Exercise 6

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6.2.2

The gini Δ as well as class distributions for labels 1 and 2 are shown in figure 1. The y-value of the corresponding label does not have a meaning. It just makes both labels more distinct. The x-value of the largest gini Δ is where both classes have the least overlap.

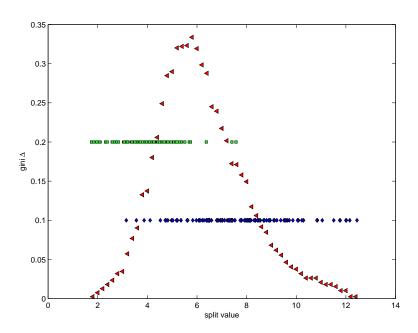


Figure 1: gini Δ as a function of the split value. The class distributions are shown for label 1 (blue) and label 2 (green).

6.3.1

The covariance is a symmetric bilinear form. Therefore the following rules apply:

$$Cov(X,Y) = Cov(Y,X) \tag{1}$$

$$Cov(aX + b, Y) = aCov(X, Y)$$
(2)

$$Cov(X+Y,Z) = Cov(X,Z) + Cov(Y,Z)$$
(3)

3 can be generalized to:

$$Cov(\sum_{i} X_i, Y) = \sum_{i} Cov(X_i, Y)$$
 (4)

Furthermore the covariance is a generalization of the variance:

$$Var(X) = Cov(X, X) \tag{5}$$

The relation between covariance and correlation is given by:

$$\rho_{ij} = \frac{cov(X_i, X_j)}{\sigma_i \sigma_j} \stackrel{i.d.}{=} \frac{cov(X_i, X_j)}{\sigma^2}$$
(6)

With this preconditions we get:

$$Var(\frac{1}{B}\sum_{i=1}^{B}X_{i}) \stackrel{5}{=} Cov(\frac{1}{B}\sum_{i=1}^{B}X_{i}, \frac{1}{B}\sum_{i=1}^{B}X_{i})$$
(7)

$$\stackrel{2,3}{=} \frac{1}{B^2} \sum_{i,j=1}^{B} (X_i, X_j) \tag{8}$$

$$= \frac{1}{B^2} sum_{i=1}^B Var(X_i) + \frac{2}{B^2} \sum_{i=1}^{B-1} \sum_{j=i+1}^B cov(X_i, X_j)$$
(9)

$$\stackrel{6,i.d.}{=} \frac{1}{B^2} B \sigma^2 + \frac{2\rho \sigma^2}{B^2} \sum_{i=1}^{B-1} \sum_{j=i+1}^{B} 1 \tag{10}$$

$$= \frac{\sigma^2}{B} + \frac{2\rho\sigma^2}{B^2} \sum_{i=1}^{B-1} B - i \tag{11}$$

$$=\frac{\sigma^{2}}{B} + \frac{2\rho\sigma^{2}}{B^{2}}\left(B\left(B-1\right) - \frac{B\left(B-1\right)}{2}\right) \tag{12}$$

$$=\frac{\sigma^2}{B} + \frac{\rho\sigma^2}{B}(B-1) \tag{13}$$

$$=\rho\sigma^2 + \frac{(1-\rho)\sigma^2}{B} \tag{14}$$

6.3.2

The probability p_{oob} for an observation to be out of bag is given by the ratio of the number N_{all} of all possible bags and the number N_{-1} of all possible bags that do not contain given observation. Let N be the number of all observations and k the number of elements contained in a bag. Then the total number of possible bags is given by the number of possible configurations $\frac{N!}{(N-k)!}$ divided by the number of corresponding permutations k! (i.e. choosing observations 1, 2 and 4 is the same as choosing 1, 4 and 2) or the binomial coefficient.

$$N_{all} = \frac{N!}{k!(N-k)!} \tag{15}$$

$$= \binom{N}{k} \tag{16}$$

The number of possible bags not containing a certain observation can be obtained in a similar fashion. Let x_i be an observation fixed to be not in a bag. Then the number of possible bags for that configuration is given by the number of possible configurations for the remaining N-1 samples $\frac{(N-1)!}{(N-k-1)!}$ divided by the number of corresponding permutations k!.

$$N_{-1} = \frac{(N-1)!}{k!(N-1-k)!} \tag{17}$$

$$= \binom{N-1}{k} \tag{18}$$

Therefore the resulting probability p_{oob} is given by:

$$p_{oob} = \frac{N_{-1}}{N_{all}}$$

$$= \frac{(N-1)!}{k!(N-1-k)!} \frac{k!(N-k)!}{N!}$$
(20)

$$=\frac{(N-1)!}{k!(N-1-k)!}\frac{k!(N-k)!}{N!}$$
(20)

$$p_{oob} = \frac{N-k}{N} = 1 - \frac{k}{N} \tag{21}$$

That probability holds for a single bootstrap sample. Given M trees based on M bootstrap samples, the probability for an observation to be out-of-bag in at least one tree can be calculated with the help of the probability that the observation is contained in every bootstrap sample. $(1 - p_{oob})^M$ is the probability for an observation to be contained in all bootstrap samples.

$$p = 1 - (1 - p_{oob})^M (22)$$

$$p = 1 - \left(\frac{k}{N}\right)^M \tag{23}$$

6.3.3

The oob error decreases with an increasing number of trees M. The test error is decreasing as well, however it's fluctuating, so it might be constant for $M > M_{min}$. Therefore choosing a good k might save a lot of computation time.

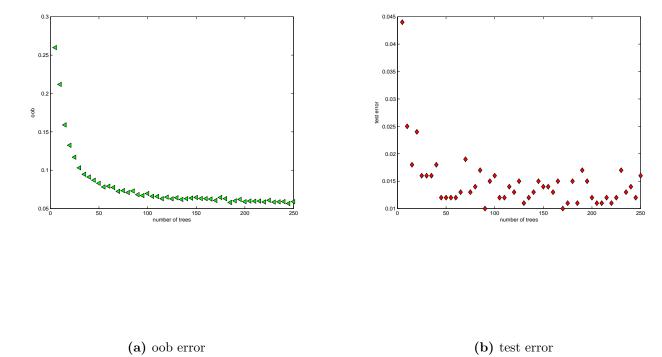


Figure 2: oob and test error as functions of the number of trees \mathbf{F}