from the test set, we use

$$prox(i, j) = \frac{1}{ntree} \sum_{t=1}^{ntree} I(q_t(i) = q_t(j)).$$

## CHAPTER 2

### PROBABILITY ESTIMATION METHODS

Let  $p_{i,k} = P(Y = k|X = \mathbf{x}_i)$ . We compare four methods of estimating  $p_{i,k}$ . The first method, based on voting the trees, is the “standard” or “default” method. The second method is a regression method introduced by Malley et al. [10]. The third and fourth methods, labeled “Proximity Weighting” and “Out-of-bag” are new methods developed for this research project.

#### 2.1 Voting

For test data,  $\hat{p}_{i,k}^{vote}$  is the proportion of trees that predict class  $k$  when observation  $\mathbf{x}_i$  is passed down the tree. For training data, the proportion is only taken over trees for which  $\mathbf{x}_i$  is out-of-bag.

#### 2.2 Probability Machines

This method only works for two-class problems ( $K = 2$ ). The two classes are denoted 0 and 1 and Random Forests is run in regression mode. Random Forests for regression are analogous to Random Forests for classification, except that the splits are chosen to minimize the mean squared error instead of Gini, the predictions for a tree are the average of the  $y$ -values of  $B_t$  in the nodes, and the predicted values for the forest are obtained by averaging over the trees for which the observation is in  $B_t^c$ . Once the Random Forests regression predictions  $\{\hat{y}_1, \dots, \hat{y}_N\}$  are obtained, we set  $\hat{p}_{i,1}^{reg} = \hat{y}_i$  and  $\hat{p}_{i,0}^{reg} = 1 - \hat{y}_i$ .

#### 2.3 Proximity Weighting

The motivation for this method comes from the fact that Random Forests can be thought of as a “nearest neighbor” classifier [4] and proximities are believed to correspond to the neighborhoods of the nearest neighbor classifier. The proximity weighting method uses the proximities defined above to find a weighted average:



$$\hat{p}_{i,k}^{prox} = \frac{\sum_{j \in A, j \neq i} prox(i, j) I(y_j = k)}{\sum_{j \in A, j \neq i} prox(i, j)}.$$

The weighted average means that observations that are “close” have more impact on the probability estimate than observations that are not “close” (where “close” is defined using the Random Forest proximities). For more information about proximities, see A. Cutler et al.[2]

#### 2.4 Out-of-bag Method

The motivation for this method comes from the fact that when fitting a classifier using a single tree, the terminal nodes are not pure and the relative frequency of class  $k$  in a terminal node can be used to estimate the probability of class  $k$  for observations in that terminal node. In Random Forests, the terminal nodes *are* pure so the information from members of  $B_t$  is not useful. However, the out-of-bag observations (those in  $B_t^c$ ) *do* give information about the underlying class probabilities.

For tree  $t$ , if a node contains members of  $B_t^c$ , we use the relative frequency of class  $k$  observations in  $B_t^c$  in node  $q_t$  to estimate the probabilities for the node:

$$\hat{p}_{q_t, k} = \frac{\sum_{j \in B_t^c} I(q_t(j) = q_t) I(\hat{y}_j = k)}{\sum_{j \in B_t^c} I(q_t(j) = q_t)}.$$

and denote the set of nodes that do not contain members of  $B_t^c$  by  $Q_t^0$ . The out-of-bag estimates of the probabilities are found by averaging over the nodes that contain out-of-bag observations:

$$\hat{p}_{i, k}^{oob} = \frac{\sum_{t=1}^{ntree} I(q_t(i) \notin Q_t^0) \hat{p}_{q_t(i), k}}{\sum_{t=1}^{ntree} I(q_t(i) \notin Q_t^0)}.$$

#### 2.5 Software

We coded everything in R and used R package ”randomForest” [9] and ”Rcpp” [3].

## CHAPTER 3 SIMULATION

The simulation designs are used to represent scenarios where a binary response variable  $\mathbf{Y}$  is predicted from a set of predictor variables.

We used five simulation models in order to compare the probability estimation methods. The first one is the XOR model. The second and the third one are from Mease et al. [11], where they considered a simple two-dimensional circle model and 10 dimensional model. The fourth one is a bivariate normal mixture model and the last one is a mixture of normal clusters taken from the Elements of Statistical Learning [5]. We also make the plots for each model to visualize them.

