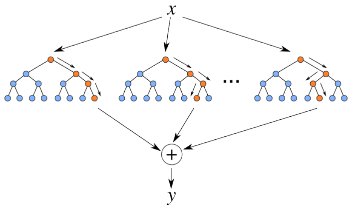
Introduction to Machine Learning

Random Forest: Introduction



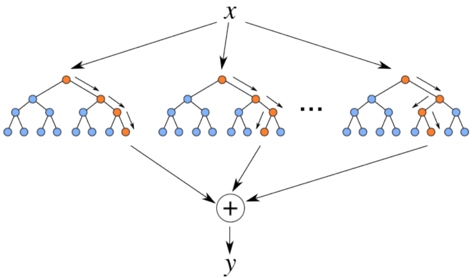
Learning goals

- Know how random forests are defined by extending the idea of bagging
- Understand that the goal is to decorrelate the trees
- Understand that the out-of-bag error is a way to obtain unbiased estimates of the generalization error during training

RANDOM FORESTS

Modification of bagging for trees proposed by Breiman (2001):

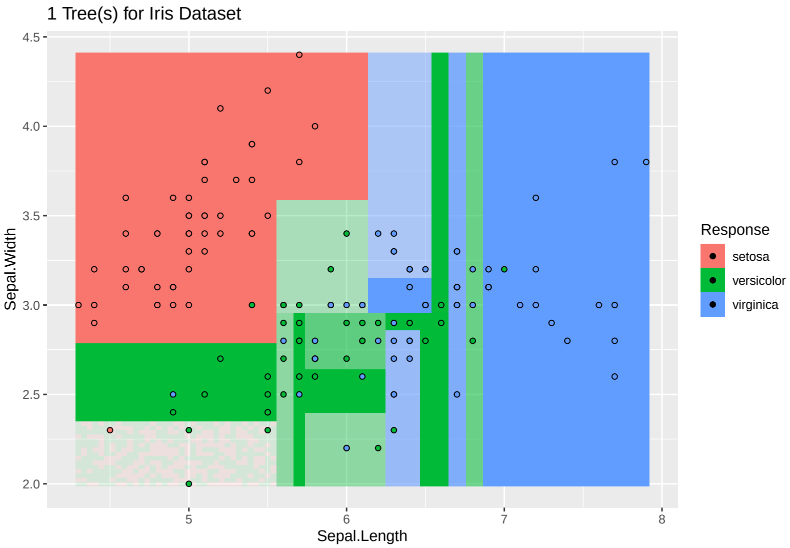
- Tree base learners on bootstrap samples of the data
- Uses **decorrelated** trees by randomizing splits (see below)
- Tree base learners are usually fully expanded, without aggressive early stopping or pruning, to **increase variance of the ensemble**



RANDOM FEATURE SAMPLING

- From our analysis of bagging risk we can see that decorrelating trees improves the ensemble
- Simple randomized approach:
  At each node of each tree, randomly draw mtry $\leq p$ candidate features to consider for splitting. Recommended values:
  - Classification: mtry $= \lfloor \sqrt{p} \rfloor$
  - Regression: mtry $= \lfloor p/3 \rfloor$

