Bagging and Random Forests

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Outline

1. Bagging (1/2 class)

2. Random Forests (1/2 class)

Bagging=bootstrap aggregation

Consider first the regression problem. Suppose we fit a model to our training data $\mathbf{Z} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$, obtaining the prediction $\hat{f}(x)$ at input x. Bootstrap aggregation or *bagging* averages this prediction over a collection of bootstrap samples, thereby reducing its variance. For each bootstrap sample $\mathbf{Z}^{*b}$, $b = 1, 2, \ldots, B$, we fit our model, giving prediction $\hat{f}^{*b}(x)$. The bagging estimate is defined by

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^{*b}(x). \tag{8.51}$$

"Model averaging"

An average of B i.i.d. random variables, each with variance σ^2, has variance $\frac{1}{B}\sigma^2$. If the variables are simply i.d. (identically distributed, but not necessarily independent) with positive pairwise correlation ρ, the variance of the average is (Exercise 15.1)

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2. \tag{15.1}$$

Trees are variable

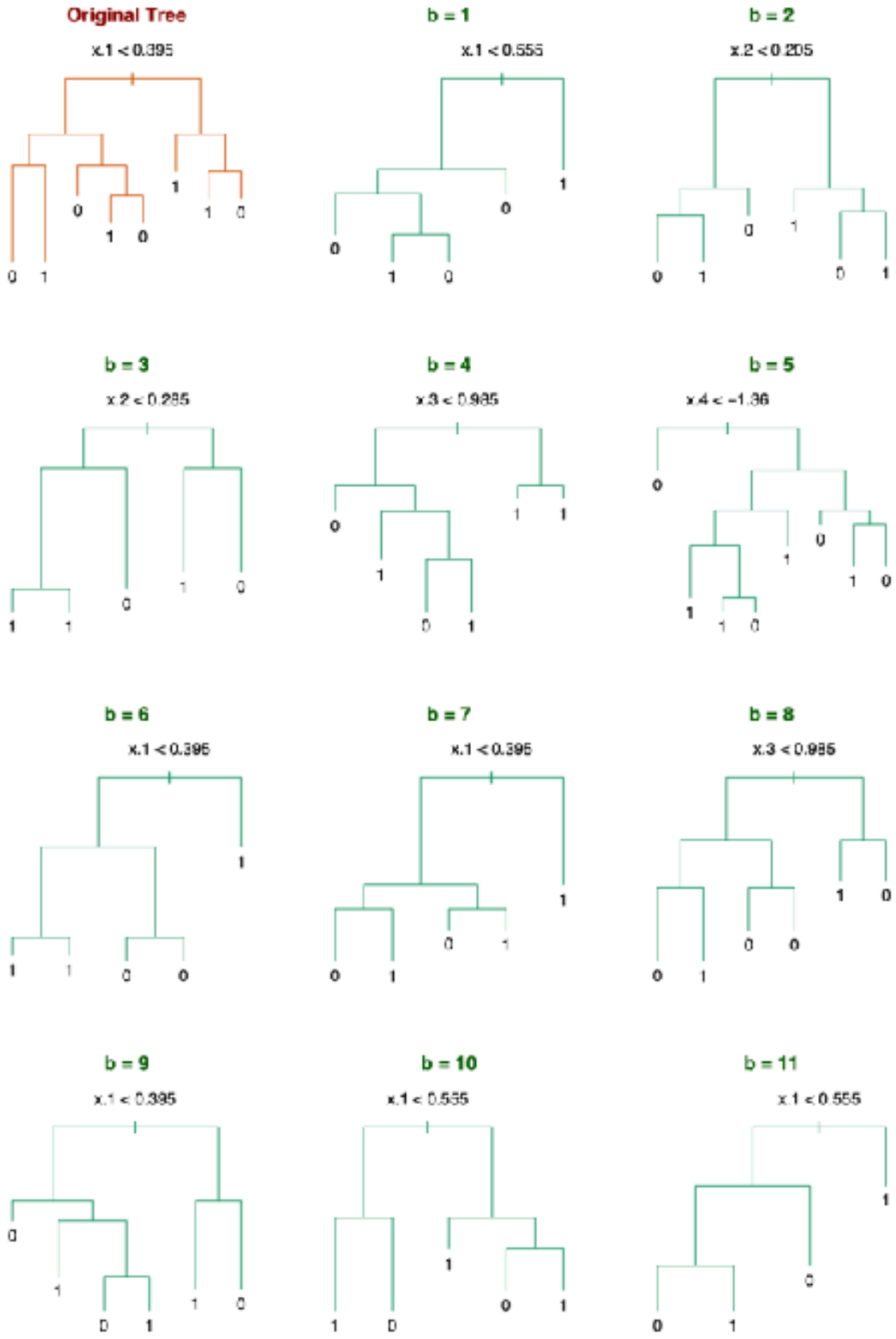

FIGURE 8.9. *Bagging trees on simulated dataset. The top left panel shows the original tree. Eleven trees grown on bootstrap samples are shown. For each tree, the top split is annotated.*

