



# A random forests quantile classifier for class imbalanced data

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## ABSTRACT

Extending previous work on quantile classifiers ( $q$ -classifiers) we propose the  $q^*$ -classifier for the class imbalance problem. The classifier assigns a sample to the minority class if the minority class conditional probability exceeds  $0 < q^* < 1$ , where  $q^*$  equals the unconditional probability of observing a minority class sample. The motivation for  $q^*$ -classification stems from a density-based approach and leads to the useful property that the  $q^*$ -classifier maximizes the sum of the true positive and true negative rates. Moreover, because the procedure can be equivalently expressed as a cost-weighted Bayes classifier, it also minimizes weighted risk. Because of this dual optimization, the  $q^*$ -classifier can achieve near zero risk in imbalance problems, while simultaneously optimizing true positive and true negative rates. We use random forests to apply  $q^*$ -classification. This new method which we call RFQ is shown to outperform or is competitive with existing techniques with respect to  $G$ -mean performance and variable selection. Extensions to the multiclass imbalanced setting are also considered.

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## 1. Introduction

Random forests, introduced by Leo Breiman [1], is an increasingly popular learning algorithm that offers fast training, excellent performance, and great flexibility in its ability to handle all types of data [2,3]. It provides its own internal generalization error estimate (i.e., out-of-bag error) as well as measures of variable importance [1,4–6] and class probability estimates [7]. Random forests has been used for predictive tasks as varied as modeling mineral prospectivity [8], lake water level forecasting [9], identifying potentially salvageable tissue after acute ischemic stroke [10], identifying biomarkers for diagnosis of Kawasaki disease [11], classifying childhood onset schizophrenia [12], electrical load forecasting [13], and for pedestrian detection [14]. The random forests algorithm has also been generalized beyond classification and regression, most importantly to random survival forests, where each terminal node of a tree in the forest provides a survival function estimate [15,16]. Random survival forests has been used to analyze survival problems with great success; for example, in esophageal cancer staging [17,18].

In biomedical and other real world applications, a common problem is the occurrence of imbalanced data, defined as data featuring high-imbalance in the frequency of the observed class labels (see Section 2 for a formal definition). Some examples are

disease prediction [19] and diagnosing aviation turbulence [20]. Imbalanced data has been observed to seriously hinder the classification performance of learning algorithms, including random forests and other ensemble methods because their decisions are based on classification error [21] and where there is high-imbalance in the frequency of the observed class labels a low error rate can be achieved by classifying all of the samples as members of the majority class.

Classification of class imbalanced data sets has been identified as a top problem in machine learning [22] and there is an ever increasing body of literature devoted to this extremely important problem. He and Garcia [23] and Sun et al. [24] systematically reviewed classification in the presence of class imbalance. As examples of more specialized reviews, Galar et al. [21] focused specifically on using ensembles to learn class imbalanced data and Lopez et al. [25,26] explored imbalanced data characteristics. Finally, three very recent, useful reviews deserve mentioning: Krawczyk [27] thoroughly reviewed open research challenges in learning imbalanced data; Haixiang et al. [28] exhaustively reviewed existing papers on imbalanced data published between 2006 and 2016 and categorized them with respect to method and the journals in which they were published; and Das et al. [29] provided a comprehensive review of current approaches to imbalanced data and class overlap and open issues with the same in the broader context of data irregularities.

Section 2 formally defines the class imbalance problem and provides a breakdown of methods that have been used to address this problem. As discussed there, of the various methods proposed,

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undersampling the majority class so that its cardinality matches that of the minority class is among the most popular. In the context of random forests, undersampling the majority class provides improved classification performance with respect to the minority class [30] and appears to be the most common approach when using random forests to learn imbalanced data due to the fact that it was implemented in Breiman's original Fortran code [4] used by the `randomForest` R-package [31]. This method is called *balanced random forests* (BRF) and it is an example of what has been referred to in the literature [32] as a data level method, which transform the distributions of the classes in the training data. We will show that BRF has an important connection to our approach even though our method is not an example of a data level method.

In Section 3, we propose our new approach to the class imbalance problem using a density-based argument. This results in a classifier that can be seen to be an example of a *quantile classifier*, or *q-classifier* [33], which classifies samples based on whether the conditional probability of the minority class exceeds a specified threshold  $0 < q < 1$ . Theorem 2 shows that the specific threshold value  $q^*$  of this classifier ( $q^*$ -classifier) has the useful property that it maximizes the true positive and true negative rates. Moreover, because it can be equivalently expressed as a cost-weighted Bayes classifier, it is also shown to minimize weighted risk. Because of this dual optimization, unlike the traditional Bayes classifier (which is a  $q = 0.5$  median classifier), the  $q^*$ -classifier can achieve near zero risk in highly imbalanced data, while simultaneously optimizing true positive and true negative rates. Furthermore, we show surprisingly that balanced sampling as used by BRF also has this optimality property of maximizing the true positive and true negative rates (Theorem 3). Moreover, we show that the  $q^*$ -classifier's optimality continues to hold even if sampling strategies are imposed (Theorem 4). Because we choose to implement  $q^*$ -classification using the full data, this means balanced sampling, while achieving the same optimality property, comes at the cost of efficiency since it only uses a fraction of the data. We apply  $q^*$ -classification with random forests, which we call RFQ, using a large comparative benchmark study (Section 4) and find it highly competitive and not only that but we are able to identify conditions under which RFQ significantly outperforms BRF (Section 5). These findings are further confirmed using synthetic data and through in-depth case study analyses. Section 6 shows RFQ also outperforms BRF with respect to variable selection. Section 7 considers the extension of RFQ to the multiclass imbalanced setting. Section 8 compares RFQ to boosting methods. Section 9 concludes with a discussion of our findings.

## 2. Imbalanced data setting

We now formally define the imbalanced data setting and introduce notation to be used throughout the paper. Denote the learning data by  $\mathcal{L} = (X_i, Y_i)_{1 \leq i \leq N}$ , where  $X_i \in \mathcal{X}$  is the  $d$ -dimensional feature and  $Y_i \in \{0, 1\}$  is the binary ordinal response. It is assumed that  $(X_i, Y_i)$  are i.i.d. from a common distribution  $\mathbb{P}$ . Let  $(X, Y)$  denote an independent generic data point with distribution  $\mathbb{P}$ .

Our goal is to build an accurate classifier for  $Y$  given  $X = x$  when the learning data is imbalanced. To help quantify what is meant by “imbalancedness”, we start by first defining the imbalance ratio (IR). Following the convention in the literature, we assume that the majority class labels are 0, and outnumber the minority class labels, 1.

**Definition 1.** The imbalance ratio (IR) is defined as  $IR = N_0/N_1$  where  $N_0$  and  $N_1$  denote the cardinality of the majority and minority samples, respectively. A data set is imbalanced if  $IR \gg 1$ .

It has been observed that class imbalance is not a problem in and of itself and does not necessarily lead to poor generalization

in classification. If the training data is such that the classes can be separated in the feature space, then good classification will be achieved irrespective of IR. Rather the problem is that of training the classifier on too few minority examples in the presence of class overlap and small subgroups of minority class examples surrounded by majority class examples in the data space (sometimes referred to as “small disjuncts”), which frequently characterize imbalanced data. This combination of characteristics, termed “concept complexity,” [34] make it difficult for a classifier to construct a good decision boundary leading to poor classification performance [35–37].

In order to quantify the complexity of imbalanced data, we adopt the approaches in [38] and [36], where they evaluate the distribution of the two classes in the local neighborhood of each minority example using  $k = 5$  nearest neighbors. We adopt their taxonomy of types of minority examples except that we make no distinction between minority examples with 4/5 and 5/5 nearest neighbors of the majority class.

**Definition 2.** A minority class example is *safe*, *borderline*, or *rare* if 0 to 1, 2 to 3, or 4 to 5 of its 5 nearest neighbors are of the majority class, respectively.

We show in Section 5 that the percentage of minority class samples that are rare plays an important role in explaining differences between the  $q^*$ -classifier and BRF.

Now we define some formal notions of imbalancedness. Following [39], we distinguish between *marginally imbalanced* and *conditionally imbalanced* data.

**Definition 3.** The data is marginally imbalanced if  $p(x) \ll 1/2$  for all  $x \in \mathcal{X}$  where  $p(x) = \mathbb{P}\{Y = 1|X = x\}$ .

Thus, marginally imbalanced data is data for which the probability of the minority class is close to zero throughout the feature space.

**Definition 4.** The data is conditionally imbalanced if there exists a set  $A \subset \mathcal{X}$  with nonzero probability,  $\mathbb{P}\{X \in A\} > 0$ , such that  $\mathbb{P}\{Y = 1|X \in A\} \approx 1$  and  $p(x) \ll 1/2$  for  $x \notin A$ .

In contrast to marginally imbalanced data, conditional imbalancedness occurs when the probability of the minority class is close to 1 given the features lie in a certain set, and approximately zero otherwise. In both cases, it is assumed that the minority class is rare.

### 2.1. Related work

As briefly mentioned in the Introduction, there is a vast literature on methods that have been used for the class imbalance problem. Methods to address the problem can be broadly grouped into data level methods, which transform the distributions of the classes in the training data, and algorithmic level methods, which adapt existing learning algorithms or develop new ones [32].

#### 2.1.1. Data level methods

Data level methods, by far the most popular approach to imbalanced data [28], can be further subdivided into those that undersample the majority class or oversample the minority class to achieve balanced training data.

- One-Sided Sampling [40] selectively subsamples the majority class, removing only majority class instances that are either redundant with other majority class instances or have minority class instances as their 1-NN. These “Tomek links” are removed since a small amount of attribute noise can push these examples to the incorrect side of the decision boundary.

- Balanced Random Forests (BRF) [30], discussed in the Introduction, undersamples the majority class so that its cardinality matches that of the minority class in each bootstrap sample. BRF is a common approach when using random forests due to the fact it is implemented in the popular `randomForest` R-package [31].
- Neighborhood Balanced Bagging [38] focuses bootstrap sampling toward minority examples that are difficult to learn while simultaneously decreasing probabilities of selecting examples from the majority class. The extent to which an example is considered difficult to learn is quantified by determining the number of majority examples among its  $k$ -nearest neighbors.
- Synthetic Minority Over-sampling Technique (SMOTE) [41,42] generates new artificial minority class examples by interpolating among the  $k$ -nearest neighbors that are of the minority class (i.e., artificial minority instances are introduced on the lines between each minority instance and its  $k$ -nearest minority class neighbors until the class frequencies are approximately balanced).
- A number of methods that combine boosting with sampling the data at each boosting iteration have been developed; SMOTEBoost [43] combines SMOTE with boosting, RUSBoost [44] combines random undersampling with boosting, and EUSBoost [45] combines evolutionary undersampling with boosting.

### 2.1.2. Algorithmic level methods

As an alternative to sampling the data to balance the cardinality of the classes, learning algorithms can be modified to improve classification over the minority class.

- SHRINK [46] labels all the instances in a region as minority class provided the region contains at least one minority class example. SHRINK then searches over these regions for the optimal minority class region with the greatest number of minority class samples relative to majority class samples. However, SHRINK fails in data sets where there exists more than one substantial cluster of minority class instances and it provides no advantage in data sets without significant class overlap.
- Hellinger Distance Decision Trees (HDDT) [47] use Hellinger distance, a measure of distributional divergence, as the splitting criterion. The authors argue that the skew insensitivity of Hellinger distance makes it superior to standard splitting rules such as the Gini index in the presence of imbalanced data.
- Near-Bayesian Support Vector Machines (NBSVM) [48] combines decision boundary shifting with unequal regularization costs for the majority and minority classes. NBSVM uses the empirical relative frequencies of the two classes as estimates of the prior probabilities to shift the decision boundary toward the Bayes optimal decision boundary. However, the performance of NBSVM is kernel-dependent (as with standard SVM) and is poor when the minority class is compact in comparison to the majority class.
- Class Switching according to Nearest Enemy Distance [49] adapts a technique proposed by Breiman [50] to highly imbalanced data by switching the labels of majority class samples with a probability proportional to their Euclidean distance to the closest minority class sample.

## 3. An optimal quantile classifier for class imbalanced data

Our approach falls under the class of algorithmic level procedures. Following [33], we define a quantile classifier ( $q$ -classifier)

as

$$\delta_q(x) = \mathbf{1}_{\{p(x) \geq q\}},$$

where  $0 < q < 1$  is a prespecified quantile threshold. If we have  $q = 1/2$ , which [33] term a *median classifier*, we obtain the familiar Bayes classifier:

$$\delta_B(x) = \mathbf{1}_{\{p(x) \geq 1/2\}}.$$

As noted in [33], minimizing loss subject to unequal misclassification costs is equivalent to classification based on  $p(x) \geq q$  using thresholds  $q$  other than  $1/2$ . This will be demonstrated presently and in so doing explain why imbalanced data is so challenging for classifiers.

Define the risk for a classifier  $\hat{\delta}(x)$  as

$$r(\hat{\delta}, \ell_0, \ell_1) = \mathbb{E} \left[ \ell_0 \mathbf{1}_{\{\hat{\delta}(X)=1, Y=0\}} + \ell_1 \mathbf{1}_{\{\hat{\delta}(X)=0, Y=1\}} \right]. \quad (1)$$

Here  $\ell_0, \ell_1 > 0$  are fixed constants associated with the cost of making one of the two classification errors:  $\ell_0$  is the cost of misclassifying a majority class instance;  $\ell_1$  is the cost for misclassifying a minority class instance. Assigning specific losses leads to the interpretation of (1) as a cost-weighted risk function. Under uniform weights  $\ell_0 = \ell_1 = 1$ , the risk (1) simplifies to classification error,  $\mathbb{P}\{\hat{\delta}(X) \neq Y\}$ , which we denote as  $r(\hat{\delta})$ .