### 3.1 XOR model ( **XOR1** and **XOR2** )

Let  $\mathbf{X} = (X_1, X_2)$  be a two-dimensional random vector uniformly distributed on the square  $[-1, 1]^2$  and let  $y$  be a categorical variable with values 0 or 1 defined as

$$y = \begin{cases} 0 & x_1x_2 \leq 0; \\ 1 & x_1x_2 > 0. \end{cases}$$

$Y = 0$  corresponds to class 0 and  $Y = 1$  corresponds to class 1. Therefore, the conditional probability of  $Y = 1$  given  $X$  is

$$P(y = 1|X = x) = \begin{cases} 0 & x_1x_2 \leq 0; \\ 1 & x_1x_2 > 0. \end{cases}$$

A second case of the XOR model is overlapping 10% based on the the model described above. We sample 10% observations from class 0 without replacement and switch it with the same number of observations from class 1. The conditional probability  $Y = 1$  given  $X$  is:

$$P(y = 1|X = x) = \begin{cases} 0.1 & x_1x_2 \leq 0; \\ 0.9 & x_1x_2 > 0. \end{cases}$$

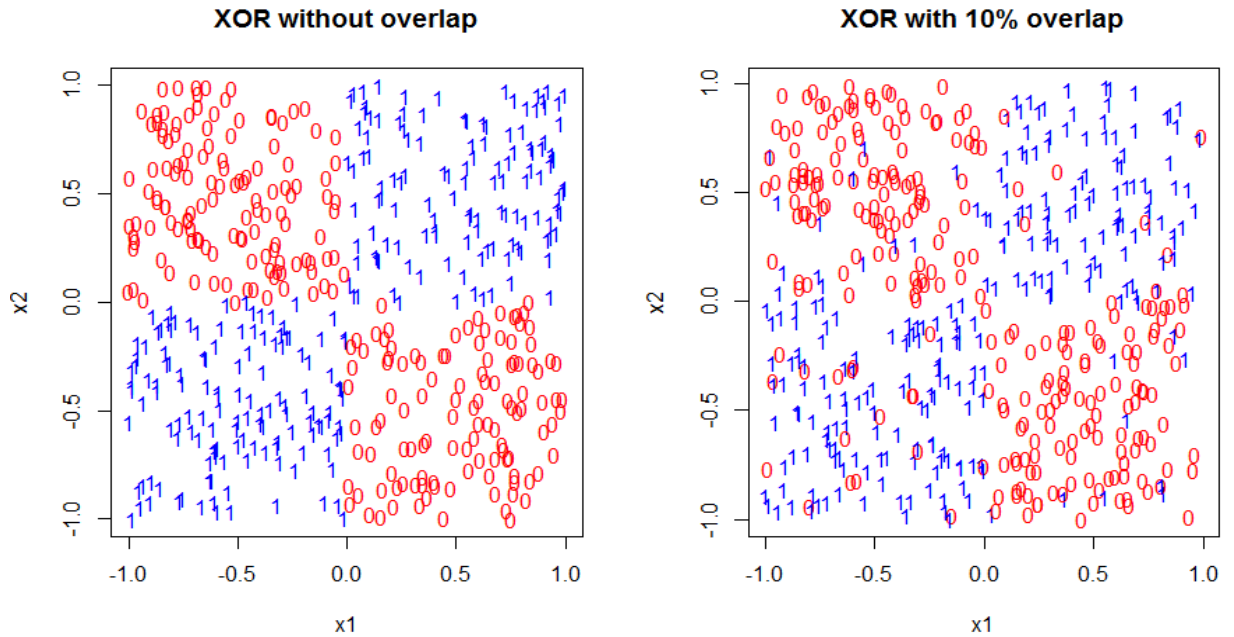


Figure 3.1. XOR Model

### 3.2 2-dimensional Circle Model (**2D Circle**)

Let  $\mathbf{X}$  be a two-dimensional random vector uniformly distributed on the square  $[0, 50]^2$  and  $Y$  be a categorical variable with values 0 or 1 depending on  $X$ . We construct level curves of  $p(x)$  to be concentric circles with center  $(25, 25)$ . The conditional probability of  $Y = 1$  given  $X = x$  is defined as:

$$P(Y = 1|X = x) = \begin{cases} 1 & r(x) < 8; \\ \frac{28-r(x)}{20} & 8 \leq r(x) \leq 28; \\ 0 & r > 28. \end{cases}$$

where  $r(x)$  is the distance from  $x$  to the point  $(25, 25)$  in  $R^2$ . This is called the 2-Dimensional Circle model. The right panel of figure 3.2 shows these probabilities for a hold-out sample with that is a grid 2000 evenly spaced points on  $[0, 50]^2$ . The greyness of the plot shows the probabilities: the lighter the color is, the smaller the probabilities are.