Bagging improves over one tree

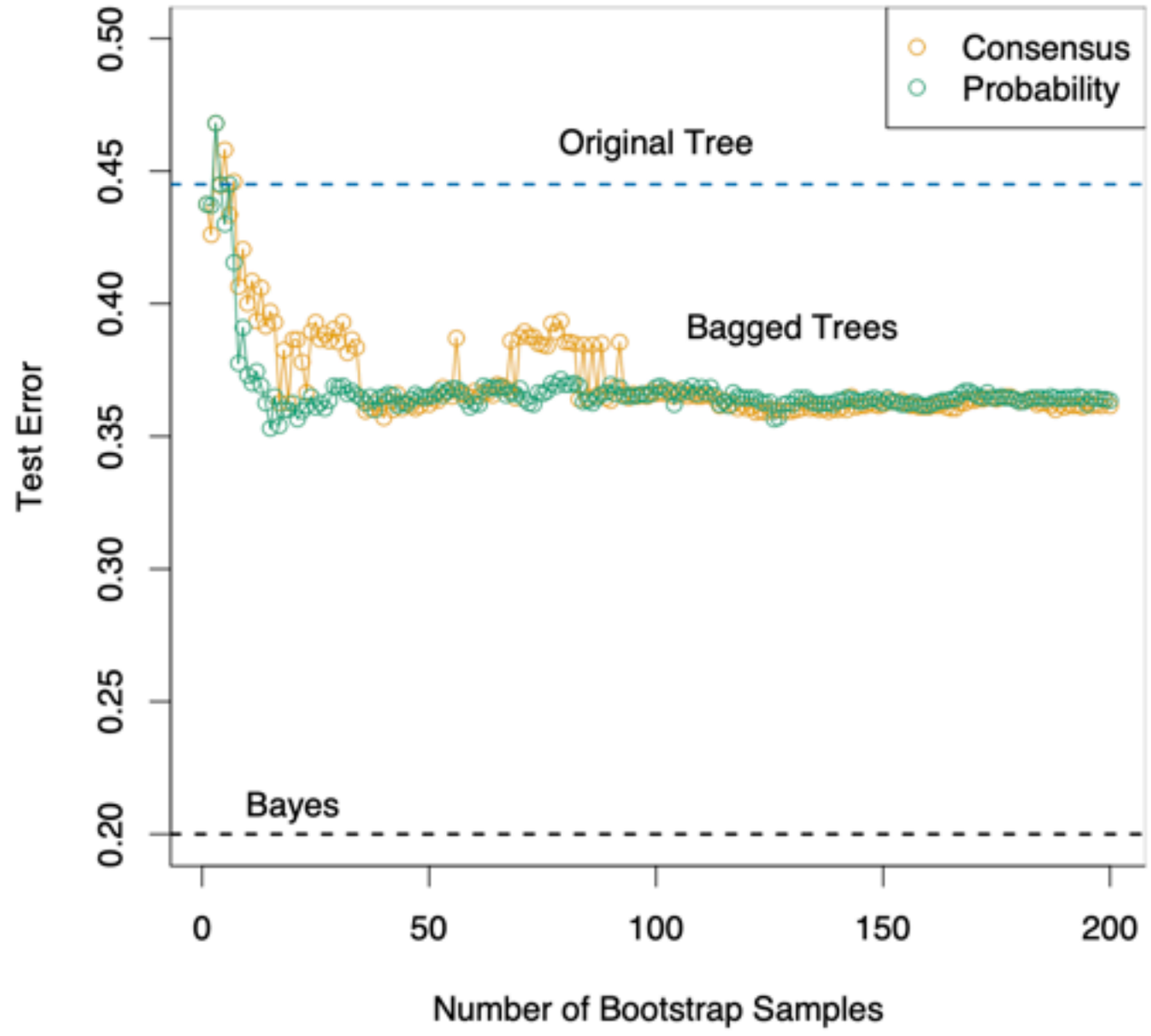

FIGURE 8.10. *Error curves for the bagging example of Figure 8.9. Shown is the test error of the original tree and bagged trees as a function of the number of bootstrap samples. The orange points correspond to the consensus vote, while the green points average the probabilities.*