Under the cost-weighted risk (1), the optimal classifier is the cost-weighted Bayes rule, defined as

$$\delta_{WB}(x) = \mathbf{1}_{\{p(x) \geq \ell_0/(\ell_0 + \ell_1)\}}, \quad (2)$$

which we recognize as a quantile classifier with  $q = \ell_0/(\ell_0 + \ell_1)$ . The following well known result establishes the optimality of the cost-weighted Bayes classifier [51]. For convenience we provide a proof in [Appendix A](#).

**Theorem 1.** *The cost-weighted Bayes rule is optimal in that its risk satisfies  $r(\delta_{WB}, \ell_0, \ell_1) \leq r(\hat{\delta}, \ell_0, \ell_1)$  for any classifier  $\hat{\delta} : \mathcal{X} \rightarrow \{0, 1\}$ . Its risk equals*

$$r(\delta_{WB}, \ell_0, \ell_1) = \mathbb{E}[\min\{\ell_1 p(X), \ell_0(1 - p(X))\}]. \quad (3)$$

Thus, (3) is the smallest weighted risk achievable by a decision rule.

Now consider what happens in imbalanced data if performance is measured using classification error,  $\ell_0 = \ell_1 = 1$ . In this case, the cost-weighted Bayes classifier reduces to the (unweighted) Bayes classifier. Assuming marginal imbalance, i.e.  $p(x) \ll 0.5$ , the Bayes rule is  $\delta_B(x) = 0$ , thereby classifying all observations as majority class labels. Under classification error we know this must be the optimal rule. In particular by (3), the Bayes error equals  $r(\delta_B) = \mathbb{E}[\min\{p(X), 1 - p(X)\}] = \mathbb{E}[p(X)] \approx 0$  which is essentially perfect.

### 3.1. A density-based approach

We see that classification error provides a strong incentive for learning algorithms to correctly classify majority class samples at the expense of misclassifying minority class samples. This is obviously problematic and a better approach is to demand good performance from a classifier under both types of classification errors. Define the TNR (true negative rate) and TPR (true positive rate) for a classifier  $\hat{\delta}$  as follows:

$$\text{TNR}(\hat{\delta}) = \mathbb{P}\{\hat{\delta}(X) = 0 | Y = 0\}, \quad \text{TPR}(\hat{\delta}) = \mathbb{P}\{\hat{\delta}(X) = 1 | Y = 1\}.$$

Our goal is to find a classifier that achieves both high TNR and TPR values in imbalance problems. The Bayes rule,  $\delta_B$ , does not achieve this goal because it has a TNR value of 1 but a TPR value of 0.

**Definition 5.** A classifier  $\hat{\delta} : \mathcal{X} \rightarrow \{0, 1\}$  is said to be TNR+TPR-optimal if it maximizes the sum of the rates,  $\text{TNR} + \text{TPR}$ .

To achieve the goal of TNR+TPR optimality, we introduce the following classifier derived from a density-based approach. The

**Table 1**  
Notation used throughout the paper.

$\hat{\delta}(x)$	Generic classifier
$\ell_0, \ell_1$	misclassification costs for majority and minority classes
$r(\hat{\delta}, \ell_0, \ell_1)$	risk for $\hat{\delta}(x)$
$\pi$	the marginal probability that $Y = 1$ , $\pi = \mathbb{P}\{Y = 1\}$
$\hat{\pi} = N_1/N$	relative frequency of minority class
$p(x)$	conditional class probability function, $p(x) = \mathbb{P}\{Y = 1 X = x\}$
$f_X(x)$	density for $X$
$\delta_q(x)$	quantile classifier ( $q$ -classifier)
$\delta_B(x)$	Bayes classifier
$\delta_{WB}(x)$	cost-weighted Bayes classifier
$\delta_{q^*}(x)$	$q^*$ -classifier (quantile classifier with $q = \pi$ )

classifier, denoted by  $\delta_D(x)$ , assigns an instance  $x$  to the minority class if its data density for minority class labels,  $f_{X|Y}(x|1)$ , is larger than the data density for majority class labels,  $f_{X|Y}(x|0)$ :

$$\delta_D(x) = \mathbf{1}_{\{f_{X|Y}(x|1) \geq f_{X|Y}(x|0)\}}.$$

Basing the classifier on the conditional density of the features,  $f_{X|Y}$ , rather than the conditional density of the response,  $p(x)$ , removes the effect of the prevalence of the minority class labels. This is one way to see how  $\delta_D$  is able to handle imbalancedness. More directly we can show that  $\delta_D$  is TNR+TPR-optimal. Here is an informal argument showing this. First notice that for a classifier  $\hat{\delta}$  to achieve TNR+TPR-optimality it should maximize the probability of the events  $\{\hat{\delta}(X) = 0|Y = 0\}$  and  $\{\hat{\delta}(X) = 1|Y = 1\}$ ; this being equivalent to tracking the regions of the data space where the respective conditional densities are maximized. The value of TNR + TPR conditional on  $\mathcal{L}$  for the classifier  $\hat{\delta}$  equals

$$\begin{aligned} & \int_{\hat{\delta}(x)=0} f_{X|Y}(x|0) dx + \int_{\hat{\delta}(x)=1} f_{X|Y}(x|1) dx \\ & \leq \int_{f_{X|Y}(x|0) > f_{X|Y}(x|1)} f_{X|Y}(x|0) dx + \int_{f_{X|Y}(x|0) \leq f_{X|Y}(x|1)} f_{X|Y}(x|1) dx. \end{aligned}$$

The right-hand side is the TNR + TPR value for  $\delta_D$ , which shows that it is the optimal TNR+TPR-rule. A more formal proof of this fact is given shortly.

Before proceeding, we introduce a table of notation that will be particularly useful in this and subsequent sections (see Table 1).

### 3.2. The $q^*$ -classifier

While it is convenient theoretically to describe the density-based classifier in terms of the conditional density of the data, in practice it will be difficult to implement the classifier as stated. However, we can rewrite  $\delta_D(x)$  using the following identity:

$$\frac{f_{X|Y}(x|1)}{f_{X|Y}(x|0)} = \frac{f_{X,Y}(x, 1)/\mathbb{P}\{Y = 1\}}{f_{X,Y}(x, 0)/\mathbb{P}\{Y = 0\}} = \frac{\mathbb{P}\{Y = 1|X = x\}f_X(x)/\mathbb{P}\{Y = 1\}}{\mathbb{P}\{Y = 0|X = x\}f_X(x)/\mathbb{P}\{Y = 0\}}.$$

Cancelling the common value  $f_X(x)$  in the numerator and denominator, and using the notation of Table 1, we have

$$\delta_D(x) = \mathbf{1}_{\{\Delta_D(x) \geq 1\}}, \quad \text{where} \quad \Delta_D(x) = \frac{f_{X|Y}(x|1)}{f_{X|Y}(x|0)} = \frac{p(x)(1-\pi)}{(1-p(x))\pi}. \quad (4)$$

With a little bit of rearrangement, we now see that (4) is a  $q$ -classifier with  $q = \pi$  (notice analogously for the Bayes classifier that  $\delta_B(x) = \mathbf{1}_{\{\Delta_B(x) \geq 1\}}$  where  $\Delta_B(x) = p(x)/(1-p(x))$ , which is a  $q$ -classifier with  $q = 0.5$ ). This leads to the following definition of the proposed classifier.

**Definition 6.** Call  $\delta_{q^*}(x) = \mathbf{1}_{\{p(x) \geq \pi\}}$  the  $q^*$ -classifier (and keep in mind  $\delta_{q^*} = \delta_D$ ).

Although [33] introduced the extremely useful concept of a quantile classifier, they did not address how to select the optimal

$q$ . In deriving the  $q^*$ -classifier, we have informally argued that  $q$  should be  $\pi$ . In the following result, we formally justify our selection of  $q$  by showing that the  $q^*$ -classifier is able to achieve a near zero risk while jointly optimizing TNR and TPR.

**Theorem 2.** The  $q^*$ -classifier is TNR+TPR-optimal. Furthermore, it is the cost-weighted Bayes rule (2) under misclassification costs  $\ell_0 = \pi$  and  $\ell_1 = (1 - \pi)$ .

Theorem 2 shows that the  $q^*$ -classifier is not only TNR+TPR-optimal, but also weighted risk optimal under misclassification costs  $\ell_0 = \pi$  and  $\ell_1 = (1 - \pi)$ . In particular, by (3) of Theorem 1 we have

$$\begin{aligned} r(\delta_{q^*}, \pi, 1 - \pi) &= \mathbb{E}[\min\{(1 - \pi)p(X), \pi(1 - p(X))\}] \\ &\leq \mathbb{E}[\pi(1 - p(X))] \leq \pi. \end{aligned}$$

Notice that the right-hand side will be nearly zero for both types of imbalanced data: marginally and conditionally imbalanced. Moreover, unlike the Bayes rule, which also achieves a near zero risk, Theorem 2 shows the  $q^*$ -classifier is able to do this while satisfying the requirement of a jointly optimized TNR and TPR.

**Proof of Theorem 2.** Maximizing TNR and TPR is equivalent to minimizing FPR = 1 – TNR and FNR = 1 – TPR. For any classifier  $\hat{\delta}$ , we have by definition

$$\begin{aligned} & \text{FPR}(\hat{\delta}) + \text{FNR}(\hat{\delta}) \\ &= \mathbb{P}\{\hat{\delta}(X) = 1|Y = 0\} + \mathbb{P}\{\hat{\delta}(X) = 0|Y = 1\} \\ &= \frac{\mathbb{P}\{\hat{\delta}(X) = 1, Y = 0\}}{\mathbb{P}\{Y = 0\}} + \frac{\mathbb{P}\{\hat{\delta}(X) = 0, Y = 1\}}{\mathbb{P}\{Y = 1\}} \\ &= \mathbb{E}\left[\frac{\mathbf{1}_{\{\hat{\delta}(X)=1, Y=0\}}}{\ell_1} + \frac{\mathbf{1}_{\{\hat{\delta}(X)=0, Y=1\}}}{\ell_0}\right]. \end{aligned}$$

Minimizing the above expression does not change if we multiply by  $\ell_0\ell_1$  throughout. Therefore, minimizing the FPR and FNR rate is equivalent to minimizing

$$\mathbb{E}\left[\ell_0 \mathbf{1}_{\{\hat{\delta}(X)=1, Y=0\}} + \ell_1 \mathbf{1}_{\{\hat{\delta}(X)=0, Y=1\}}\right]$$

which is the weighted risk  $r(\hat{\delta}, \ell_0, \ell_1)$  where  $\ell_0 = \pi$  and  $\ell_1 = 1 - \pi$ . By Theorem 1, this is minimized by the weighted Bayes rule (2), which equals the  $q^*$ -classifier under the stated choices for  $\ell_0$  and  $\ell_1$ .  $\square$

### 3.3. Response-based sampling: Balancing the data

One common strategy to overcome the imbalance problem is to undersample the majority class to evenly balance the data. We can describe this process more formally by introducing auxiliary variables  $S_i \in \{0, 1\}$  where values  $S_i = 1$  indicate subsampled cases. The subsampled learning data is defined as  $\mathcal{L}_S = \{(X_i, Y_i) : S_i = 1, i = 1, \dots, N\}$  where data values are selected with probabilities that depend only on the value of  $Y$  and not  $X$ . This is called response-based sampling. In particular,

$$\mathbb{P}\{S = 1|Y\} = \begin{cases} \pi_S(1), & \text{if } Y = 1 \\ \pi_S(0), & \text{otherwise,} \end{cases} \quad (5)$$

where  $0 < \pi_S(Y) < 1$ .