### 3.3 10-dimensional Model (**Friedman**)

Let  $\mathbf{X}$  be a 10-dimensional random vector  $\mathbf{X} = (X_1, X_2, \dots, X_{10})$  distributed according to  $N_{10}(0, I)$  and let  $Y$  be a categorical variable with values 0 or 1 depending on  $\mathbf{X}$ . The

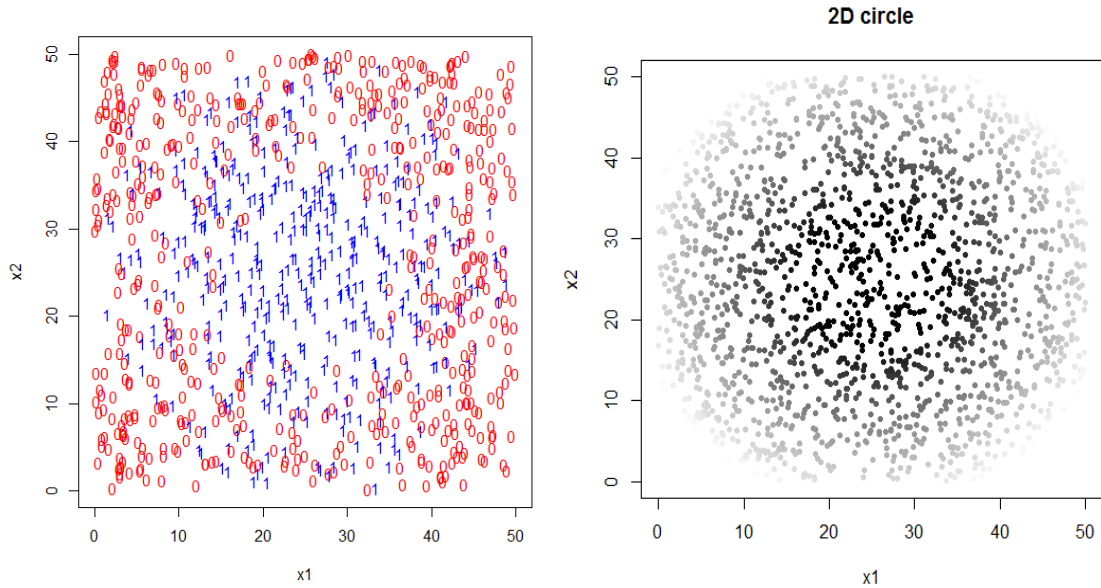


Figure 3.2. Training data (left) and true probabilities of being in class 1 (right) for the 2-Dimensional Circle Model

conditional probability that  $Y = 1$  given  $X = \mathbf{x}$  (which we denote  $p(\mathbf{x})$ ) is defined as follows:

$$\log \frac{p(\mathbf{x})}{1 - p(\mathbf{x})} = r[1 - x_1 + x_2 - x_3 + x_4 - x_5 + x_6] \sum_{j=1}^6 x_j$$

We choose  $r=10$ , which mimics the simulation of Friedman's model exactly. [6]

### 3.4 Bivariate Normal Model (**Binorm**)

Let  $\mathbf{X}$  be a random matrix consisting of two classes that belong to two different bivariate normal distributions with mean  $\mu_0$  and  $\mu_1$  and covariance  $\Sigma_0$  and  $\Sigma_1$ . Let  $Y$  be a dichotomous dependent variable with  $Y = 0$  corresponding to class 0 and  $Y = 1$  corresponding to class 1. The conditional probability that  $Y = 1$  given  $\mathbf{X} = x$  is defined as:

$$f(Y = 1|X = \mathbf{x}) = \frac{\pi_1 f_1(\mathbf{x})}{\pi_0 f_0(\mathbf{x}) + \pi_1 f_1(\mathbf{x})}$$

where  $\pi_0$  and  $\pi_1$  are the probabilities that  $Y = 0$  and  $Y = 1$  respectively,  $f_0(\mathbf{x})$  and  $f_1(\mathbf{x})$  are the probability density functions of class 0 and class 1.

We simulate 3 different representative cases for this model, labeled as binorm1, binorm2

and binorm3. Binorm1 has class 0 with mean  $\mu_0 = (0, 0)^T$ , covariance  $\Sigma_0 = \begin{pmatrix} 1 & 0.55 \\ 0.55 & 1 \end{pmatrix}$  and class 1 with mean  $\mu_1 = (0, 2.5)^T$ , covariance  $\Sigma_1 = \begin{pmatrix} 1 & -0.55 \\ -0.55 & 1 \end{pmatrix}$ . Binorm2 has class 0 with mean  $\mu_0 = (0, 0)^T$ , covariance  $\Sigma_0 = \begin{pmatrix} 1 & 0.47 \\ 0.47 & 1 \end{pmatrix}$  and class 1 with mean  $\mu_1 = (1, 1)^T$ , covariance  $\Sigma_1 = \begin{pmatrix} 1 & -0.47 \\ -0.47 & 1 \end{pmatrix}$ . Binorm3 has class 0 with mean  $\mu_0 = (0, 0)^T$ , covariance  $\Sigma_0 = \begin{pmatrix} 1 & -0.8 \\ -0.8 & 1 \end{pmatrix}$  and class 1 with mean  $\mu_1 = (1, 1)^T$ , covariance  $\Sigma_1 = \begin{pmatrix} 1 & -0.8 \\ -0.8 & 1 \end{pmatrix}$ . Class 0 is generated with probability  $\pi_0 = 2/3$  for the three cases.