Inductive bias of trees (or stumps) is hard to wash out

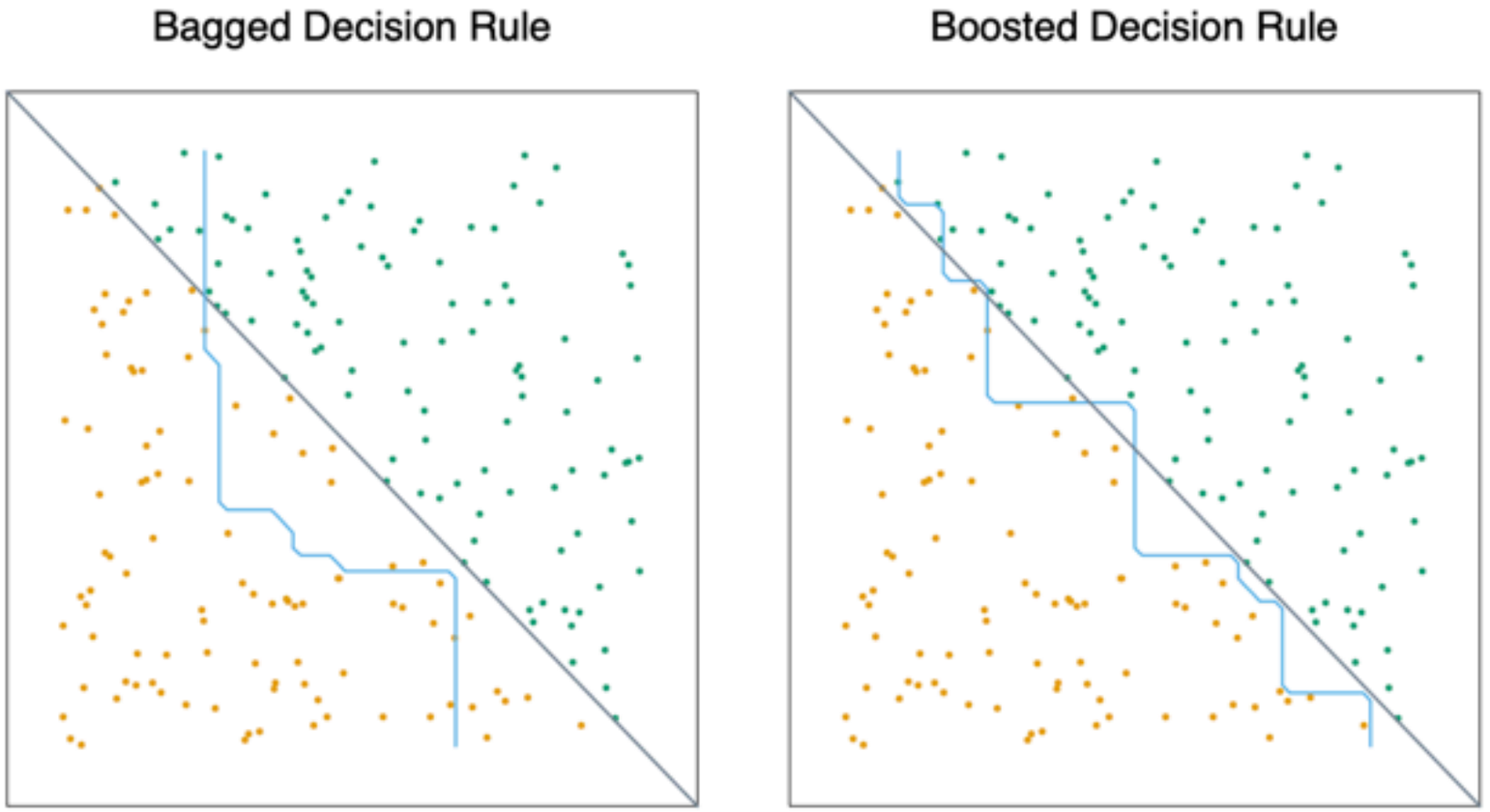

FIGURE 8.12. *Data with two features and two classes, separated by a linear boundary. (Left panel:) Decision boundary estimated from bagging the decision rule from a single split, axis-oriented classifier. (Right panel:) Decision boundary from boosting the decision rule of the same classifier. The test error rates are* 0.166, *and* 0.065, *respectively. Boosting is described in Chapter 10.*

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2. Random Forests (1/2 class)

Algorithm 15.1 *Random Forest for Regression or Classification.*

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\mathrm{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\mathrm{rf}}^B(x) = \textit{majority vote } \{\hat{C}_b(x)\}_1^B$.

Typically values for m are $\sqrt{p}$ or even as low as 1.

An average of B i.i.d. random variables, each with variance σ^2, has variance $\frac{1}{B}\sigma^2$. If the variables are simply i.d. (identically distributed, but not necessarily independent) with positive pairwise correlation ρ, the variance of the average is (Exercise 15.1)