By (5), the probability a randomly selected  $Y$  from  $\mathcal{L}_S$  equals  $Y = 1$  is

$$\pi^S := \mathbb{P}\{Y = 1|S = 1\} = \frac{\mathbb{P}\{S = 1|Y = 1\}\mathbb{P}\{Y = 1\}}{\mathbb{P}\{S = 1\}} = \frac{\pi_S(1)\pi}{\mathbb{P}\{S = 1\}}. \quad (6)$$

Likewise,  $1 - \pi^S = \mathbb{P}\{Y = 0|S = 1\} = \pi_S(0)(1 - \pi)/\mathbb{P}\{S = 1\}$ . In order to have balanced labels we must have  $\pi^S = 1/2$ , or equivalently



$\pi^S = 1 - \pi^S$ , which implies by (6)

$$\frac{\pi_S(1)}{\pi_S(0)} = \frac{1 - \pi}{\pi}. \quad (7)$$

The factor (7) calls to mind the factor in (4) that modulates the difference between  $\delta_B$  and  $\delta_D$ . This is not a coincidence as we now show. In what follows, we expand upon the justification for under-sampling provided by [33], which can be inferred from [52]. Let  $\delta_B^S$  be the Bayes rule constructed using  $\mathcal{L}_S$  (call this the subsampled Bayes rule). For a given  $x$ ,

$$\delta_B^S(x) = 1 \quad \text{if} \quad \frac{p^S(x)}{(1 - p^S(x))} \geq 1,$$

where by definition  $p^S(x) = \mathbb{P}\{Y = 1|X = x, S = 1\}$ . By Bayes theorem,

$$p^S(x) = \frac{f_{X,Y}^S(x, 1)}{f_X^S(x)}, \quad 1 - p^S(x) = \frac{f_{X,Y}^S(x, 0)}{f_X^S(x)}.$$

Consequently,

$$\delta_B^S(x) = 1 \quad \text{if} \quad \frac{f_{X,Y}^S(x, 1)}{f_{X,Y}^S(x, 0)} \geq 1.$$

By definition,

$$f_{X,Y}^S(x, 1) = \mathbb{P}\{X = x, Y = 1|S = 1\} = \frac{\mathbb{P}\{X = x, Y = 1, S = 1\}}{\mathbb{P}\{S = 1\}}.$$

Noting that

$$\begin{aligned} \mathbb{P}\{X = x, Y = 1, S = 1\} &= \mathbb{P}\{S = 1|X = x, Y = 1\}\mathbb{P}\{X = x, Y = 1\} \\ &= \mathbb{P}\{S = 1|Y = 1\}f_{X,Y}(x, 1) \\ &= \pi_S(1)p(x)f_X(x), \end{aligned}$$

we have

$$f_{X,Y}^S(x, 1) = \frac{\pi_S(1)p(x)f_X(x)}{\mathbb{P}\{S = 1\}}.$$

Applying a similar argument to  $f_{X,Y}^S(x, 0)$ , and cancelling the common value  $f_X(x)$  and  $\mathbb{P}\{S = 1\}$ , deduce that

$$\frac{p^S(x)}{(1 - p^S(x))} = \frac{f_{X,Y}^S(x, 1)}{f_{X,Y}^S(x, 0)} = \frac{p(x)\pi_S(1)}{(1 - p(x))\pi_S(0)}. \quad (8)$$

Therefore,

$$\delta_B^S(x) = 1 \quad \text{if} \quad \frac{p(x)}{(1 - p(x))} \geq \frac{\pi_S(0)}{\pi_S(1)}.$$

Under (7), the right-hand side equals  $\pi/(1 - \pi)$ . Hence,  $\delta_B^S(x) = \delta_D(x)$  under (7). This implies that the subsampled Bayes rule is TNR+TPR-optimal under (7).

**Theorem 3.** Under balanced subsampling (7), the subsampled Bayes rule  $\delta_B^S$  is TNR+TPR-optimal.

### 3.4. The $q^*$ -classifier is invariant to response-based sampling

In contrast, the  $q^*$ -classifier is unaffected by response-based sampling and retains its TNR+TPR-optimality no matter what the target balance ratio is. Let  $\delta_{q^*}^S(x)$  be the  $q^*$ -classifier constructed using  $\mathcal{L}_S$ . By definition,  $\delta_{q^*}^S(x) = \mathbf{1}_{\{p^S(x) \geq \pi^S\}}$  where  $\pi^S = \mathbb{P}\{Y = 1|S = 1\}$ . Equivalently,

$$\delta_{q^*}^S(x) = 1 \quad \text{if} \quad \frac{p^S(x)(1 - \pi^S)}{(1 - p^S(x))\pi^S} \geq 1.$$

Therefore, using (8),

$$\delta_{q^*}^S(x) = 1 \quad \text{if} \quad \frac{p(x)\pi_S(1)(1 - \pi^S)}{(1 - p(x))\pi_S(0)\pi^S} = \frac{p(x)/\pi}{(1 - p(x))/(1 - \pi)} \geq 1, \quad (9)$$

where we have used the following identity which follows from (6)

$$\frac{\pi_S(1)/\pi^S}{\pi_S(0)/(1 - \pi^S)} = \frac{\mathbb{P}\{S = 1\}/\pi}{\mathbb{P}\{S = 1\}/(1 - \pi)}.$$

In other words,  $\delta_{q^*}^S = \delta_{q^*}$  (compare (9) to (4)). We can therefore conclude that  $\delta_{q^*}^S$  remains TNR+TPR-optimal. Combined with Theorem 3 we have therefore established the following.

**Theorem 4.** Under response-based sampling of the form (5),  $\delta_{q^*}^S = \delta_{q^*}$ , and therefore  $\delta_{q^*}^S$  is TNR+TPR-optimal. Moreover, under balanced sampling (7), all three methods are equivalent:

$$\delta_B^S = \delta_{q^*}^S = \delta_{q^*},$$

and all three methods are TNR+TPR-optimal.

## 4. Application to random forests

In practice, the value of  $p(x)$  is unknown and therefore must be estimated. In this scenario, when we refer to  $q^*$ -classification we mean classification using an estimated value for  $p(x)$  to classify observations using the quantile  $q = \pi$ . In general, we can apply  $q$ -classification based on any specified  $0 < q < 1$ . Here we investigate the performance of  $q^*$ -classification when applied with random forests. We refer to this procedure as RFQ. As a comparison procedure, we will use balanced random forests, which we continue to refer to as BRF. We also use the standard random forests algorithm as comparison and refer to this as RF.

Algorithm 1 provides a description of the RF classification al-

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### Algorithm 1 Random Forest Classification (RF).

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**Input:**

- 1: Learning data  $\mathcal{L} = (X_i, Y_i)_{1 \leq i \leq N}$
- 2: User specified values of `ntree`, `nodesize`, `mtry`

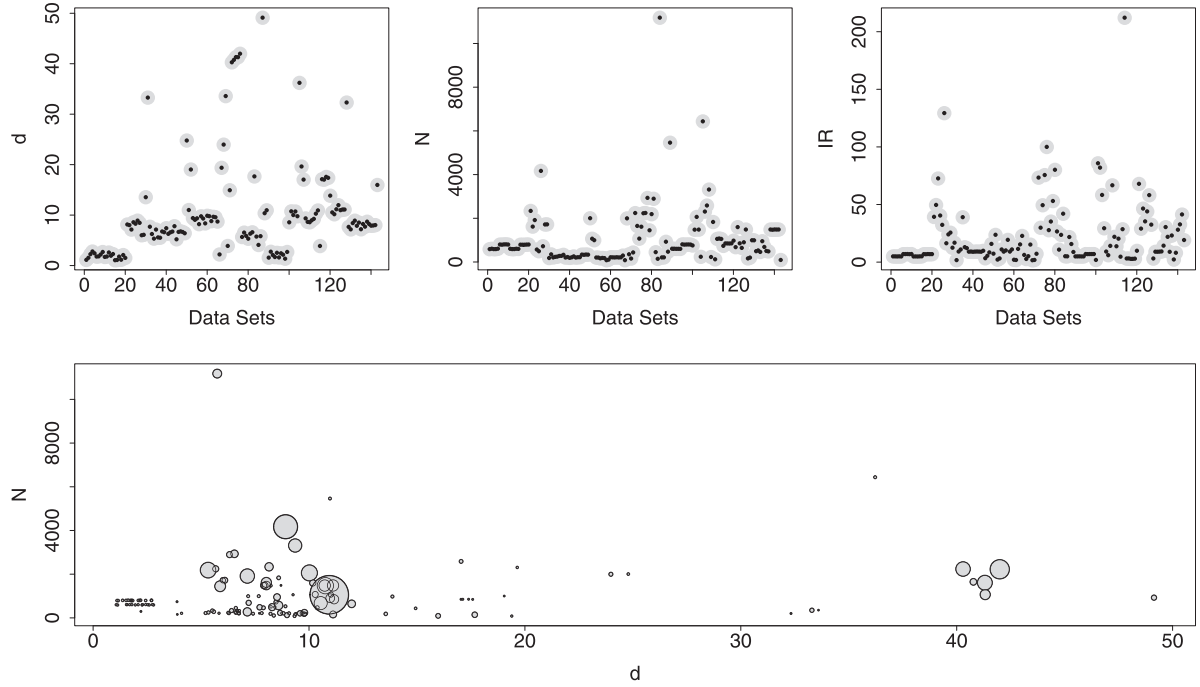
**Learning Phase:**

- 3: **procedure** RF( $\mathcal{L}$ , `ntree`, `nodesize`, `mtry`)
- 4:   **for**  $m = 1, \dots, \text{ntree}$  **do**
- 5:     Select  $N$  values with replacement from  $\mathcal{L}$  and grow a tree using this data as follows
- 6:     **for** all tree nodes **do**
- 7:       **while** observations in node  $>$  `nodesize` & impurity present **do**
- 8:         Randomly select without replacement `mtry` features for splitting
- 9:         Determine decrease in impurity for each selected feature for splitting
- 10:        Split on the variable whose optimal split decreases impurity the most
- 11:        **end while**
- 12:     **end for**
- 13:     Calculate  $\hat{p}_m(\cdot)$ , the tree estimated value for  $p(\cdot)$
- 14:   **end for**
- 15:   Let  $\hat{p}_{\text{RF}}(\cdot) = \sum_{m=1}^{\text{ntree}} \hat{p}_m(\cdot) / \text{ntree}$  be the RF ensemble estimator for  $p(\cdot)$
- 16: **end procedure**

**Classification Phase:**

- 17: Classify  $x$  using the ensemble classifier  $\hat{\delta}_{\text{RF}}(x) = \mathbf{1}_{\{\hat{p}_{\text{RF}}(x) \geq 1/2\}}$
- 

gorithm. The algorithm requires the following parameters: `ntree` (number of trees trained in the forest), `nodesize` (target terminal node size), and `mtry` (number of random features used to split a tree node). RFQ and BRF apply Algorithm 1 exactly as RF does but with the following one line modifications:



**Fig. 1.** Summary of 143 benchmark imbalanced data sets. Top figures display dimension of feature space  $d$ , sample size  $N$ , and imbalance ratio  $IR$ . Bottom figure displays  $d$  versus  $N$  with symbol size displaying value of  $IR$ . This identifies several interesting data sets with large  $IR$  values, with some of these having larger  $d$ .

**RFQ:** Line 17 of [Algorithm 1](#) is modified as follows. In place of median (Bayes) classification,  $\hat{\delta}_{RF}(x) = \mathbf{1}_{\{\hat{p}_{RF}(x) \geq 1/2\}}$ , RFQ applies  $q^*$ -classification,  $\hat{\delta}_{RFQ}(x) = \mathbf{1}_{\{\hat{p}_{RF}(x) \geq \pi\}}$ .

**BRF:** Line 5 of [Algorithm 1](#) is modified as follows. Rather than selecting a bootstrap sample of size  $N$ , a sample of size  $2N_1$  is used, where the probabilities for minority and majority class instances to be selected for the bootstrap sample are  $\pi_S(1) = (N_0/N_1)\pi_S(0)$ , thus satisfying the balancing condition (7). Keep in mind that BRF uses the Bayes rule for classification; thus the classification rule used in Line 17 is the same for BRF.

#### 4.1. Performance comparisons on benchmark imbalanced data

In theory, both BRF and RFQ will possess the TNR+TPR-property: this is true for BRF by [Theorem 3](#) because it satisfies the balancing condition (7), while for RFQ this holds by [Theorem 2](#) because it applies  $q^*$ -classification. However this is predicated on knowledge of the true probability function  $p(x)$ , which in practice must be estimated, and therefore performance in practice may be very different. In particular, an advantage of RFQ is that it uses a much larger sample size than BRF which should increase its efficiency in estimating  $p(x)$ .

To see how the two methods performed in practice we tested them using a diverse collection of 143 benchmark imbalanced data sets (see [Fig. 1](#) for summary statistics of the data sets; Supplementary Materials Appendix C provides background information on the data). Analyses were performed in R [53] using the R-package `randomForestSRC` [54]. Forests of size `ntree` = 1000 were used for each training data set. Default settings for random forests were used: trees were grown to purity (`nodesize` = 1), and random feature selection was set at `mtry` =  $d/3$ . Tree node splits (Lines 6–12 of [Algorithm 1](#)) were implemented using Gini splitting. The value  $q^* = \pi$  required for RFQ was estimated using the empirical relative frequency of the minority class labels,  $\hat{\pi} = N_1/(N_0 + N_1)$ . In

addition to BRF and RF, we also considered standard random forests under Hellinger distance splitting [47], and BRF with Hellinger splitting.