### 3.5 Normal Cluster Mixtures (**Clusters**)

Let a 2-dimensional vector  $\mathbf{X} = \{X_1, X_2\}$ . Firstly 10 means  $\mu_j = \{mu_{j1}, \dots, \mu_{j10}\}$  are generated from a bivariate normal distribution  $N_2((1, 0)^T, \mathbf{I})$  and 10 more means  $\mu_i = \{mu_{i1}, \dots, \mu_{i10}\}$  are drawn from another bivariate normal distribution  $N_2((0, 1)^T, \mathbf{I})$ . We are generating a sample with N observations in total and the sample sizes for class 0 and class 1 are  $n_0$  and  $n_1$ . Then for each class, we generate  $n_0$  and  $n_1$  observations as follows: for each observation, a mean  $\mu$  is picked at random with probability  $1/10$  from  $\{mu_{j1}, \dots, \mu_{j10}\}$  for class 0 and from  $\{mu_{i1}, \dots, \mu_{i10}\}$  for class 1. Then the observation is drawn from a new bivariate normal distribution with the selected mean and covariance  $\Sigma = \mathbf{I}/5$ .  $Y$  is the binary response variable, where  $Y = 0$  corresponds to class 0 and  $Y = 1$  corresponds to class 1.

The conditional probability that  $Y = 1$  given  $X = \mathbf{x}$  is calculated using the same formula given above in the multivariate normal model. However,  $f_0(x)$  and  $f_1(x)$  are not directly given and they are the average of the pdf's of 10 different bivariate normal distributions.

In our simulation, class 0 is generated with probability  $\pi_0 = 2/3$ . The plot below is a sample with N=500.