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2. \tag{15.1}$$

Typically, RF beats Bagging

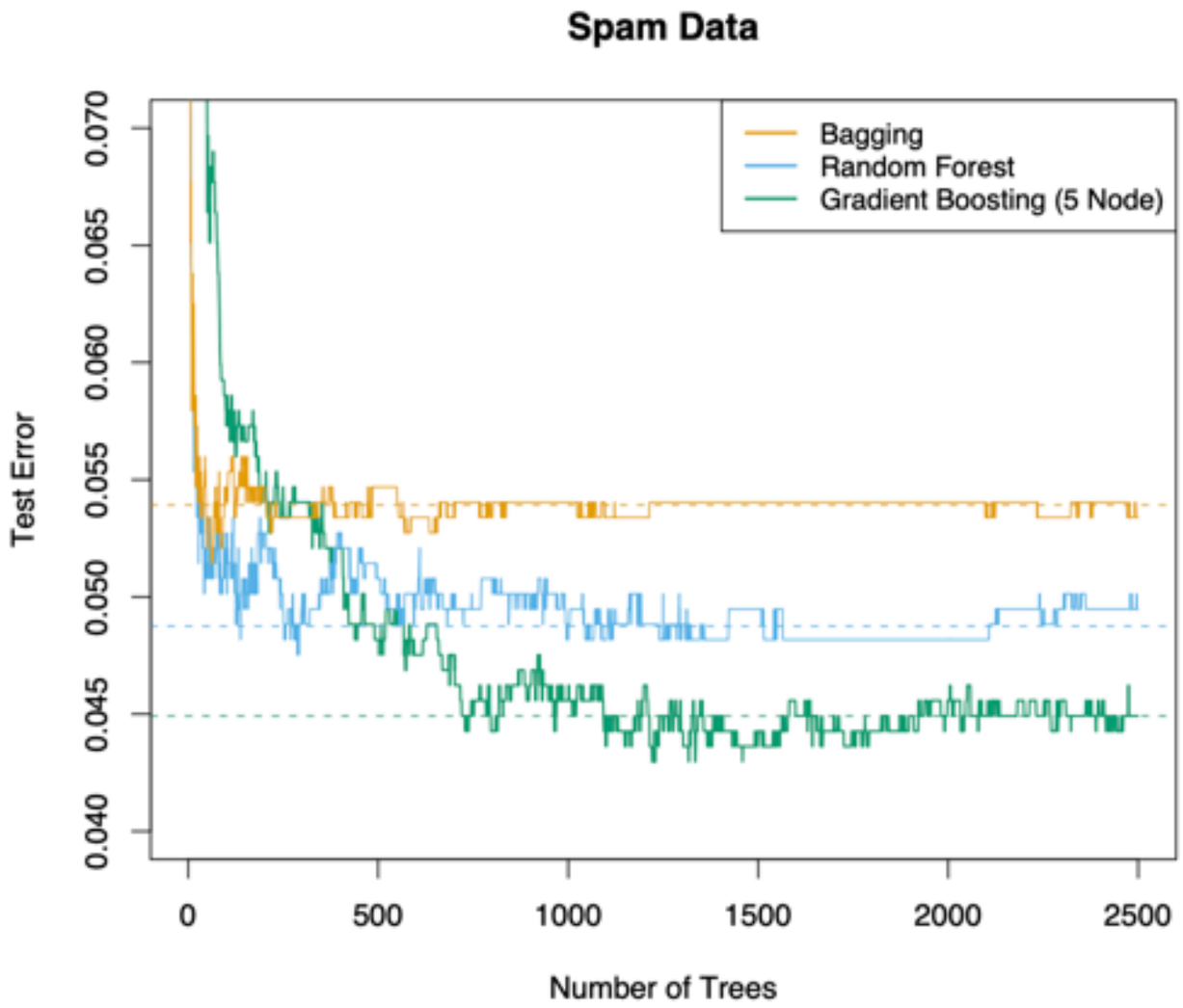


FIGURE 15.1. *Bagging, random forest, and gradient boosting, applied to the spam data. For boosting,* 5*-node trees were used, and the number of trees were chosen by* 10*-fold cross-validation (*2500 *trees). Each "step" in the figure corresponds to a change in a single misclassification (in a test set of* 1536*).*

Effect of depth

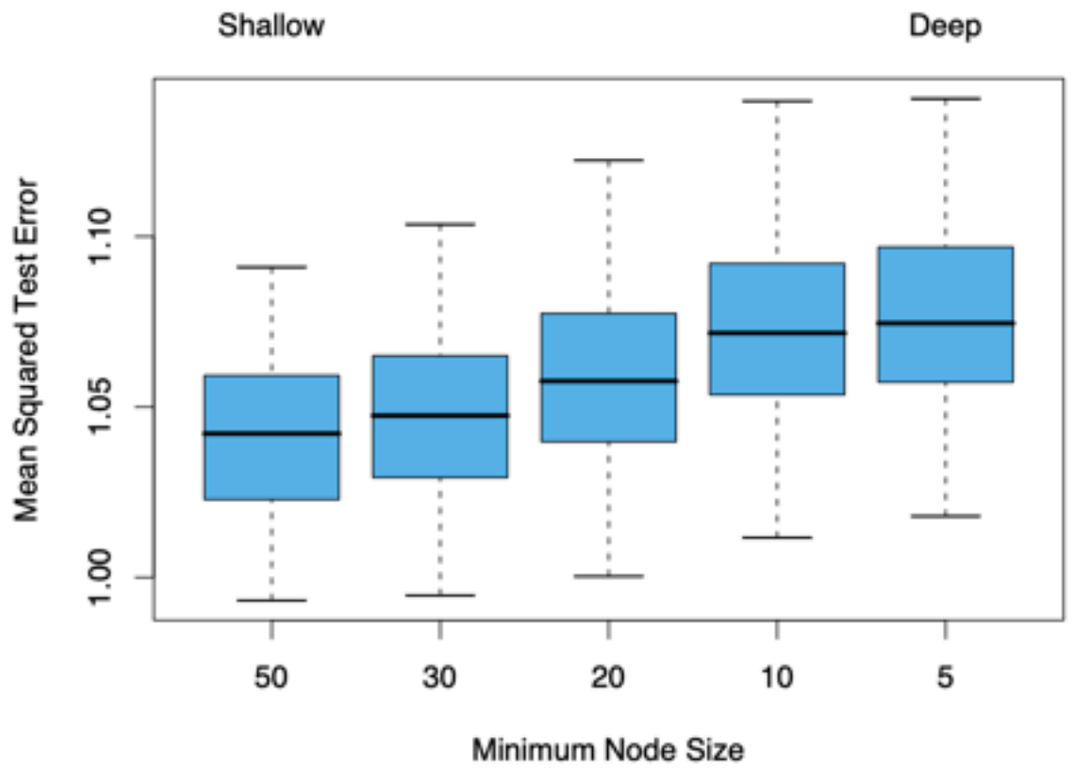
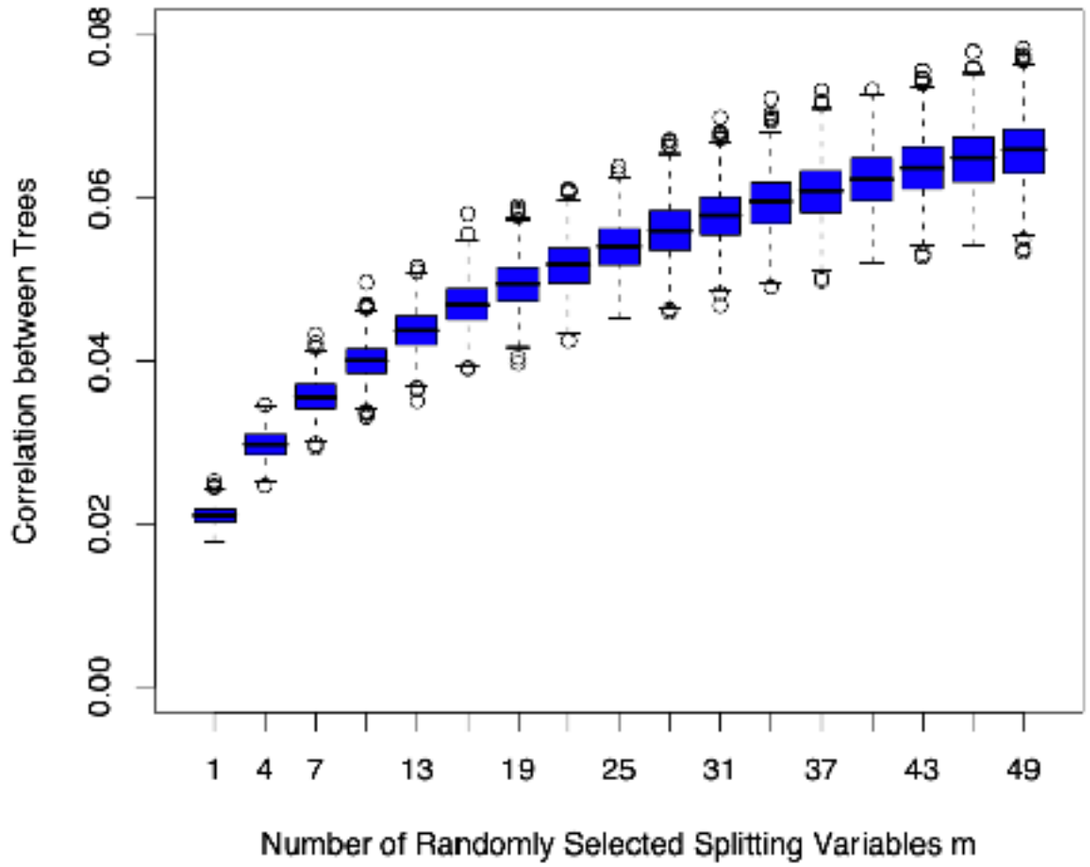