##### 4.1.1. Performance metrics: The G-mean

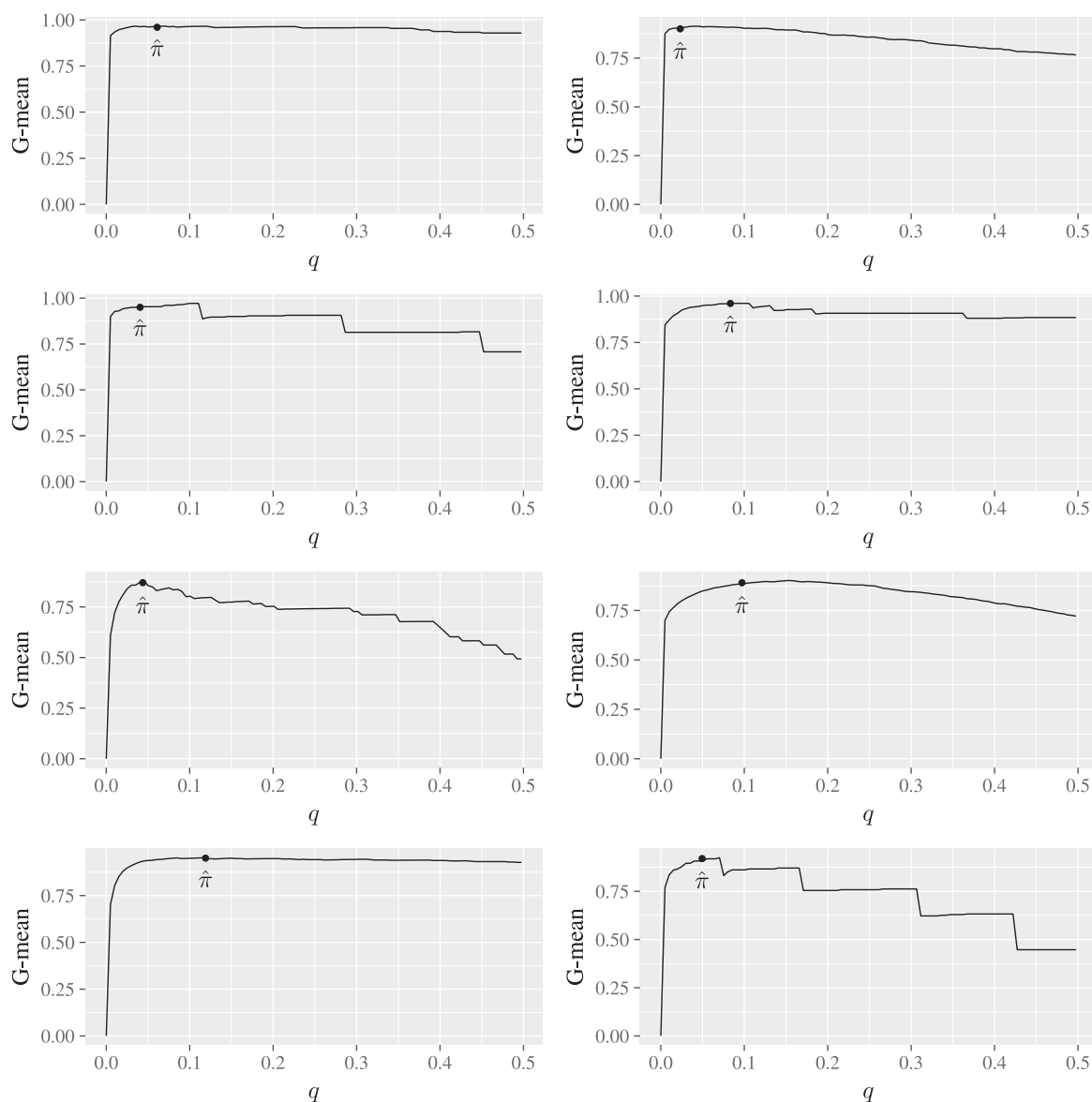
In assessing performance, we used TNR, TPR, and the G-mean. The G-mean is the geometric mean of TNR and TPR, i.e.,  $G\text{-mean} = (TNR \times TPR)^{1/2}$  and it is meant to replace misclassification rate in imbalanced data settings, since an overall accuracy close to 1 can be achieved by classifying all data points as majority class labels for heavily imbalanced data as previously noted. By way of contrast, the G-mean is close to 1 only when both the true negative and true positive rates are close to 1 and the difference between the two is small [46].

##### 4.1.2. The $q^*$ -classifier appears to optimize the G-mean

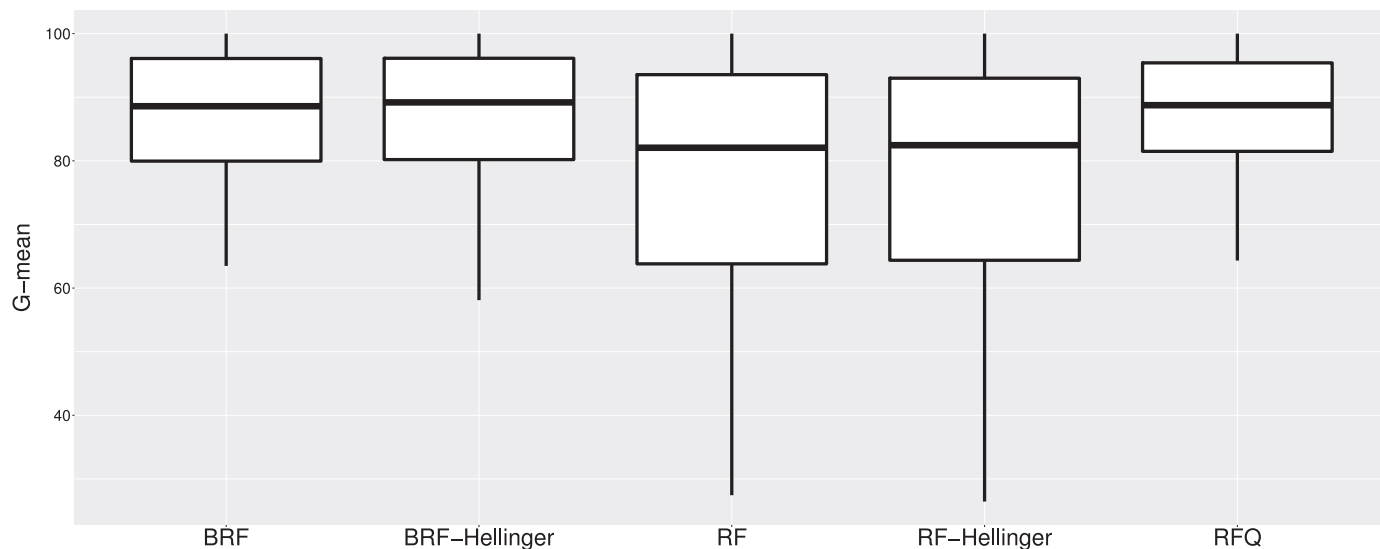
Before discussing the results, it is worth noting that even though the  $q^*$ -classifier was not specifically developed to maximize the G-mean, we observed that by applying random forests  $q$ -classification under different values of  $q$ , that the maximum G-mean is achieved when  $q$  is approximately  $\hat{\pi}$  (i.e., the G-mean appears to be maximized by RFQ). This is illustrated in [Fig. 2](#) using 8 selected benchmark data sets. This is strong evidence that TNR+TPR-optimality is a useful property for a classifier.

##### 4.1.3. Results

For the analysis of the 143 benchmark data sets, we used 10-fold cross-validation repeated 250 times. The G-mean for each procedure is reported in [Fig. 3](#). We observe that RFQ and BRF outperform all other methods. We also observe that using Hellinger distance as the splitting criterion instead of the Gini index does not noticeably improve performance, and thus we did not include it in further experiments.



**Fig. 2.** G-mean from random forests  $q$ -classification using various  $q$  for thresholding (including  $q = \hat{\pi}$ ) for 8 different benchmark data sets. Notice that the maximum value is near  $\hat{\pi}$  in all instances.



**Fig. 3.** G-mean performance of different classifiers across 143 benchmark imbalanced data sets. (BRF=Balanced Random Forests; RF=Random Forests; RFQ = Random Forests  $q^*$ -classifier).

## 5. Analyzing performance differences between RFQ and BRF

From Fig. 3 it appears that RFQ and BRF have roughly similar performance overall. However, upon further investigation (Fig. 4), we found that when the imbalance ratio is high, and when the percent of minority class examples of the rare type is high, and when  $d$  is high, RFQ outperformed BRF. We investigate this effect further in this section.

### 5.1. An explanation of why RFQ is better

As we have noted previously, while RFQ and BRF both possess the TNR+TPR optimality property, in practice the difference between the two methods is that RFQ utilizes all  $N$  data points, whereas BRF uses the smaller sample size of  $2N_1$ , which it must in order to balance the data.

We suggested that the reduced sample size of BRF reduces its efficiency in estimating unknown model parameters. We now provide a more detailed explanation of how this affects BRF's performance for the scenarios described above. We consider a simple logistic regression setting where the true conditional class probability function is

$$p(x) = \frac{1}{1 + \exp(-\alpha - \beta^T x)}.$$

By (4),  $\delta_{q^*}(x) = 1$  if  $\log(\Delta_D(x)) \geq 0$ . Hence  $x$  is classified as a minority class instance if

$$\log\left(\frac{p(x)}{1 - p(x)}\right) \geq \log\left(\frac{\pi}{1 - \pi}\right).$$

Under the logistic model this simplifies to  $\alpha + \beta^T x \geq \gamma$ , where  $\gamma = \log(\pi/(1 - \pi))$  (as comparison, the Bayes rule,  $\delta_B(x)$ , classifies  $x$  as a minority class sample if  $\log(\Delta_B(x)) \geq 0$ , which simplifies to  $\alpha + \beta^T x \geq 0$ ). To gain more insight into  $\delta_{q^*}(x)$ , first note the following identity for  $\pi$ :

$$\pi = \mathbb{P}\{Y = 1\} = \int f_{Y|X}(1|x) f_X(x) dx = \int p(x) f_X(x) dx.$$

Now in the setting of marginal imbalance, since  $p(x) \approx 0$ , we must have  $\alpha \ll 0$ , and therefore,

$$\begin{aligned} \pi &= \int \left[ \frac{1}{1 + \exp(-\alpha - \beta^T x)} \right] f_X(x) dx \\ &= \exp(\alpha) \int \left[ \frac{1}{\exp(\alpha) + \exp(-\beta^T x)} \right] f_X(x) dx \\ &\approx \exp(\alpha) \int \exp(\beta^T x) f_X(x) dx. \end{aligned}$$

Combining this with  $\pi \approx 0$ , deduce that

$$\gamma = \log\left(\frac{\pi}{1 - \pi}\right) \approx \log(\pi) \approx \alpha + \log\left[\int \exp(\beta^T x) f_X(x) dx\right].$$

The  $q^*$ -classifier classifies  $x$  as a minority class instance if  $\alpha + \beta^T x \geq \gamma$ . Hence,  $\delta_{q^*}(x) = 1$  if

$$\beta^T x \geq \log\left[\int \exp(\beta^T x) f_X(x) dx\right].$$

For example, if  $X \sim N(\mu, \Sigma)$

$$\int \exp(\beta^T x) f_X(x) dx = \exp\left(\beta^T \mu + \frac{1}{2} \beta^T \Sigma \beta\right).$$

Therefore,  $\delta_{q^*}(x) = 1$  if  $\beta^T x \geq \beta^T \mu + (1/2) \beta^T \Sigma \beta$ .

The above represents the theoretical boundary for achieving TNR+TPR optimality, but RFQ and BRF must classify the data according to an estimated  $\delta_{q^*}$ . Suppose the two procedures directly estimate  $\delta_{q^*}(x)$  by estimating  $\theta = (\beta, \beta^T \mu, \beta^T \Sigma \beta)$  (i.e., instead of

**Table 2**

Simulated data sets.

	$N^a$	Signal <sup>b</sup>	Noise <sup>c</sup>	IR <sup>d</sup>	% Rare <sup>e</sup>
Two Norm <sup>f</sup>	1250	20	500	49	99%
Waveform <sup>g</sup>	1250	21	500	49	99%
TwoClassSim <sup>h</sup>	1250	20	500	9	92%
Friedman 1 <sup>i</sup>	1250	5	500	49	99%
Friedman 2 <sup>i</sup>	1250	4	500	48	99%
Friedman 3 <sup>i</sup>	1250	4	500	49	99%

<sup>a</sup> The sample size for training data and test data.

<sup>b</sup> The number of signal (true) variables.

<sup>c</sup> The number of resampled noise variables.

<sup>d</sup> As defined in Definition 1.

<sup>e</sup> As defined in Definition 2.

<sup>f</sup> Class 2 is randomly downsampled to 25 instances.

<sup>g</sup> Classes 1 + 2 form the majority class; class 3 is randomly downsampled to 25 instances.

<sup>h</sup> Intercept = -16 and 100 of the 500 noise variables correlated with  $\rho = 0.7$ .

<sup>i</sup> Where  $y \geq y_{q=0.98}$  are classified as 1 and 0 otherwise.

indirectly estimating  $p(x)$ ). Then RFQ will have an advantage because estimating  $\theta$  uses data across both classes and RFQ uses all  $N$  data points whereas BRF uses a sample size of  $2N_1$  evenly split across the two classes. Furthermore, performance differences will become magnified as the imbalance ratio increases (since  $2N_1$  becomes even smaller compared with  $N$ ) and when the dimension  $d$  increases (since estimation becomes more difficult). This also explains why RFQ is better in rare instance settings. Recall from Definition 2 that a minority class example  $x$  is rare if 4 to 5 of its nearest neighbors are majority class examples. We can imagine a setting where rare instances are a by product of indistinguishable conditional densities. That is, for  $x'$  close to  $x$  we have  $f(x'|1) = f(x'|0)$ . If this region has positive measure, then by the identification of finite mixtures of multivariate normals,  $f(x|1) = f(x|0) = f(x)$  almost everywhere. This shows data from both classes are important for estimating all components of  $\theta$ , thus further favoring RFQ.