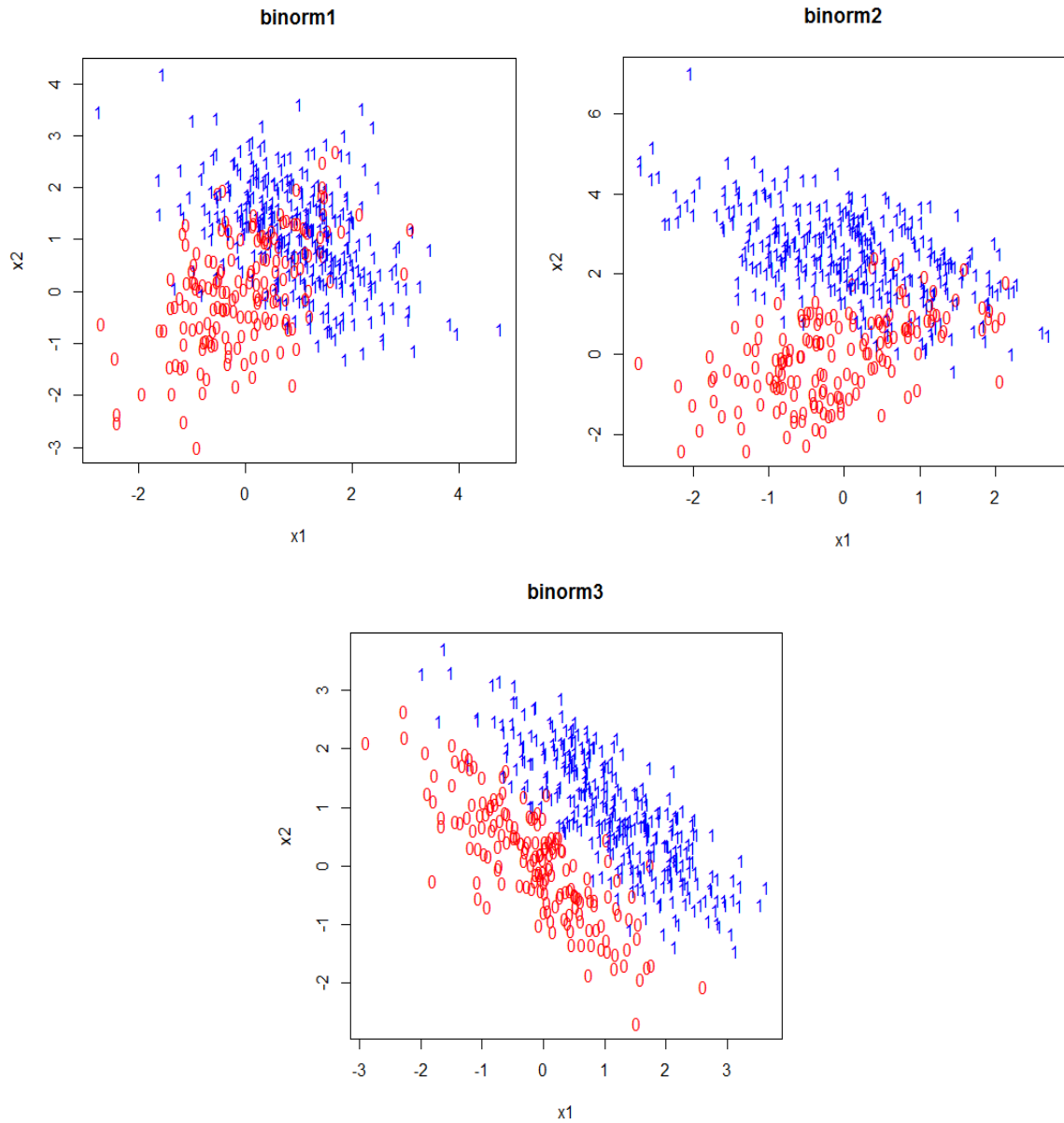


Figure 3.3. Bivariate Normal Model

### 3.6 Method to Measure the Performance of Class Probability Estimators

#### 3.6.1 Mean Squared Loss Function

We choose mean squared loss function to quantify the accuracy of the probability estimates for the simulations. It is defined:

$$\frac{1}{N} \sum_{i=1}^N (p(x_i) - \hat{p}(x_i))^2$$

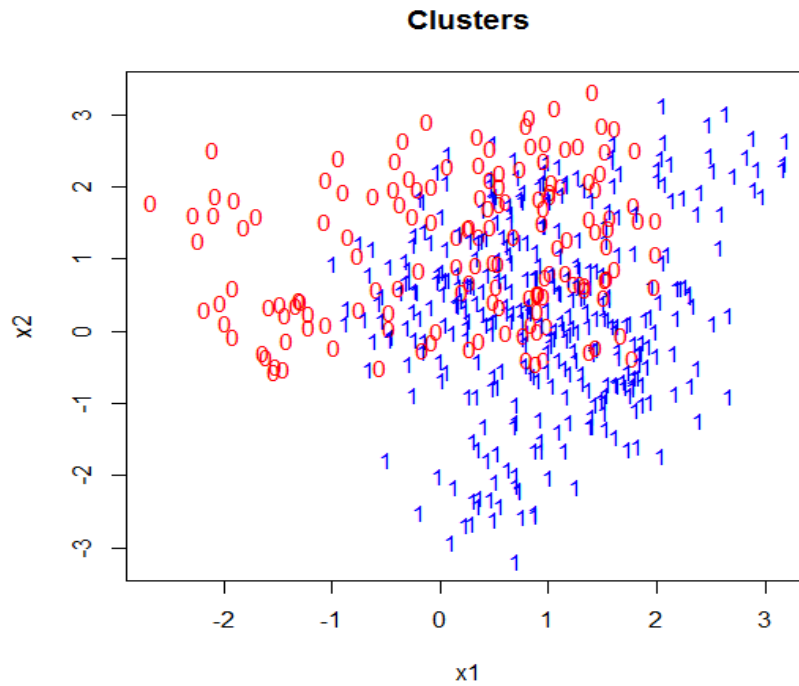


Figure 3.4. Normal Cluster Mixtures

### 3.6.2 Misclassification Error Rate

Another way we use to measure the accuracy of the probability estimates for the simulations is misclassification error rate. We give the classification results according to the probability estimations, i.e. an observation belongs to the class with bigger probability.

The trees are built based on the simulation training data with sample size  $N$ . There are 500 trees in total for each case, i.e.  $n_{tree}=500$ . Changing  $n_{tree}$  didn't change the squared loss for each method from the early experiments we did (Section 3.7.3), therefore, we are only showing the results when  $n_{tree}=500$ . We use the test data from 100 independent sample with sample size 1000 to evaluate the probability estimates. The final mean squared loss of the sample is the average of the losses for the 100 times' simulations. So does the misclassification error rate.

## 3.7 Simulation results

## 3.7.1 Results for Mean Squared Loss

Table 3.1. Mean Squared Loss N=100

Data	Dim	vote	prox	regrf	oob
XOR1	2	47.42	<b>40.25</b>	49.68	47.42
XOR2	2	97.29	92.16	94.51	<b>84.65</b>
2D Circle	2	38.26	32.21	32.63	<b>29.82</b>
Freidman	10	<b>204.72</b>	215.53	205.21	215.35
Binorm1	2	42.67	50.20	40.36	<b>38.33</b>
Binorm2	2	84.86	91.83	80.04	<b>68.25</b>
Binorm3	2	<b>41.35</b>	59.72	41.50	47.51
Clusters	2	131.2791	140.1213	124.6173	<b>108.87</b>

Table 3.2. Mean Squared Loss N=500

Data	Dim	vote	prox	regrf	oob
XOR1	2	7.85	<b>4.89</b>	7.99	7.72
XOR2	2	80.09	74.65	77.09	<b>66.39</b>
2D Circle	2	28.93	21.74	24.18	<b>13.36</b>
Freidman	10	<b>164.46</b>	168.69	165.19	184.75
Binorm1	2	37.94	43.02	35.60	<b>30.23</b>
Binorm2	2	77.3477	86.0702	72.7500	<b>60.79</b>
Binorm3	2	23.78	32.54	<b>22.66</b>	22.88
Clusters	2	135.38	144.36	130.67	<b>115.27</b>