FIGURE 15.8. *The effect of* tree size *on the error in random forest regression. In this example, the true surface was additive in two of the* 12 *variables, plus additive unit-variance Gaussian noise. Tree depth is controlled here by the minimum node size; the smaller the minimum node size, the deeper the trees.*

Figure 15.8 shows the modest effect of depth control in a simple regression example. Classifiers are less sensitive to variance, and this effect of overfitting is seldom seen with random-forest classification.

Effect of #split parameters m



Number of Randomly Selected Splitting Variables m

FIGURE 15.9. *Correlations between pairs of trees drawn by a random-forest regression algorithm, as a function of m. The boxplots represent the correlations at* 600 *randomly chosen prediction points x.*

The following demonstrations are based on a simulation model

the training data $\mathbf{Z}$

$$Y = \frac{1}{\sqrt{50}} \sum_{j=1}^{50} X_j + \varepsilon, \tag{15.8}$$

with all the X_j and ε iid Gaussian. We use 500 training sets of size 100, and a single set of test locations of size 600. Since regression trees are nonlinear in $\mathbf{Z}$, the patterns we see below will differ somewhat depending on the structure of the model.

Figure 15.9 shows how the correlation (15.6) between pairs of trees decreases as m decreases: pairs of tree predictions at x for different training sets $\mathbf{Z}$ are likely to be less similar if they do not use the same splitting variables.

Effect of #irrelevant variables (true sparsity)