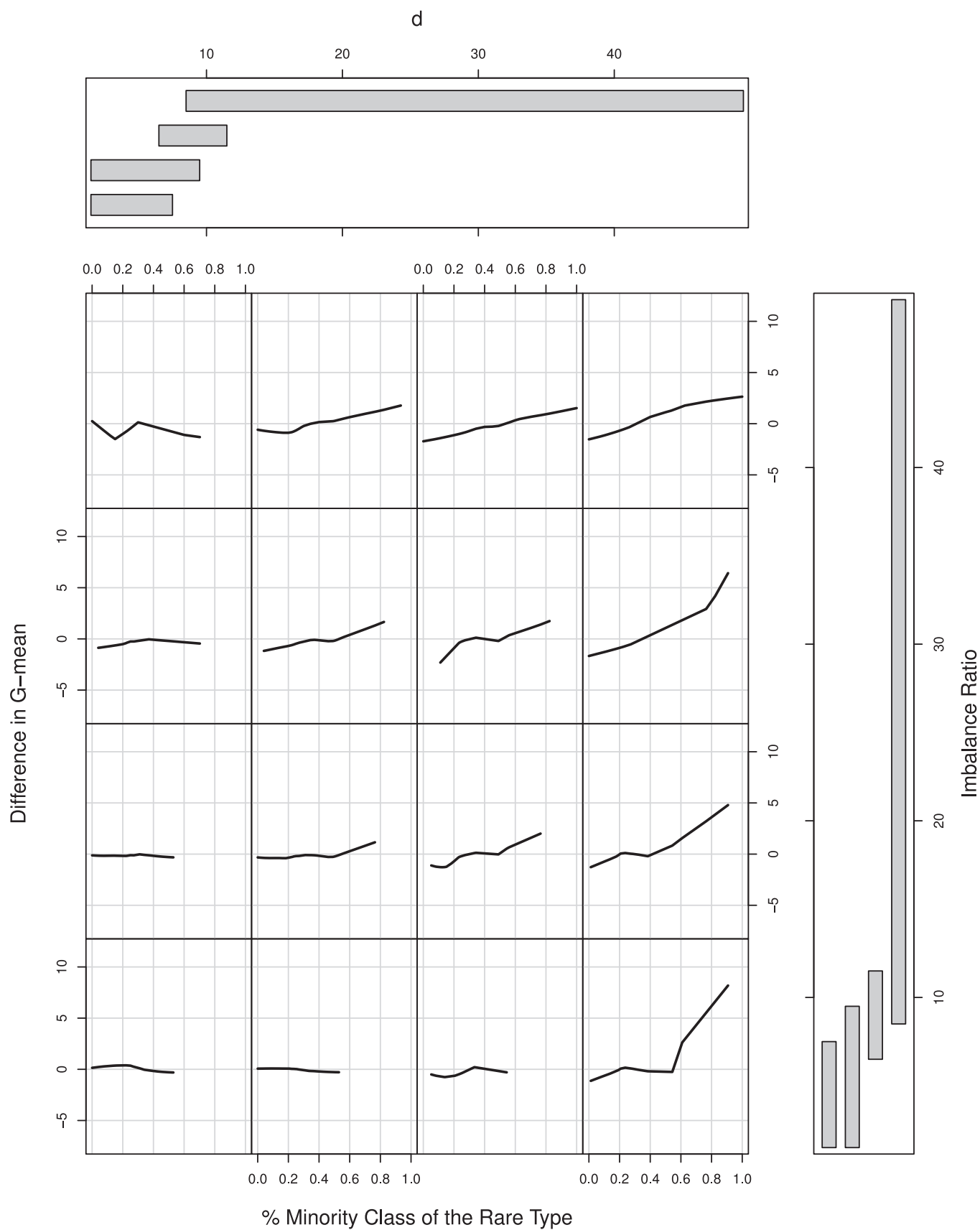
### 5.2. Performance comparisons on simulated data

To provide further evidence for the above, we converted five simulations from the mlbench R-package [55] into imbalanced data in addition to simulating imbalanced data directly using the caret package [56] as detailed in Table 2. We repeated each experiment 250 times with forests of 5000 trees grown on each training data set (nodesize=1, mtry=d/3). We compared the performance of RFQ to BRF and standard random forests (RF) and obtained the following results reported in Table 3. The results are consistent with what we observed across the 143 benchmark data sets. Clearly, RFQ outperforms BRF (as well as RF) with respect to the G-mean, across all of the six simulated high-dimensional imbalanced data models (Wilcoxon signed rank test  $p$ -value = 0.03). This shows RFQ can offer significant improvement for complex imbalanced data in high-dimensional settings.

### 5.3. Cognitive impairment data

We chose the Alzheimers Disease CSF Data from the AppliedPredictiveModeling R-package [57] to further explore performance of RFQ in difficult settings. This data set is a modified version of the data in [58]. There are  $N = 333$  observations with  $d = 130$  predictors; the outcome is presence/absence of cognitive impairment with  $N_0 = 242$  controls and  $N_1 = 91$  impaired, for an IR of 2.66. We explored the relationship among





**Fig. 4.** A closer look at difference in G-mean performance of RFQ and BRQ for benchmark data sets. Vertical axis plots difference in G-mean as a function of % rare minority class examples, feature dimension  $d$ , and imbalance ratio  $IR$ . There is an increasing trend upwards (thus favoring RFQ) as % rare minority class examples increases with increasing  $d$  and increasing  $IR$ .

**Table 3**

Performance comparisons on simulated data sets.

	RFQ			BRF			RF		
	TPR	TNR	G-mean	TPR	TNR	G-mean	TPR	TNR	G-mean
Two Norm	86.71	58.88	<b>71.34</b>	13.55	100	35.37	1.96	100	14.00
Waveform	91.58	56.04	<b>71.56</b>	53.98	94.29	70.87	1.96	100	14.00
TwoClassSim	84.73	56.32	<b>69.00</b>	7.38	99.79	26.28	1.86	99.98	11.49
Friedman 1	68.20	54.13	<b>60.46</b>	2.93	99.97	16.43	2.00	100	14.12
Friedman 2	95.54	56.26	<b>73.27</b>	11.35	99.89	31.99	1.98	100	14.02
Friedman 3	48.71	54.84	<b>51.33</b>	2.06	100	14.26	2.01	100	14.14

**Table 4**

Performance on cognitive impairment data.

	RFQ			BRF			RF		
	TPR	TNR	G-mean	TPR	TNR	G-mean	TPR	TNR	G-mean
Scenario 1 <sup>a</sup>	88.78	71.48	79.34	75.82	88.14	<b>81.33</b>	49.66	96.42	68.34
Scenario 2 <sup>b</sup>	89.72	69.21	<b>78.50</b>	65.83	89.82	76.35	27.83	98.86	50.93
Scenario 3 <sup>c</sup>	89.09	66.89	<b>76.87</b>	59.11	90.84	72.64	14.45	99.64	36.19
Scenario 4 <sup>d</sup>	87.92	62.58	<b>73.78</b>	48.67	92.44	66.24	8.23	100	27.57
Scenario 5 <sup>e</sup>	88.82	65.87	76.13	65.68	89.78	<b>76.19</b>	13.79	99.59	35.14
Scenario 6 <sup>f</sup>	89.37	60.48	<b>73.11</b>	52.82	92.55	69.09	7.27	99.99	26.06
Scenario 7 <sup>g</sup>	88.94	55.19	<b>69.56</b>	39.03	94.53	59.36	5.75	100	23.68
Scenario 8 <sup>h</sup>	88.83	47.01	<b>64.01</b>	22.25	97.11	44.33	5.27	100	22.92
Scenario 9 <sup>i</sup>	84.54	62.10	<b>71.97</b>	56.98	89.57	70.61	6.85	99.95	25.38
Scenario 10 <sup>j</sup>	84.94	53.33	<b>66.73</b>	38.26	94.42	58.45	5.46	100	23.23
Scenario 11 <sup>k</sup>	85.17	45.42	<b>61.56</b>	20.99	97.14	42.53	5.23	100	22.86
Scenario 12 <sup>l</sup>	84.46	36.85	<b>55.01</b>	9.46	99.24	28.80	5.21	100	22.83
Scenario 13 <sup>m</sup>	78.76	61.26	<b>68.88</b>	49.17	88.42	64.65	5.55	100	23.37
Scenario 14 <sup>n</sup>	78.33	51.41	<b>62.84</b>	25.64	95.35	46.63	5.22	100	22.84
Scenario 15 <sup>o</sup>	79.15	43.84	<b>58.21</b>	12.10	98.41	31.94	5.21	100	22.83
Scenario 16 <sup>p</sup>	78.96	36.10	<b>52.63</b>	6.49	99.74	24.68	5.21	100	22.83

<sup>a</sup> Original data<sup>b</sup> Original data + 200 noise variables<sup>c</sup> Original data + 500 noise variables<sup>d</sup> Original data + 1000 noise variables<sup>e</sup> Subsampled data with 40 cases randomly selected and all controls<sup>f</sup> Subsampled data with 40 cases randomly selected and all controls + 200 noise variables<sup>g</sup> Subsampled data with 40 cases randomly selected and all controls + 500 noise variables<sup>h</sup> Subsampled data with 40 cases randomly selected and all controls + 1000 noise variables<sup>i</sup> Subsampled data with 20 cases randomly selected and all controls<sup>j</sup> Subsampled data with 20 cases randomly selected and all controls + 200 noise variables<sup>k</sup> Subsampled data with 20 cases randomly selected and all controls + 500 noise variables<sup>l</sup> Subsampled data with 20 cases randomly selected and all controls + 1000 noise variables<sup>m</sup> Subsampled data with 10 cases randomly selected and all controls<sup>n</sup> Subsampled data with 10 cases randomly selected and all controls + 200 noise variables<sup>o</sup> Subsampled data with 10 cases randomly selected and all controls + 500 noise variables<sup>p</sup> Subsampled data with 10 cases randomly selected and all controls + 1000 noise variables

performance, dimensionality, and IR by adding progressively more noise variables (obtained by resampling the predictor variables) and by progressively subsampling the minority class, where each smaller subsample of the minority class was randomly sampled from the subsample of the previous iteration (i.e., nested subsamples). Table 4 contains the results of 10-fold cross-validation repeated 250 times under the various scenarios with forests of 5000 trees grown on each training data set with  $\text{nodesize}=1$ ,  $\text{mtry}=d/3$  for each scenario.

Even though the unaltered cognitive impairment data features a modest IR of 2.66, standard random forests (RF) only classifies slightly less than half of the patients with cognitive impairment correctly and its performance rapidly deteriorates with the addition of noise and increasing IR through subsampling the minority class. While BRF tends to perform well on the unaltered data and under increasing IR, its performance rapidly deteriorates in higher dimensions (i.e., with increasing noise) to the point that its performance is not much better than RF and significantly inferior to RFQ. In contrast, RFQ outperforms BRF (and RF) with respect to the G-mean under all scenarios considered except for the unaltered data

with no noise and the data with 40 of the 91 cognitively impaired patients randomly selected with no noise (Wilcoxon signed rank test  $p$ -value  $< 0.001$ ). Under all scenarios the performance of RFQ over the minority class remains constant and is superior to BRF and RF, although with the cost of an increased FPR with increasing dimensions.

#### 5.4. Customer churn data

As another example, we looked at the Customer Churn Data from the C50 R-package [59]. This is artificial customer churn data modeled on real world data where the outcome is customer churn yes/no. The data is already split into training and test data, so no cross-validation is required. In the training data there are  $N = 3333$  observations of which  $N_1 = 483$  are instances of customer churn, for an IR of 5.90.

As with the cognitive impairment data, we progressively add more noise variables and progressively subsample the minority class. Table 5 contains the results of running the test data through the forests under the various scenarios with forests of 5000 trees

**Table 5**  
Performance on customer churn data.

	RFQ			BRF			RF		
	TPR	TNR	G-mean	TPR	TNR	G-mean	TPR	TNR	G-mean
Scenario 1 <sup>a</sup>	86.19	90.02	88.09	83.52	95.64	<b>89.37</b>	73.72	99.79	85.77
Scenario 2 <sup>b</sup>	89.31	75.55	<b>82.14</b>	64.37	94.11	77.83	30.07	100	54.83
Scenario 3 <sup>c</sup>	91.09	71.60	<b>80.76</b>	42.98	96.33	64.35	18.49	100	42.99
Scenario 4 <sup>d</sup>	90.20	69.80	<b>79.34</b>	34.08	97.64	57.68	6.46	100	25.41
Scenario 5 <sup>e</sup>	87.08	87.88	87.48	82.18	93.21	<b>87.52</b>	61.69	99.93	78.52
Scenario 6 <sup>f</sup>	88.42	71.46	<b>79.49</b>	47.44	94.94	67.11	9.13	100	30.22
Scenario 7 <sup>g</sup>	88.42	67.16	<b>77.06</b>	35.41	97.02	58.61	2.45	100	15.65
Scenario 8 <sup>h</sup>	85.75	62.94	<b>73.46</b>	21.16	99.17	45.81	0.22	100	4.72
Scenario 9 <sup>i</sup>	81.29	84.55	<b>82.91</b>	73.27	91.83	82.03	46.55	100	68.23
Scenario 10 <sup>j</sup>	80.40	67.93	<b>73.90</b>	31.85	95.98	55.29	2.00	100	14.16
Scenario 11 <sup>k</sup>	81.29	64.81	<b>72.58</b>	25.61	97.37	49.94	0.22	100	4.72
Scenario 12 <sup>l</sup>	78.62	59.82	<b>68.58</b>	8.69	99.58	29.41	0.22	100	4.72
Scenario 13 <sup>m</sup>	82.63	84.34	<b>83.48</b>	65.26	91.69	77.35	12.25	100	35.00
Scenario 14 <sup>n</sup>	80.85	62.11	<b>70.86</b>	30.96	96.19	54.57	2.90	100	17.02
Scenario 15 <sup>o</sup>	79.51	59.33	<b>68.69</b>	13.59	98.96	36.67	2.45	100	15.65
Scenario 16 <sup>p</sup>	80.40	56.01	<b>67.11</b>	2.00	99.86	14.15	0.22	100	4.72

<sup>a</sup> Original data

<sup>b</sup> Original data + 200 noise variables

<sup>c</sup> Original data + 500 noise variables

<sup>d</sup> Original data + 1000 noise variables

<sup>e</sup> Subsampled data with 240 cases randomly selected and all controls

<sup>f</sup> Subsampled data with 240 cases randomly selected and all controls + 200 noise variables

<sup>g</sup> Subsampled data with 240 cases randomly selected and all controls + 500 noise variables

<sup>h</sup> Subsampled data with 240 cases randomly selected and all controls + 1000 noise variables

<sup>i</sup> Subsampled data with 120 cases randomly selected and all controls

<sup>j</sup> Subsampled data with 120 cases randomly selected and all controls + 200 noise variables

<sup>k</sup> Subsampled data with 120 cases randomly selected and all controls + 500 noise variables

<sup>l</sup> Subsampled data with 120 cases randomly selected and all controls + 1000 noise variables

<sup>m</sup> Subsampled data with 60 cases randomly selected and all controls

<sup>n</sup> Subsampled data with 60 cases randomly selected and all controls + 200 noise variables

<sup>o</sup> Subsampled data with 60 cases randomly selected and all controls + 500 noise variables

<sup>p</sup> Subsampled data with 60 cases randomly selected and all controls + 1000 noise variables

grown on each training data set with  $\text{nodesize}=1$ ,  $\text{mtry}=d/3$  for each scenario.