Table 3.3. Mean Squared Loss N=1000

Data	Dim	vote	prox	regrf	oob
XOR1	2	3.35	<b>2.00</b>	3.41	3.27
XOR2	2	79.33	64.89	76.37	<b>60.50</b>
2D Circle	2	26.96	20.25	22.36	<b>10.34</b>
Freidman	10	<b>147.14</b>	146.15	148.17	167.81
Binorm1	2	35.95	40.27	33.86	<b>28.40</b>
Binorm2	2	75.45	86.41	71.20	<b>59.81</b>
Binorm3	2	21.40	27.78	20.18	<b>19.24</b>
Clusters	2	138.87	150.15	134.50	<b>120.74</b>

The data in the tables are all in  $10^{-3}$  scale, i.e. the real mean squared lost should be the value in the table times 0.001. All the simulation data only have two classes, i.e.



response variable with 2 categories. The bolded value is the smallest mean squared loss in a row.

### 3.7.2 Results for Misclassification Error Rate

Table 3.4. Misclassification Error Rate N=100

Data	Dim	vote	prox	regrf	oob
XOR1	2	0.0419	0.0412	0.0423	<b>0.0344</b>
XOR2	2	0.1898	0.1802	0.1856	<b>0.1651</b>
2D Circle	2	0.2669	0.2585	0.2595	<b>0.2542</b>
Freidman	10	<b>0.3742</b>	0.3984	0.3760	0.4009
Binorm1	2	0.1098	0.1028	0.1067	<b>0.1026</b>
Binorm2	2	0.2041	<b>0.1853</b>	0.1972	0.1855
Binorm3	2	<b>0.0915</b>	0.1103	0.0917	0.0946
Clusters	2	0.3053	0.2841	0.2992	<b>0.2826</b>

Table 3.5. Misclassification Error Rate N=500

Data	Dim	vote	prox	regrf	oob
XOR1	2	0.00561	0.00524	0.00563	<b>0.00523</b>
XOR2	2	0.12767	0.11224	0.12136	<b>0.11089</b>
2D Circle	2	0.25486	<b>0.23485</b>	0.25008	0.23645
Freidman	10	<b>0.27142</b>	0.29845	0.27217	0.28879
Binorm1	2	0.10727	<b>0.09887</b>	0.10532	0.09888
Binorm2	2	0.00547	<b>0.00477</b>	0.00545	0.00501
Binorm3	2	0.06632	0.06742	0.06460	<b>0.06407</b>
Clusters	2	0.18684	0.17452	0.18284	<b>0.14952</b>

Table 3.6. Misclassification Error Rate N=1000

Data	Dim	vote	prox	regrf	oob
XOR1	2	0.00253	<b>0.00237</b>	0.00248	0.00244
XOR2	2	0.11813	0.10576	0.11225	<b>0.10507</b>
2D Circle	2	0.25325	<b>0.23293</b>	0.24806	0.23373
Freidman	10	<b>0.22937</b>	0.25090	0.22952	0.24129
Binorm1	2	0.10508	<b>0.09629</b>	0.10304	0.09676
Binorm2	2	0.19406	0.17520	0.18878	<b>0.17495</b>
Binorm3	2	0.06390	0.06156	0.06248	<b>0.06006</b>
Clusters	2	0.30566	<b>0.28914</b>	0.30232	0.29025

The results given by misclassification error rate are a little different from the ones

measured by mean squared loss function. See chapter 5 for detailed conclusions.

### 3.7.3 Normal Cluster Mixtures with Different Ntrees

We set  $N=500$  as the sample size for training data set to build the tree. We also use the test data from 100 independent sample with sample size 1000 to evaluate the probability estimates. The final mean squared loss of the sample is the average of the losses for the 100 times' simulations. So does the misclassification error rate.

Table 3.7. Mean Squared Loss for Normal Cluster Mixtures with Different Ntrees

ntree	vote	prox	regf	oob
100	139.75	150.10	133.81	<b>118.46</b>
500	135.38	144.36	130.67	<b>115.27</b>
1000	130.79	140.17	126.08	<b>111.14</b>
1500	134.41	144.23	129.58	<b>113.97</b>
2000	135.95	146.20	131.29	<b>116.67</b>

Table 3.8. Misclassification Error Rate for Normal Cluster Mixtures with Different Ntrees

ntree	vote	prox	regf	oob
100	0.32301	<b>0.30157</b>	0.31923	0.30653
500	0.18684	0.17452	0.18284	<b>0.14952</b>
1000	0.29892	<b>0.28013</b>	0.29689	0.28419
1500	0.3092	<b>0.28997</b>	0.30695	0.29367
2000	0.29299	<b>0.27547</b>	0.29019	0.27854

## CHAPTER 4

### DATA EXAMPLES

#### 4.1 Brier Score

The Brier score is calculated by the original definition according to Wikipedia [13]. It is defined:

$$BS = \frac{1}{N} \sum_{n=1}^N \sum_{i=1}^K (f_{ti} - o_{ti})^2,$$

where  $N$  is the number of cases and  $K$  is the number of the classes for the events.  $f_{ti}$  is the estimated probability,  $o_{ti}$  is the actual outcome of the event at case  $t$  (0 if it doesn't occur and 1 if it occurs). For binary response variables, there is an alternative definition, which would give results half as big as ours.