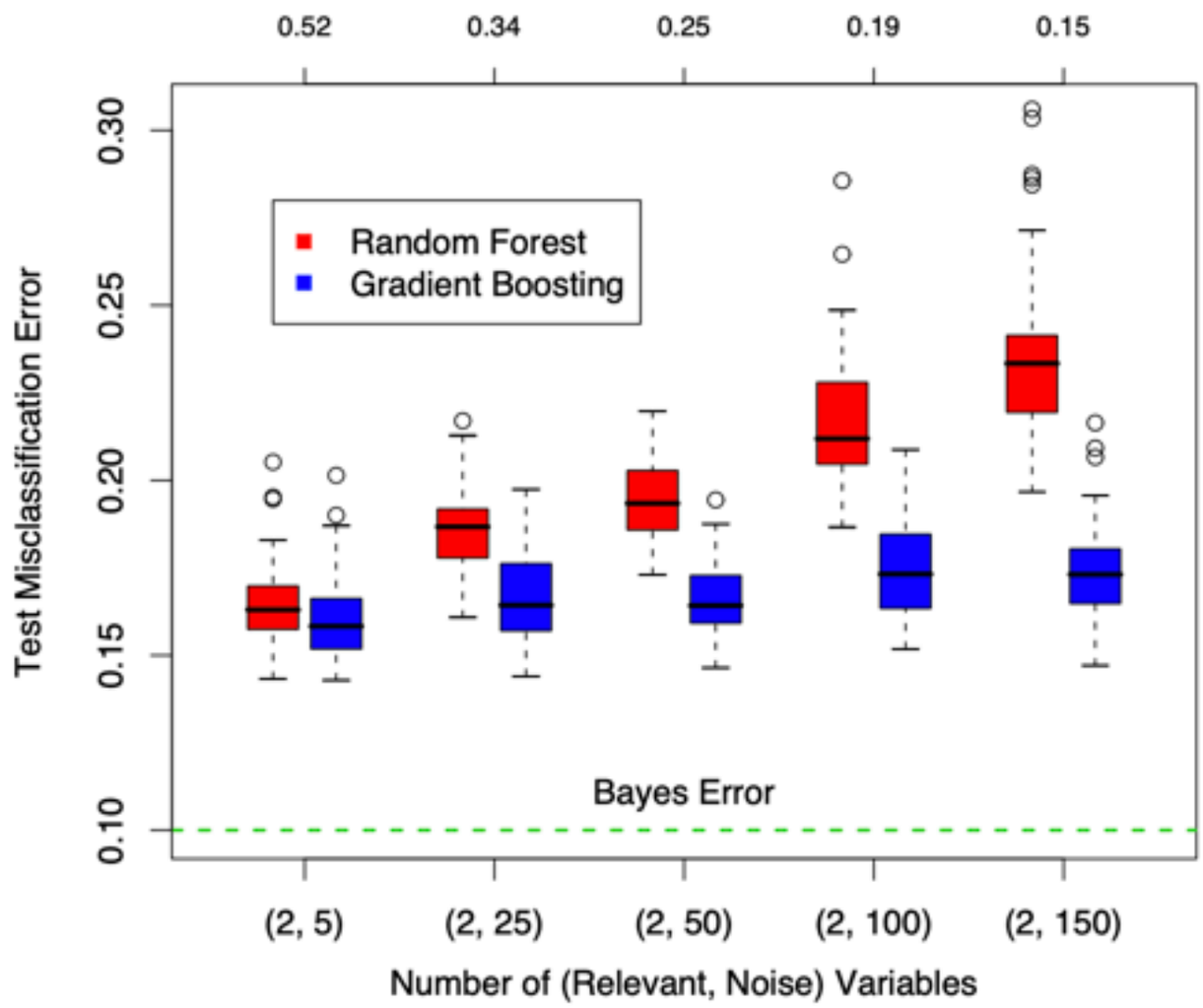


FIGURE 15.7. *A comparison of random forests and gradient boosting on problems with increasing numbers of noise variables. In each case the true decision boundary depends on two variables, and an increasing number of noise variables are included. Random forests uses its default value* $m = \sqrt{p}$. *At the top of each pair is the probability that one of the relevant variables is chosen at any split. The results are based on* 50 *simulations for each pair, with a training sample of* 300, *and a test sample of* 500.