We observe exactly the same pattern of performance with the customer churn data as with the cognitive impairment data. As before, the performance of RF rapidly deteriorates with the addition of noise and increasing IR; BRF performs decently on the unaltered data and under increasing IR but its performance rapidly deteriorates in higher dimensions; RFQ outperforms BRF and RF with respect to the G-mean under all scenarios except for the unaltered data with no noise and the data with 240 of the 483 instances of customer churn randomly selected with no noise (Wilcoxon signed rank test  $p$ -value < 0.001). Under all scenarios the performance of RFQ over the minority class remains constant and is superior to BRF and RF but with increased FPR in higher dimensions.

## 6. Variable importance

We claim that the standard variable importance (VIMP) measure in random forests introduced by Breiman and Cutler [1,4], called Breiman-Cutler importance [6], is inappropriate for RFQ in the presence of significantly imbalanced data due to the fact that almost all nodes in an individual tree will contain 0/s. We propose instead to assess variable importance using the G-mean combined with Ishwaran-Kogalur importance [15,54], the latter being an ensemble rather than tree-based measure.

In Breiman-Cutler permutation importance, a variable's OOB (out-of-bag) data is permuted and run down the tree. The original OOB prediction error is subtracted from the resulting OOB prediction error, resulting in tree importance. Averaging this value over the forest yields permutation importance. This type of importance, which is tree-based, is appropriate for BRF because each tree is a

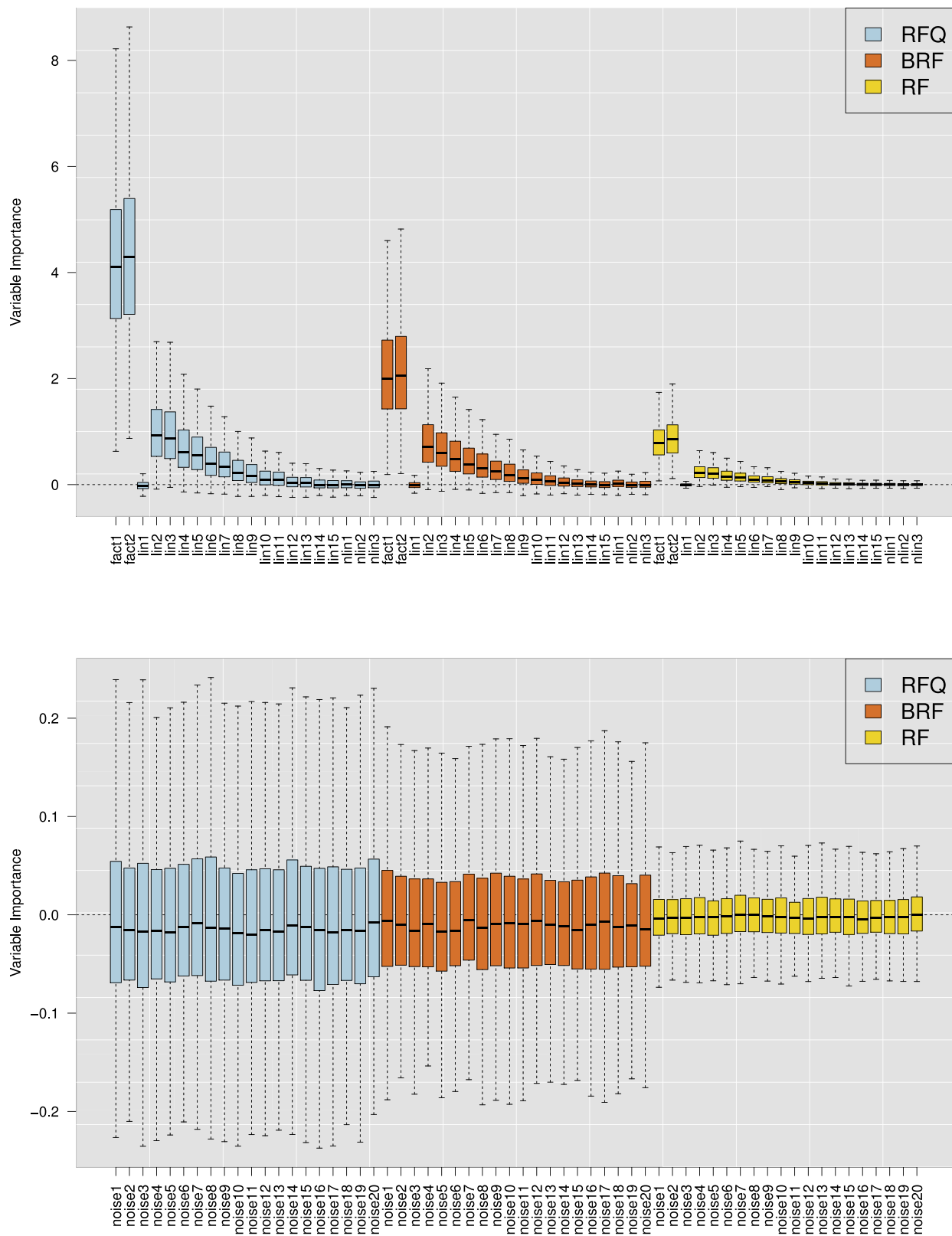
reasonably good classifier, therefore making prediction error a reasonable way to assess a variable's contribution to the model.

For RFQ this will not be a good measure because RFQ's good prediction performance arises from converting a random forest ensemble classifier into a random forest ensemble  $q$ -classifier. Therefore, we will instead use Ishwaran-Kogalur importance [15,54], an ensemble-based measure, defined as the prediction error for the original ensemble subtracted from the prediction error for the new ensemble obtained by permuting a variable's data. For RFQ, performance is measured by the G-mean. Thus, we apply Ishwaran-Kogalur importance using G-mean prediction error. Ensembles were defined in blocks of 20 trees. For BRF, we also use G-mean for prediction error, but with Breiman-Cutler importance. We also compare results to standard random forests (RF) using Breiman-Cutler importance calculated using classification error (the standard approach).

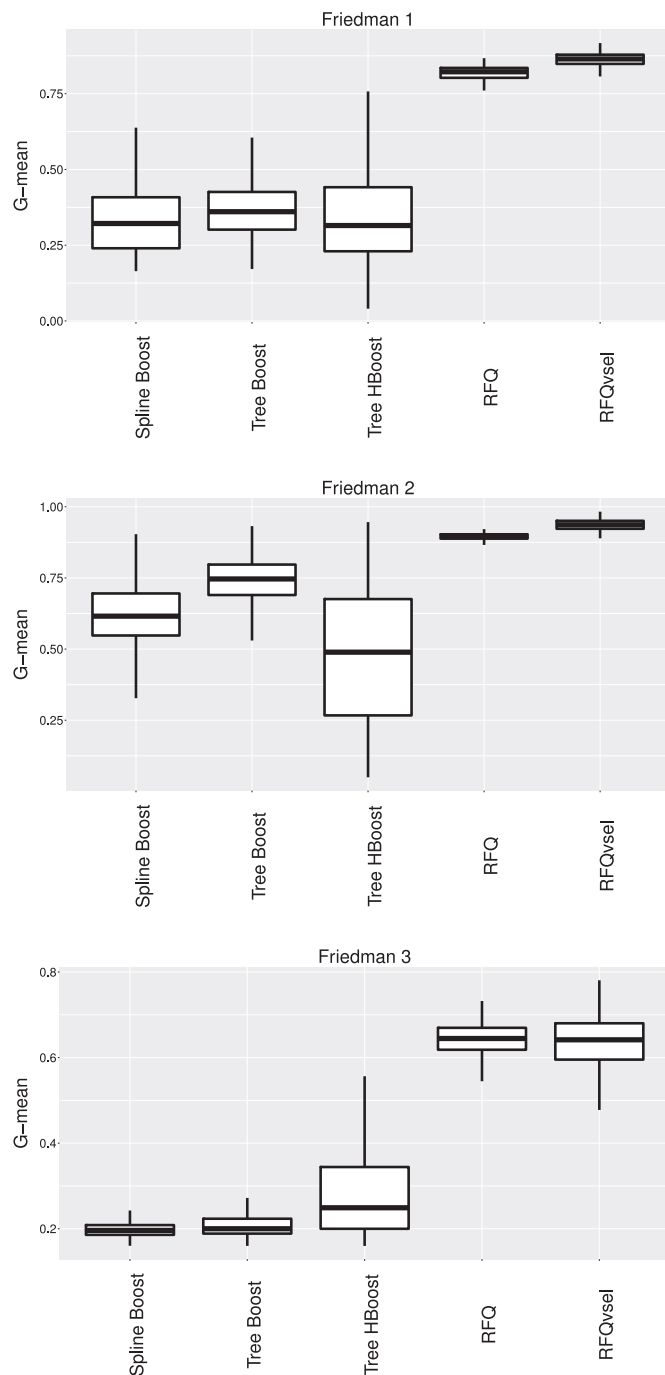
To assess performance of the proposed variable importance measures, we used the `twoClassSim` function from the `caret` package [56]: 2 factors, 15 linear variables, 3 non-linear variables, and 20 noise variables. Sample size was  $N = 1000$  with  $IR = 6$  which was induced by downsampling class 2. Results averaged from 1000 runs are displayed in Fig. 5. The results show RFQ outperforms BRF which, in turn, outperforms RF.

## 7. Multiclass imbalanced data

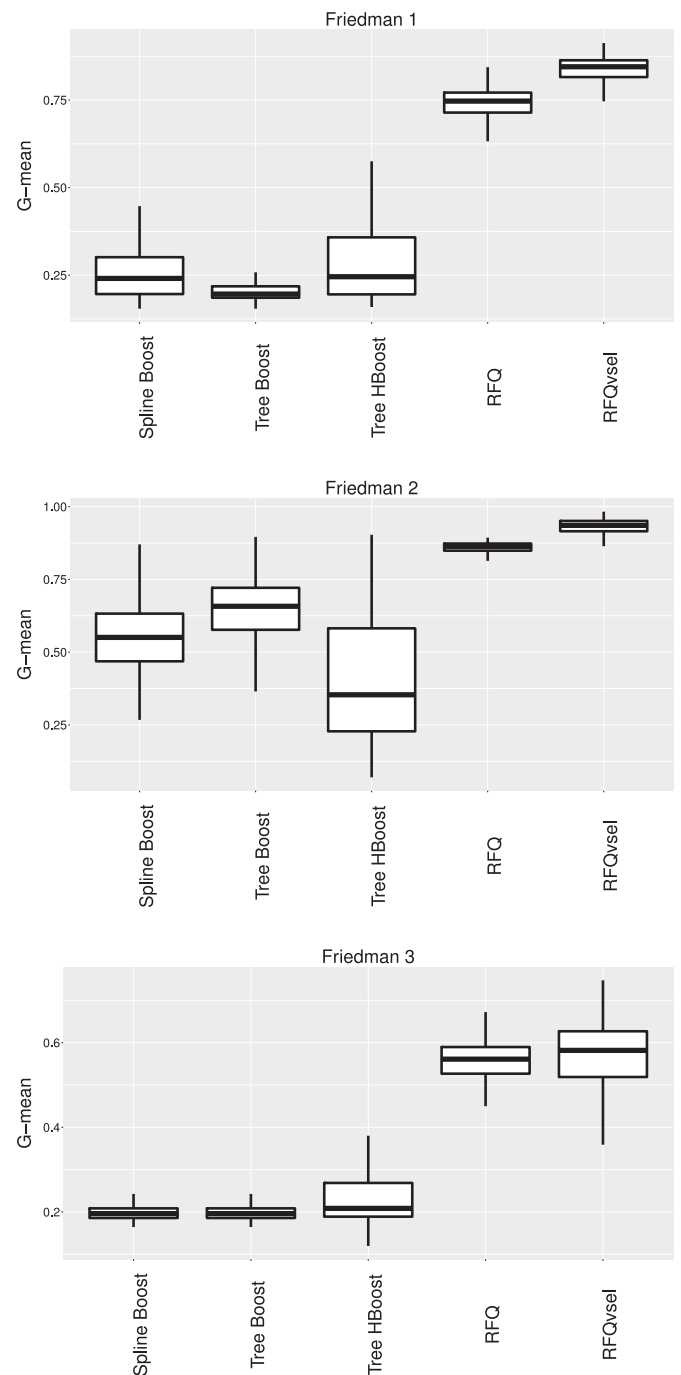
In this section we explore the performance of RFQ, BRF and RF in the multiclass imbalanced data setting. We accomplish this by decomposing the multiclass imbalanced data into  $K(K-1)/2$  two-class data sets, where  $K$  is the number of classes, obtaining classifiers on each and then taking a majority vote over the results. The empirical results that follow are based on forests of 5000 trees



**Fig. 5.** Variable importance (VIMP) for RFQ, BRF and RF from 1000 runs using simulated imbalanced data. There are 2 factors, 15 linear variables, 3 non-linear variables, and 20 noise variables (no signal). Top panel displays signal variables, bottom panel are noisy variables.