#### 4.2 10-fold Cross Validation

Cross validation is a useful statistical technique to assess the performance of a statistical model or algorithm. The general idea of cross validation is dividing the data into two parts: one is the training data set and is used to build the model; the other one is testing data set or validation set and is used to validate and evaluate the model.

10-fold cross validation is mostly commonly used in machine learning. The original data set is randomly separated into 10 subsets with equal sample size  $N/10$ . 1 subset is chosen as the testing set and the other 9 are the training sets. Each time we choose a different testing set and repeat the procedure 10 times, therefore all the observations are tested exactly once. The estimation is obtained by combining the results from each testing set. [12]

#### 4.3 Missing Values

There are many ways to deal with missing values and we replace them in two ways:

##### 4.3.1 Na.roughfix

Na.roughfix is an R function in the Random Forests package which replaces the NAs with column medians if the variables are numeric, or the most frequent levels if the variables

are categorical. [8]

#### 4.3.2 RfImpute

There is another function to deal with missing data called “rfImpute” in the Random Forest R package. The algorithm starts by imputing NAs using `na.roughfix`. Then there aren’t any missing values in the data set and `randomForest` is used to obtain the proximity matrix, therefore updating the imputation of the NAs. For continuous variables, the imputed value is the weighted average of the non-missing values, in which the weights are the proximities. For categorical variables, the imputed value is the category with the largest average proximity. The process is iterated 5 times. [7]

#### 4.4 Results for Real Data

The methods are compared on 23 datasets from UCI Repository. We use 10-fold cross validation to estimate the Brier score for each data set.

We used `ntree=500` for all the datasets. The regression method only works for a binary response variable, therefore, we put NAs in the tables when there are more than 2 classes.

Table 4.1. Brier Score(Missing values are replaced using rfImpute)

Data	Classes	N	Dim	vote	prox	regrf	oob
Appendicitis	2	106	8	0.2149	<b>0.2064</b>	0.2153	0.2142
Pima	2	768	8	0.3178	0.3216	0.3163	<b>0.3139</b>
Wcancer	2	569	30	<b>0.0633</b>	0.0752	0.0635	0.0728
Iris	3	150	4	0.0720	0.0715	NA	<b>0.0704</b>
Glass	7	214	9	<b>0.3202</b>	0.3646	NA	0.3628
Spectf	2	80	44	0.3145	0.3245	<b>0.2949</b>	0.3747
tic	2	958	9	0.1166	<b>0.1151</b>	0.1284	0.1225
ltpd	2	583	10	0.3486	0.3641	<b>0.3470</b>	0.3521
Wine	3	178	13	<b>0.0558</b>	0.0571	NA	0.0709
Balance	3	625	4	0.2221	<b>0.1848</b>	NA	0.2201
Contraceptive	3	1473	9	0.5649	<b>0.5409</b>	NA	0.5417
ecoli	8	336	7	<b>0.2282</b>	0.2536	NA	0.2302
Fertility	2	100	9	0.2426	<b>0.2197</b>	0.2367	0.2218
Vote	2	435	17	0.0053	<b>0.0025</b>	0.0031	0.0051
Car	4	1728	6	<b>0.0900</b>	0.1161	NA	0.0926
Flag	6	194	28	0.4019	<b>0.3954</b>	NA	0.4347
Haberman	2	306	3	0.3840	0.3743	0.3757	<b>0.3664</b>
Roth	3	132	5	0.2729	0.2671	NA	<b>0.2651</b>
lens	3	24	5	<b>0.3475</b>	0.3730	NA	0.3531
Lung	3	32	57	0.3916	<b>0.3528</b>	NA	0.3737
Post-operative	3	90	9	0.3365	<b>0.3250</b>	NA	0.3322
Zoo	7	1484	16	<b>0.0583</b>	0.0899	NA	0.0743
Yeast	10	101	8	<b>0.5141</b>	0.5317	NA	0.5232

Table 4.2. Brier Score(Missing values are replaced using na.roughfix)