Bias and variance, vs m

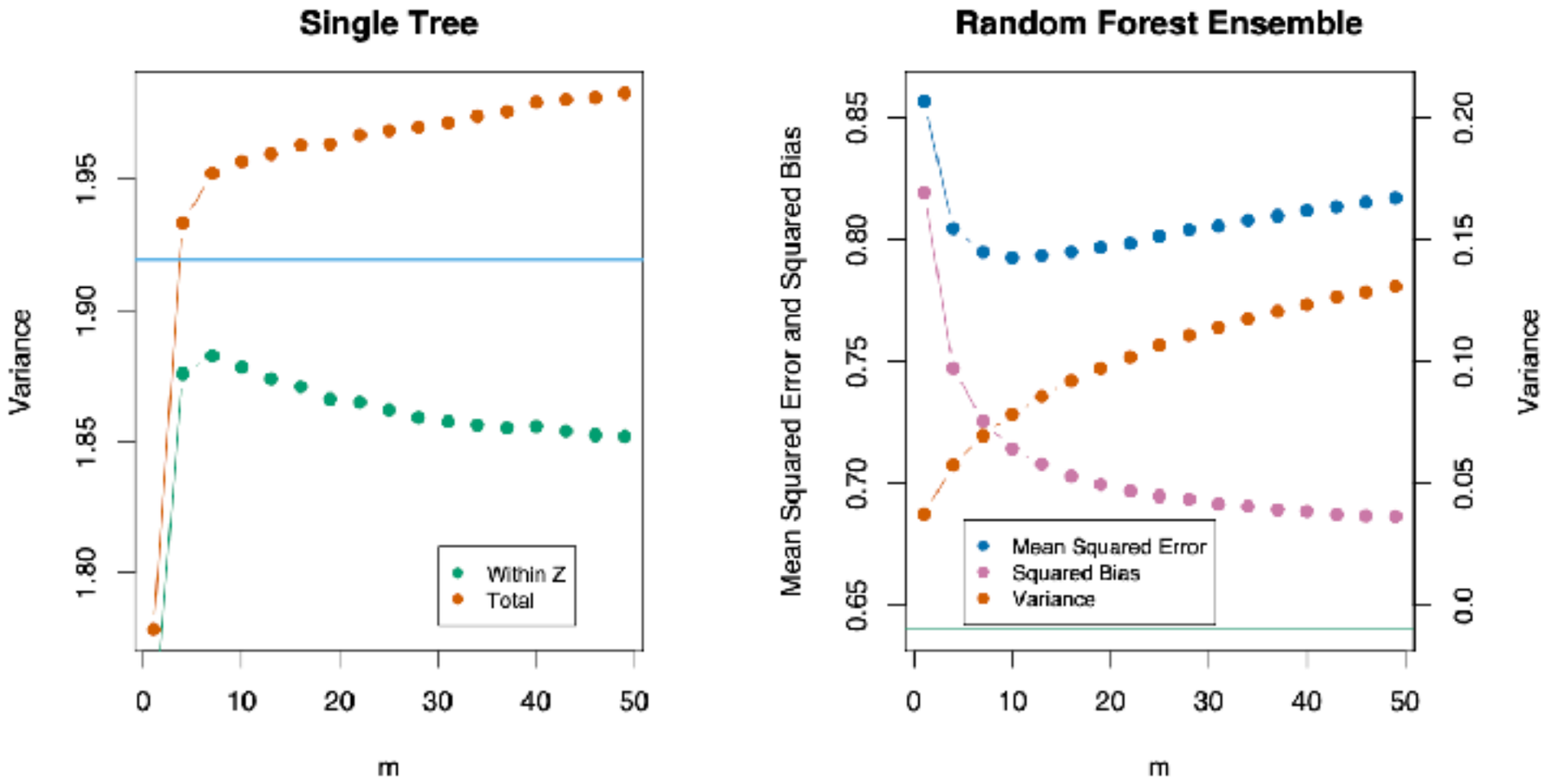


FIGURE 15.10. *Simulation results. The left panel shows the average variance of a single random forest tree, as a function of m. "Within* $\mathbf{Z}$*" refers to the average within-sample contribution to the variance, resulting from the bootstrap sampling and split-variable sampling (15.9). "Total" includes the sampling variability of* $\mathbf{Z}$*. The horizontal line is the average variance of a single fully grown tree (without bootstrap sampling). The right panel shows the average mean-squared error, squared bias and variance of the ensemble, as a function of m. Note that the variance axis is on the right (same scale, different level). The horizontal line is the average squared-bias of a fully grown tree.*