**Fig. 6.** G-mean performance of boosting classifiers versus RFQ for Friedman low dimensional simulations. (Spline Boost, Tree Boost are boosted splines and boosted trees using binomial loss; Tree HBoost are boosted trees with Huber loss; RFQvsel is RFQ with variable selection filtering).



**Fig. 7.** G-mean performance of boosting classifiers versus RFQ for Friedman high dimensional simulations. (Spline Boost, Tree Boost are boosted splines and boosted trees using binomial loss; Tree HBoost are boosted trees with Huber loss; RFQvsel is RFQ with variable selection filtering).

grown on each training data set with `nodesize=1`, `mtry=d/3` and 50 resampled noise variables.

### 7.1. Waveform simulations

As a preliminary exploration of the more challenging multiclass imbalance data setting [60], we chose the waveform data simulation from the `mlbench` R-package [55], which produces three classes of (approximately) equal size. We generated  $N = 1000$  samples for the training (initially) and test data sets. To obtain multi-

class imbalanced data, we subsampled the second and third classes to obtain different class ratios. For each of the three class imbalanced data sets derived from the waveform simulation, we adopted the approach of [61] and trained RFQ, BRF and RF on  $\binom{3}{2} = 3$  two-class data sets. The multiclass classifier was obtained by taking a majority vote over the three predicted class labels for the test data. We compared the performance of the RFQ, BRF and RF multiclass classifier using Friedman's one-vs-one approach using the true positive rate for each of the three classes and the G-Mean. This we did 250 times, averaging the results, which are listed in



Table B.1 of Appendix B, where the “true positive rates” (i.e., the performance metrics within each class) are denoted by TPR1, TPR2 and TPR3, respectively.

The (unweighted) G-mean is not necessarily the appropriate metric for measuring classification performance in the multiclass imbalanced data setting, especially in cases of extreme imbalance. For the imbalanced data sets with the ratios 100:25:1, 100:10:1 and 100:5:1 the G-means for RFQ and BRF are similar but TPR for the third class with the fewest instances is in the range 85–86 for RFQ whereas the range is 42–44 for BRF. Granted, TPR over the first class with far more instances than the other classes is approximately 52–55 for RFQ whereas it is approximately 86–87 for BRF, but in real-world settings the cost associated with misclassifying the class with the fewest instances is likely to be far higher, as with two class imbalanced data. To account for this, we also looked at the G-means for two classes at a time, denoted as  $G\text{-mean}_{kk'}$  for classes  $k$  and  $k'$ , as well as the weighted G-mean, which in the three class setting we define as

$$\text{Weighted G-Mean} = (\text{TPR1}^{\beta_1} \times \text{TPR2}^{\beta_2} \times \text{TPR3}^{\beta_3})^{1/(\beta_1 + \beta_2 + \beta_3)}.$$

Specifically, in Table B.2 of Appendix B, we looked at the weighted G-mean with  $\beta_1 = 1/2$  and  $\beta_2 = \beta_3 = 1$ , which is not necessarily ideal because it does not take into account the imbalance between the second and third classes; nevertheless, it is sufficient to illustrate our point.

In Table B.2 we see a pronounced difference in the weighted G-mean with  $\beta_1 = 1/2$ ,  $\beta_2 = 1$ , and  $\beta_3 = 1$  for the highly imbalanced data sets with the ratios 100:25:1, 100:10:1 and 100:5:1. To see why this is appropriate we look at the two class G-means. The performance of RFQ is superior to BRF with respect to  $G\text{-mean}_{13}$  and  $G\text{-mean}_{23}$ , whereas BRF is superior to RFQ only with respect to  $G\text{-mean}_{12}$ . Even though the performance of RFQ is superior with respect to two of the three two class G-means and the difference in  $G\text{-mean}_{23}$  in favor of RFQ is approximately the same as the difference in  $G\text{-mean}_{12}$  in favor of BRF, the unweighted G-mean is insensitive to this. For this reason, we believe that the weighted G-mean is especially appropriate in the multiclass imbalanced data setting.

## 7.2. Cassini simulations

As another example, we chose the cassini data simulation from the mlbench R-package [55], which produces three classes of in the ratio 2:2:1. As with the waveform simulation, we generated  $N = 1000$  samples for the training (initially) and test data sets with noise variables and then subsampled the second and third classes to obtain different class ratios.

The averaged results from 250 repetitions are listed in Table B.3 of Appendix B. In contrast to the waveform imbalanced data sets, for the cassini data sets with the most extreme class imbalance, i.e., 100:50:1, 100:25:1, 100:10:1 and 100:5:1, RFQ is clearly superior to BRF with respect to the unweighted G-mean.

We then looked at the weighted G-mean with  $\beta_1 = 1/2$  and  $\beta_2 = \beta_3 = 1$ . In Table B.4 of Appendix B, we see an even more pronounced difference in performance between RFQ and BRF with respect to the weighted G-mean with  $\beta_1 = 1/2$ ,  $\beta_2 = 1$ , and  $\beta_3 = 1$  for the extremely imbalanced data sets with the ratios 100:50:1, 100:25:1, 100:10:1 and 100:5:1 and essentially identical performance over most of the other imbalanced data sets.

It should be noted that these results are limited in that we only considered three class imbalanced data, which is a special case in that the number of competent classifiers (i.e., classifiers trained on a given class) outnumber non-competent classifiers (i.e., classifiers that were not trained on the class in question); for three class imbalanced data using one-vs-one there are exactly two com-

petent classifiers and one non-competent classifier, so classification by majority vote works. However, the ratio of competent to non-competent classifiers becomes 1:1 for data with four classes and monotonically decreases in favor of non-competent classifiers as the number of classes increases. In these imbalanced multiclass settings, a more sophisticated approach using some form of weighted voting should be used instead [60,62].

## 8. Comparison to boosting

Gradient boosting is another machine learning method known to possess state of the art classification performance. Therefore we sought to compare performance of RFQ to boosting. For boosting procedures, we used boosted parametric splines using binomial loss (Spline Boost). For nonparametric boosting, we boosted trees using binomial loss (Tree Boost) and Huber loss (Tree Hboost). Parametric spline boosting was implemented using the R-package mboost [63] and tree boosting by the R-package gbm [64]. In both cases, 1000 trees were boosted with regularization parameter 0.1. Depth of trees was set to three interactions and spline bases were set to default values used by mboost.

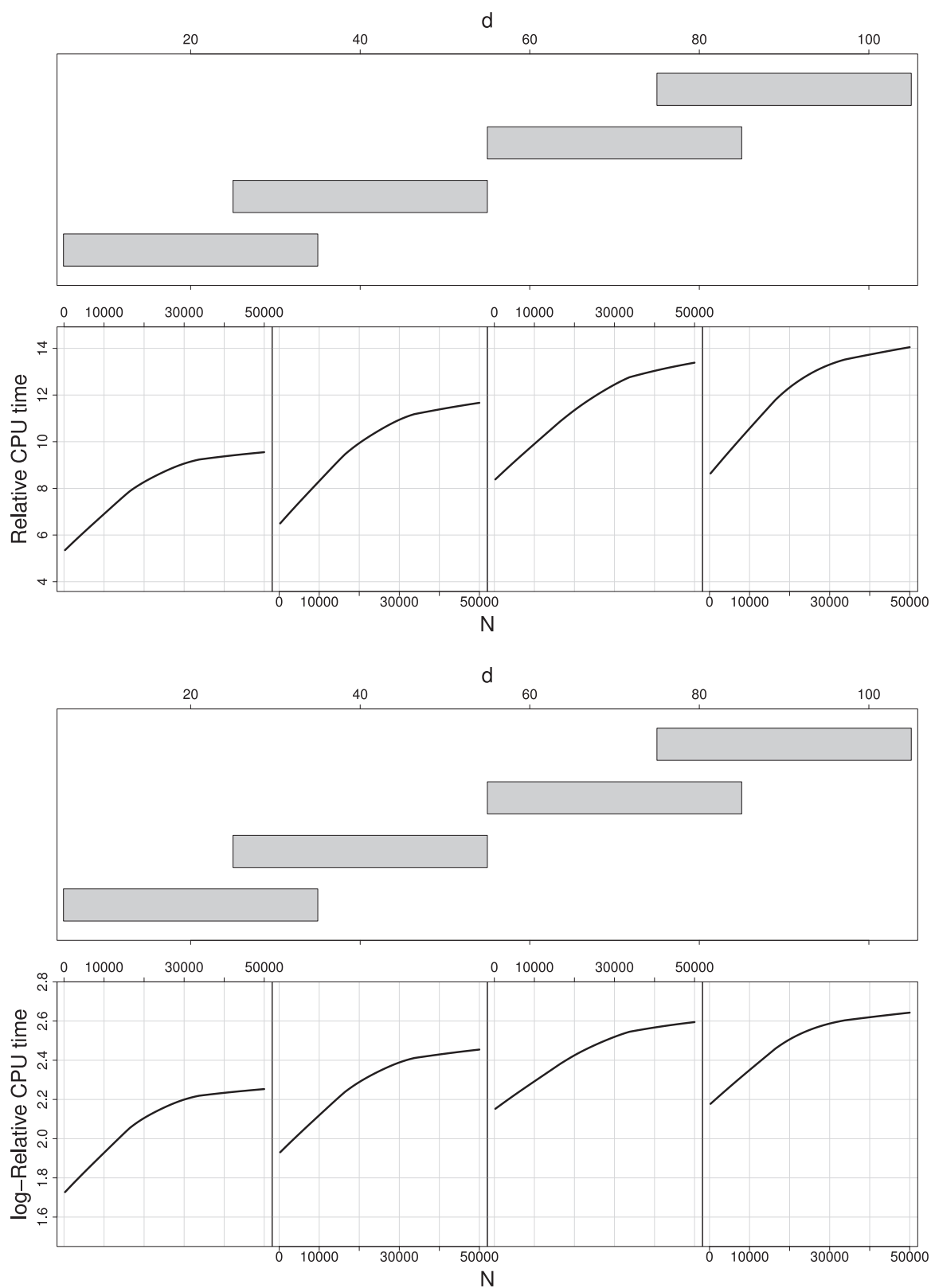
As an enhancement to RFQ we also considered an extension using variable selection. Using a preliminary RF, we calculated Ishwaran-Kogalur importance using G-mean prediction error as in Section 6. Variables were then removed if they were deemed non-significant at the 5% level, where level of significance was obtained using asymptotic confidence regions calculated using random forest variable importance subsampling [6]. Using the remaining non-filtered variables, RFQ was then run as before. We call this method RFQvsel.

We used the three Friedman simulations to test performance. Sample size was set to  $N = 1250$  with G-mean performance assessed on a test set of the same size. Low dimensional simulations with 25 noise features and high dimensional simulations with 250 noise features were used. All experiments were repeated independently 250 times.

Figs. 6 and 7 display the test set G-mean performance values for the low and high dimensional simulation scenarios, respectively. Overall, the results are very encouraging for RFQ procedures which are overwhelmingly superior to boosting procedures. Interestingly, the dimension reduction used by RFQvsel performed very well, especially in the high dimensional simulations. For example, in the Friedman 1 simulation performance of RFQvsel is more robust to increasing dimension than RFQ. In terms of the boosting procedures there appears to be no overall consensus. Sometimes Huber loss for trees is better than binomial loss. There is also no clear winner between parametric and nonparametric boosting.

## 9. Discussion

We introduced a classifier based on the ratio of data densities for learning imbalanced data and showed this resulted in a  $q$ -classifier with the property that its threshold  $q = q^*$  yielded TNR+TPR-optimality. We called this the  $q^*$ -classifier and implemented  $q^*$ -classification using random forests. We coined this method RFQ and showed RFQ to be highly competitive with the current and widely used balanced random forests (BRF) method of undersampling the majority class (used by the randomForest R-package for example). In our experiments with 143 imbalanced benchmark data sets, we observed that while BRF significantly improves classification with respect to the minority class, and unquestionably outperforms the standard random forests algorithm, its performance is roughly the same as RFQ on standard imbalanced data sets, but generally inferior in the difficult setting of high-complexity, high-imbalancedness, and high-dimensionality.



**Fig. 8.** Computational times for RFQ and BRF for Friedman 1 simulation for different sample sizes  $N$  and feature dimension  $d$ . Top plot is relative CPU time for RFQ versus BRF. Bottom plot is log-relative CPU time.

This was further confirmed by in depth experiments on simulated and real world data sets. Furthermore, we demonstrated that RFQ is better at selecting variables across imbalanced data using G-mean as the performance criterion with Ishwaran-Kogalur importance than BRF with Breiman-Cutler importance (the standard method used in random forest analyses). In the multiclass imbalanced setting, we showed that RFQ also outperforms BRF over extremely imbalanced data sets.