Data	Classes	N	Dim	vote	prox	regrf	oob
Appendicitis	2	106	8	0.2149	<b>0.2064</b>	0.2153	0.2142
Pima	2	768	8	0.3178	0.3216	0.3163	<b>0.3139</b>
Wcancer	2	569	30	<b>0.0633</b>	0.0752	0.0635	0.0728
Iris	3	150	4	0.0720	0.0715	NA	<b>0.0704</b>
Glass	7	214	9	<b>0.3202</b>	0.3646	NA	0.3628
Spectf	2	80	44	0.3145	0.3245	<b>0.2949</b>	0.3747
tic	2	958	9	0.1166	<b>0.1151</b>	0.1284	0.1225
ltpd	2	583	10	0.3669	0.3786	0.3661	<b>0.3568</b>
Wine	3	178	13	<b>0.0558</b>	0.0571	NA	0.0709
Balance	3	625	4	0.2221	<b>0.1848</b>	NA	0.2201
Contraceptive	3	1473	9	0.5649	<b>0.5409</b>	NA	0.5417
ecoli	8	336	7	<b>0.2282</b>	0.2536	NA	0.2302
Fertility	2	100	9	0.2426	<b>0.2197</b>	0.2367	0.2218
Vote	2	435	17	0.0703	0.0720	0.0698	<b>0.0683</b>
Car	4	1728	6	<b>0.0900</b>	0.1161	NA	0.0926
Flag	6	194	28	0.4019	<b>0.3954</b>	NA	0.4347
Haberman	2	306	3	0.3840	0.3743	0.3757	<b>0.3664</b>
Roth	3	132	5	0.2729	0.2671	NA	<b>0.2651</b>
lens	3	24	5	<b>0.3475</b>	0.3730	NA	0.3531
Lung	3	32	57	0.6009	0.6124	NA	<b>0.5920</b>
Post-operative	3	90	9	0.8570	<b>0.8551</b>	NA	0.8610
Zoo	7	1484	16	<b>0.0583</b>	0.0899	NA	0.0743
Yeast	10	101	8	<b>0.5141</b>	0.5317	NA	0.5232

## CHAPTER 5 CONCLUSIONS

For the Simulations, sample sizes have some effects on the performance of each methods. For the third case of the bivariate normal model: when  $N = 100$ , vote gives the smallest mean squared loss; when  $N = 500$ , the regression method makes the mean squared loss smallest; when  $N = 1000$ , the proximity weighting method turns out to be the best. For the Freidman model, vote is the best probability estimation method when the sample size is 100 and 500, however, when the sample size increases to 1000, proximity weighting performs better.

Regardless of the sample size effects, the out-of-bag method performs better than other methods in XOR with 10% over lap, 2-dimensional circle model, two bivariate normal models and normal cluster mixtures. Proximity weighting does best in the XOR model without overlap. Proximity weighting does better than votes or regression in 2-dimensional circle model.

The misclassification error rate criterion gives a little different results: When  $N = 100$  and 500, the out-of-bag method is slightly better than the proximity weighting method for XOR model without overlap; when  $N = 500$  and 1000, the proximity method gives smallest misclassification error rate instead of the out-of-bag method for 2-dimensional circle model and the Binorm1; The proximity weighting method performs best instead of the out-of-bag method for Binorm2 when  $N = 100$  and the normal cluster mixtures when  $N = 1000$ .

Only considering the misclassification error rate measurement, the out-of-bag method gives the smallest misclassification error rate. However, when the sample size of training data set increases, the proximity method tends to be better. Both the two methods apparently perform better than other methods, however, either of them can beat the other consistently.

Testing all the methods on real datasets, however, no methods did consistently better than all other methods. When we replace missing values with the rfImpute method, proximity weighting does best in more data sets. When we replace missing values with the

na.roughfix method, among the three methods, vote, proximity weighting and oob, no one is consistently better than the others. However, the regression method doesn't perform well when it is applicable, no matter what method we use to deal with missing data.



## CHAPTER 6

### DISCUSSION AND FUTURE WORK

The two new methods, proximity weighting and out-of-bag method, outperform the current methods in almost all the simulations. However, experimenting on the real data sets, the the out-of-bag method doesn't perform as well as it performs in the simulations and proximity weighting isn't significantly better than votes, based on the 23 data sets from the UCI machine learning repository. I would like to experiment on more data sets to have more confidence in the conclusions in the future.

In the simulations, sample size has very significant influence on the third case of the bivariate normal model according to mean squared loss measurement. I would like to further explore why this happens by doing more different simulations for the binorm model and thinking about it theoretically. Sample size has even more influence according to the misclassification error rate measurement, it is worthwhile to find out the reasons. Also I would like to figure out why proximity weighting performs better than the out-of bag method in XOR model without overlap. The 10-dimensional model is another simulation I would like to do more theoretical research on to figure out why the out-of-bag method performs so bad on this model.

The current version of the code for the out-of-bag method only works for numeric predictors, we have to convert the non-numeric predictors into numeric ones. Hence, we would like to improve the code for categorical predictors.

One interesting feature of the real data comparisons is that the missing value imputation method makes such a big difference.

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