RF classification is like adaptive nearest neighbors

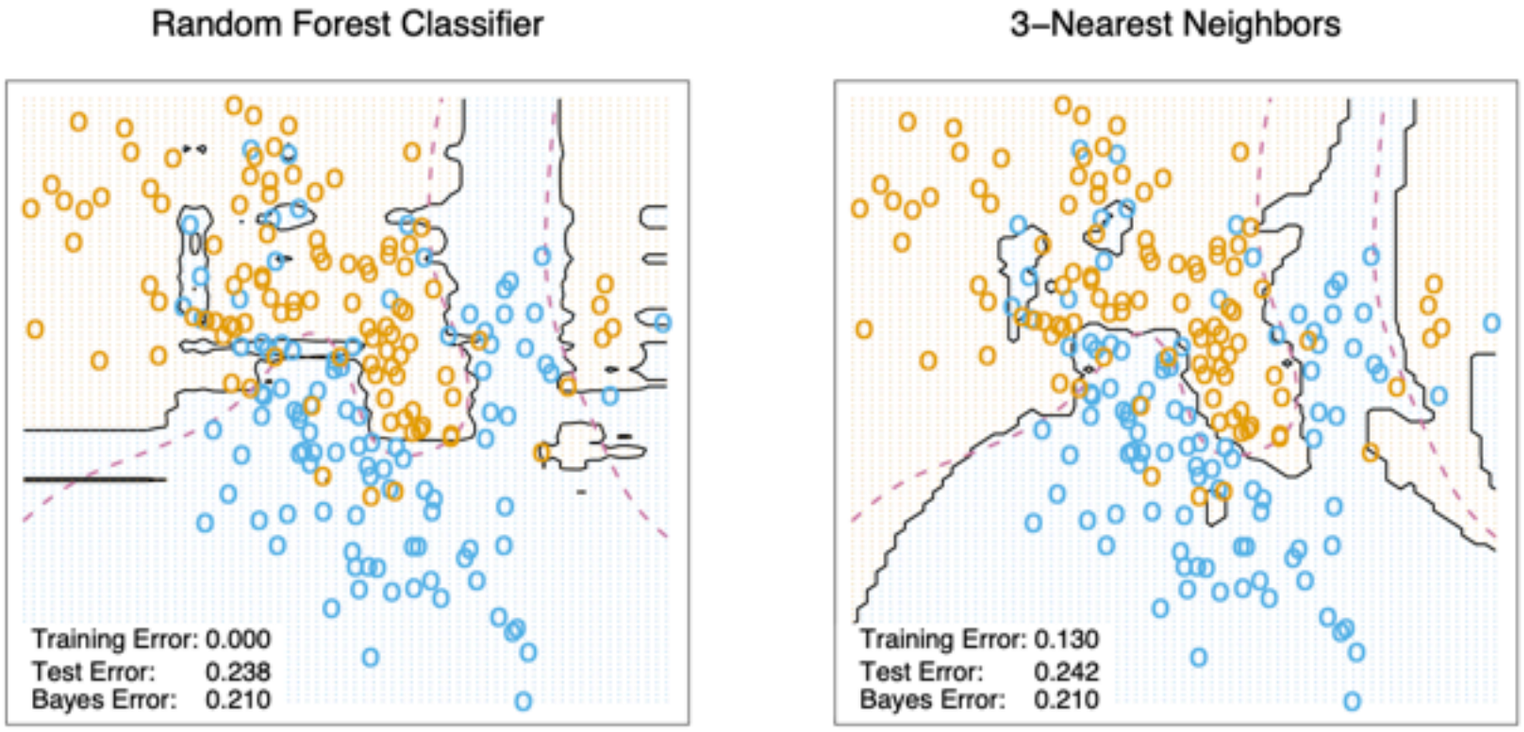


FIGURE 15.11. *Random forests versus 3-NN on the mixture data. The axis-oriented nature of the individual trees in a random forest lead to decision regions with an axis-oriented flavor.*

(If trees are grown to max depth, each tree picks out one "nearest neighbor", but in a data-dependent distance metric)

Out-of-bag error (OOB)

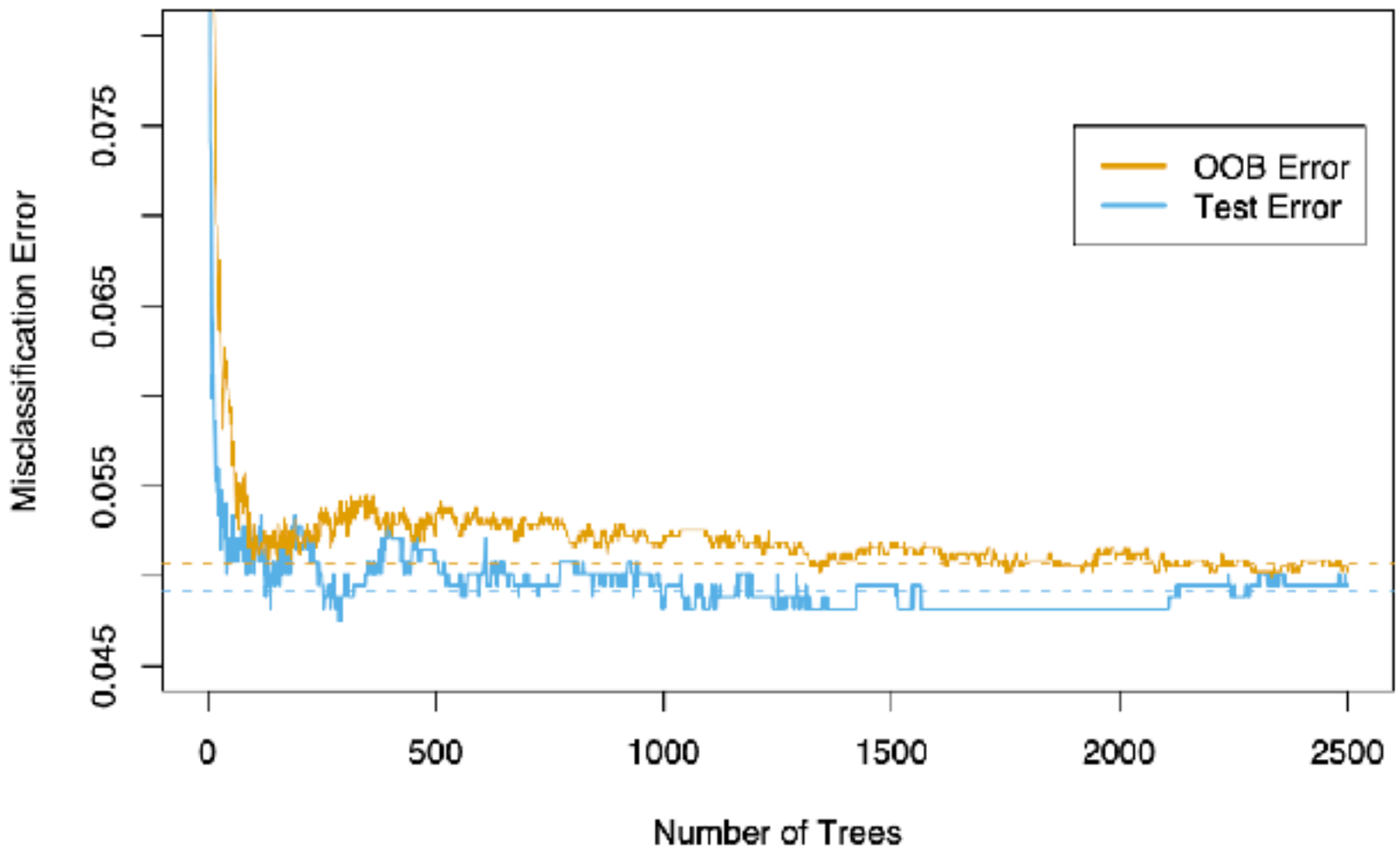


FIGURE 15.4. OOB *error computed on the* spam *training data, compared to the test error computed on the test set.*

For each observation $z_i = (x_i, y_i)$*, construct its random forest predictor by averaging* only *those trees corresponding to bootstrap samples in which* z_i did not *appear.*

Next class

Minimax theorem