However one advantage of BRF is that it is computationally faster due to the low sample size used to construct its trees. At the same time, this advantage does not appear to be large. Fig. 8 displays relative CPU times and log-relative CPU times for RFQ versus BRF for the Friedman 1 simulation as  $N$  and  $d$  are varied. Even when  $d = 100$  and  $N = 50,000$ , the relative CPU time is only 14. We also observe that as  $N$  increases, relative CPU times asymptote which suggests that in big data settings these differences may not be insurmountable. In fact, Theorem 4 suggests subsampling could be used as a simple remedy for RFQ in big  $N$  settings. Recall that Theorem 4 shows as long as the data is subsampled according to a response based sampling scheme, RFQ will continue to maintain its TNR+TPR optimality property. Subsampling will greatly reduce computational time and importantly the sampling can be devised so that the majority class label cardinality is much larger than the value of  $N_1$  used by BRF, thereby also ensuring good classification performance.

### Conflict of interest

None declared.

### Acknowledgments

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### Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.patcog.2019.01.036.

### Appendix A: Proof of Theorem 1

Although Theorem 1 is well known we provide a proof here for the convenience of the reader.

**Proof.** We will show that

$$\mathbb{E} \left[ \sum_{j=0}^1 \ell_j \left( \mathbf{1}_{\{\hat{\delta}(X)=1-j, Y=j\}} - \mathbf{1}_{\{\delta_{WB}(X)=1-j, Y=j\}} \right) \right] \geq 0 \quad (\text{A.1})$$

which implies that  $r(\hat{\delta}, l_0, l_1) - r(\delta_{WB}, l_0, l_1) \geq 0$ . The first term in the sum (A.1) when  $j = 0$  equals

$$\begin{aligned} & \ell_0 \left[ \mathbf{1}_{\{\hat{\delta}(X)=1, Y=0\}} - \mathbf{1}_{\{\delta_{WB}(X)=1, Y=0\}} \right] \\ &= \ell_0 \left[ \mathbf{1}_{\{\hat{\delta}(X)=1\}} - \mathbf{1}_{\{\delta_{WB}(X)=1\}} \right] \mathbf{1}_{\{Y=0\}} \\ &= \ell_0 \left[ \left( 1 - \mathbf{1}_{\{\hat{\delta}(X)=0\}} \right) - \left( 1 - \mathbf{1}_{\{\delta_{WB}(X)=0\}} \right) \right] \left[ 1 - \mathbf{1}_{\{Y=1\}} \right] \\ &= \ell_0 \left[ \mathbf{1}_{\{\delta_{WB}(X)=0\}} - \mathbf{1}_{\{\hat{\delta}(X)=0\}} \right] \left[ 1 - \mathbf{1}_{\{Y=1\}} \right]. \end{aligned}$$

Similarly, the second term in the sum (A.1) when  $j = 1$  is

$$\begin{aligned} & \ell_1 \left[ \mathbf{1}_{\{\hat{\delta}(X)=0, Y=1\}} - \mathbf{1}_{\{\delta_{WB}(X)=0, Y=1\}} \right] \\ &= \ell_1 \left[ \mathbf{1}_{\{\hat{\delta}(X)=0\}} - \mathbf{1}_{\{\delta_{WB}(X)=0\}} \right] \mathbf{1}_{\{Y=1\}} \\ &= \ell_1 \left[ \left( 1 - \mathbf{1}_{\{\hat{\delta}(X)=1\}} \right) - \left( 1 - \mathbf{1}_{\{\delta_{WB}(X)=1\}} \right) \right] \mathbf{1}_{\{Y=1\}} \\ &= \ell_1 \left[ \mathbf{1}_{\{\delta_{WB}(X)=1\}} - \mathbf{1}_{\{\hat{\delta}(X)=1\}} \right] \mathbf{1}_{\{Y=1\}}. \end{aligned}$$

Taking the expectation of  $Y$  conditional on  $X$  and  $\mathcal{L}$  of the sum in (A.1), yields

$$\begin{aligned} & \ell_0 \left[ \mathbf{1}_{\{\delta_{WB}(X)=0\}} - \mathbf{1}_{\{\hat{\delta}(X)=0\}} \right] [1 - p(X)] \\ &+ \ell_1 \left[ \mathbf{1}_{\{\delta_{WB}(X)=1\}} - \mathbf{1}_{\{\hat{\delta}(X)=1\}} \right] p(X), \end{aligned}$$

where recall that  $p(X) = \mathbb{P}\{Y = 1|X\}$ . We will show that the above sum is greater than or equal to zero. Taking the expectation over  $X$  and  $\mathcal{L}$  completes the argument.

When  $p(X) \geq \ell_0/(\ell_0 + \ell_1)$ , we have

$$\ell_0 \left[ 0 - \mathbf{1}_{\{\hat{\delta}(X)=0\}} \right] [1 - p(X)] + \ell_1 \left[ 1 - \mathbf{1}_{\{\hat{\delta}(X)=1\}} \right] p(X).$$

If  $\hat{\delta}(X) = 1$ , we have  $\ell_0[0 - 0][1 - p(X)] + \ell_1[1 - 1]p(X) = 0$ . If  $\hat{\delta}(X) = 0$ , we have  $(\ell_0 + \ell_1)p(X) - \ell_0 \geq 0$ .

When  $p(X) < \ell_0/(\ell_0 + \ell_1)$ , we have

$$\ell_0 \left[ 1 - \mathbf{1}_{\{\hat{\delta}(X)=0\}} \right] [1 - p(X)] + \ell_1 \left[ 0 - \mathbf{1}_{\{\hat{\delta}(X)=1\}} \right] p(X).$$

If  $\hat{\delta}(X) = 1$ , we have  $\ell_0 - (\ell_0 + \ell_1)p(X) \geq 0$ . If  $\hat{\delta}(X) = 0$ , we have  $\ell_0[1 - 1][1 - p(X)] + \ell_1[0 - 0]p(X) = 0$ .

This establishes (A.1). To complete the proof, we have to show

$$r(\delta_{WB}, \ell_0, \ell_1) = \mathbb{E}[\min\{\ell_1 p(X), \ell_0(1 - p(X))\}].$$

The proof above reveals that  $r(\delta_{WB}, l_0, l_1)$  is the expected value of

$$\begin{aligned} & \ell_0[1 - p(X)] \mathbf{1}_{\{\delta_{WB}(X)=1\}} + \ell_1 p(X) \mathbf{1}_{\{\delta_{WB}(X)=0\}} \\ &= \ell_0[1 - p(X)] \mathbf{1}_{\{p(X) \geq \ell_0/(\ell_0 + \ell_1)\}} + \ell_1 p(X) \mathbf{1}_{\{p(X) < \ell_0/(\ell_0 + \ell_1)\}} \\ &= \min\{\ell_0(1 - p(X)), \ell_1 p(X)\}, \end{aligned}$$

where the last line follows because  $\ell_0(1 - p(X)) \leq \ell_1 p(X)$  if and only if  $p(X) \geq \ell_0/(\ell_0 + \ell_1)$ .  $\square$

### Appendix B: Results from multiclass imbalanced data

Section 7 explored the performance of RFQ, BRF, and RF in the multiclass imbalanced data setting. This was accomplished by decomposing the multiclass imbalanced data into 3 two-class data sets, obtaining classifiers on each and then taking a majority vote over the results. Here we list the tables from the empirical analysis which were based on forests of 5000 trees grown on each training data set with  $\text{nodesize}=1$ ,  $\text{mtry}=d/3$  and 50 resampled noise variables.

**Table B.1**

Performance comparisons on simulated 3 class imbalanced data sets derived from waveform.

Class ratios	RFQ				BRF				RF			
	TPR1	TPR2	TPR3	G-mean	TPR1	TPR2	TPR3	G-mean	TPR1	TPR2	TPR3	G-mean
5:4:1	64.65	84.46	94.51	80.16	80.20	90.80	79.87	83.41	90.38	91.28	37.84	67.72
10:5:1	60.12	83.86	94.18	77.94	82.52	88.44	77.46	82.61	96.10	81.83	19.46	53.18
10:1:1	53.25	90.26	91.79	76.03	83.75	81.63	81.40	82.15	99.92	36.03	35.78	50.24
20:5:1	55.12	83.26	92.48	75.05	83.65	87.11	74.10	81.32	99.26	64.88	6.71	33.47
20:1:1	51.84	87.39	89.97	74.00	84.08	78.20	78.42	80.03	99.99	17.95	18.57	30.41
50:25:1	57.77	76.55	87.45	72.72	83.74	89.53	59.34	76.05	95.98	82.10	0.02	0.68
50:5:1	52.78	78.06	88.90	71.35	85.97	83.66	61.61	75.94	99.97	41.09	0.25	4.25
100:25:1	54.74	71.80	85.38	69.28	86.25	87.99	43.94	68.54	99.27	65.01	0.00	0.00
100:10:1	52.27	73.24	86.09	68.84	86.68	85.10	42.24	66.77	99.96	40.93	0.00	0.00
100:5:1	51.63	74.82	84.82	68.67	86.98	81.04	43.05	66.16	99.99	20.46	0.00	0.00

**Table B.2**Performance comparisons on simulated 3 class imbalanced data sets derived from waveform with respect to two class (unweighted) G-means and the weighted G-mean with  $\beta_1 = 1/2$  and  $\beta_2 = \beta_3 = 1$  (cf. Table B.1).

Class ratios	RFQ				BRF			
	G-mean <sub>12</sub>	G-mean <sub>13</sub>	G-mean <sub>23</sub>	Wt. G-mean	G-mean <sub>12</sub>	G-mean <sub>13</sub>	G-mean <sub>23</sub>	Wt. G-mean
5:4:1	73.84	78.13	89.32	86.22	85.29	79.98	85.13	86.55
10:5:1	70.92	75.19	88.84	84.86	85.38	79.88	82.71	85.31
10:1:1	69.25	69.83	90.97	84.48	82.60	82.49	81.45	84.64
20:5:1	67.64	71.31	87.71	82.91	85.30	78.63	80.27	83.80
20:1:1	67.19	68.18	88.59	82.61	80.97	81.07	78.19	82.40
50:25:1	66.38	70.97	81.73	79.71	86.53	70.22	72.60	78.35
50:5:1	64.01	68.34	83.21	79.43	84.71	72.49	71.53	77.91
100:25:1	62.51	68.23	78.10	76.65	87.04	60.76	61.44	70.29
100:10:1	61.66	66.95	79.22	76.75	85.77	59.53	59.00	68.42
100:5:1	61.94	66.03	79.43	76.72	83.85	60.20	58.10	67.75

**Table B.3**

Performance comparisons on simulated 3 class imbalanced data sets derived from cassini.

Class ratios	RFQ				BRF				RF			
	TPR1	TPR2	TPR3	G-mean	TPR1	TPR2	TPR3	G-mean	TPR1	TPR2	TPR3	G-mean
10:5:1	90.66	97.41	97.55	95.13	98.58	100	94.76	97.73	99.52	100	92.93	97.40
25:5:1	78.98	86.91	95.10	86.69	97.22	100	84.54	93.57	99.66	100	72.17	89.36
50:25:1	73.67	73.41	91.15	78.87	96.49	100	55.95	80.82	99.50	100	1.41	17.62
50:10:1	72.60	70.85	92.32	77.90	96.33	99.99	57.54	81.63	99.67	100	1.86	21.83
50:5:1	68.59	74.98	91.48	77.62	95.92	99.95	58.45	81.95	99.81	100	2.28	22.64
50:2:1	62.54	85.06	89.03	77.75	95.43	97.66	63.48	83.47	99.75	99.98	4.50	29.32
100:50:1	70.67	70.17	86.59	75.23	95.49	99.61	24.06	59.22	99.52	100	0.00	0.00
100:25:1	70.24	65.88	86.77	73.54	95.08	99.53	24.69	59.93	99.60	100	0.00	0.00
100:10:1	66.12	60.27	86.95	69.93	94.56	99.12	24.54	59.40	99.76	100	0.00	0.00
100:5:1	60.64	59.64	86.63	67.55	93.87	97.37	26.52	60.67	99.76	100	0.00	0.00

**Table B.4**Performance comparisons on simulated 3 class imbalanced data sets derived from cassini with respect to two class (unweighted) G-means and the weighted G-mean with  $\beta_1 = 1/2$  and  $\beta_2 = \beta_3 = 1$  (cf. Table B.3).

Class ratios	RFQ				BRF			
	G-mean <sub>12</sub>	G-mean <sub>13</sub>	G-mean <sub>23</sub>	Wt. G-mean	G-mean <sub>12</sub>	G-mean <sub>13</sub>	G-mean <sub>23</sub>	Wt. G-mean
10:5:1	93.97	94.03	97.46	96.70	99.28	96.63	97.33	97.97
25:5:1	82.82	86.62	90.87	90.17	98.60	90.55	91.84	94.01
50:25:1	73.51	81.81	81.68	83.00	98.23	72.86	74.20	81.31
50:10:1	71.67	81.76	80.76	82.17	98.14	73.92	75.33	82.14
50:5:1	71.64	79.10	82.66	82.66	97.91	74.37	75.94	82.53
50:2:1	72.85	74.40	86.79	84.09	96.53	77.36	78.23	84.13
100:50:1	70.39	78.00	77.71	79.71	97.52	46.21	47.28	59.71
100:25:1	67.96	77.86	75.33	78.00	97.28	46.99	48.14	60.46
100:10:1	63.02	75.58	72.03	74.92	96.81	46.53	47.71	59.97
100:5:1	59.95	72.30	71.42	73.43	95.59	48.42	49.33	61.34

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