EFFECT OF ENSEMBLE SIZE



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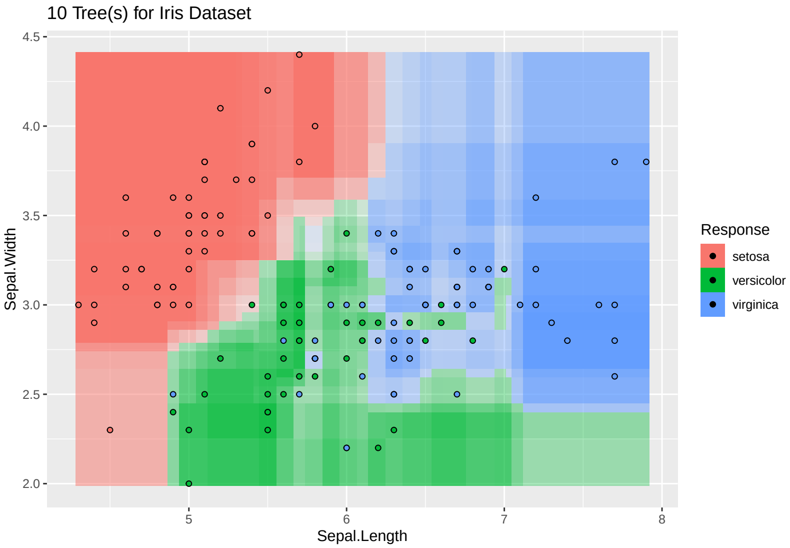
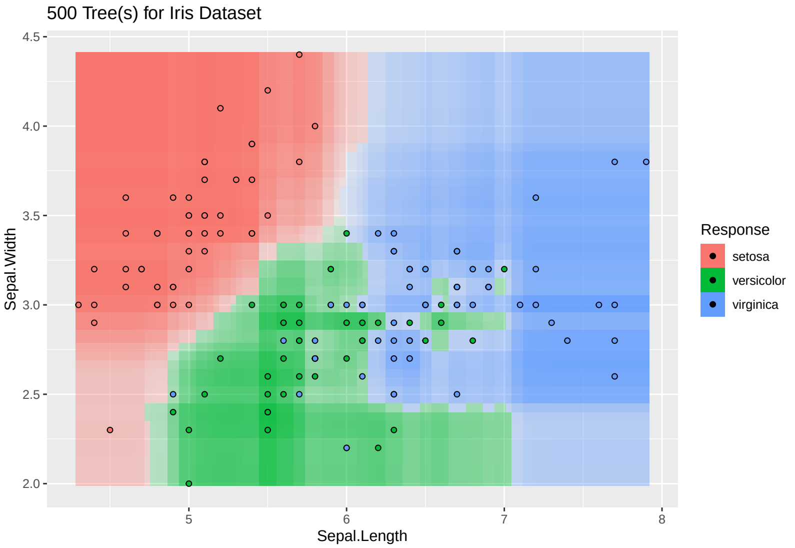
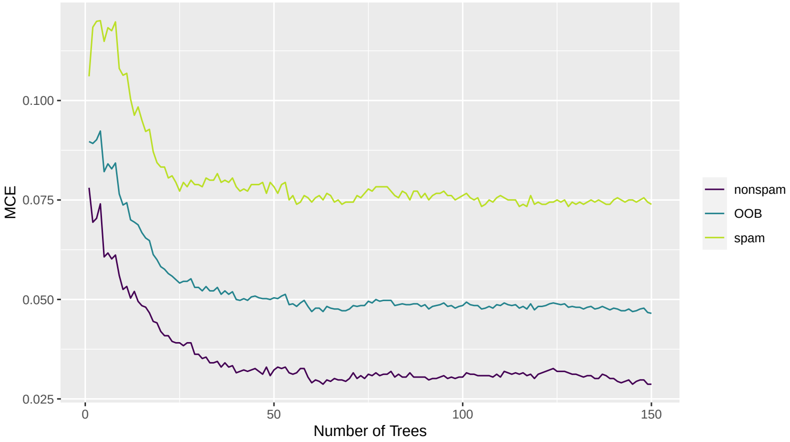


EFFECT OF ENSEMBLE SIZE

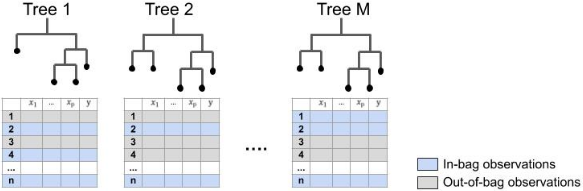


OUT-OF-BAG ERROR ESTIMATE

With the RF it is possible to obtain unbiased estimates of the generalization error directly during training, based on the out-of-bag observations for each tree:



OUT-OF-BAG ERROR ESTIMATE



- For an estimation of the generalization error, we exploit the fact that the *i*-th observation acts as unseen test point for all trees in which it is OOB.
- Let $\text{OOB}^{[m]}$ denote the index set $\left\{i \in \{1, \ldots, n\} | (\mathbf{x}^{(i)}, y^{(i)}) \text{ is OOB for } b^{[m]}(\mathbf{x})\right\}$.
- The number of trees for which the *i*-th observation is OOB is then given by $S_{\text{OOB}}^{(i)} = \sum_{m=1}^{M} \mathbb{I}(i \in \text{OOB}^{[m]})$.
- We can compute the average over predictions $\hat{y}^{(i)[m]}$ from trees $b^{[m]}(\mathbf{x})$ that have observation i in their OOB data to obtain an ensemble prediction.
- The average loss of these ensemble OOB predictions over all n observations yields an estimate for the generalization error.

OUT-OF-BAG ERROR ESTIMATE

- Compute the ensemble OOB prediction for each observation:

$$\hat{y}^{(i)}_{\text{OOB}} = \begin{cases} \frac{1}{S^{(i)}_{\text{OOB}}} \sum_{m=1}^{M} \mathbb{I}(i \in \text{OOB}^{[m]}) \cdot \hat{y}^{(i)[m]} & \text{in regression,} \\ \\ \arg\max_{k \in \{1,\ldots,g\}} \frac{\sum_{m=1}^{M} \mathbb{I}(i \in \text{OOB}^{[m]}) \cdot \mathbb{I}(\hat{h}^{(i)[m]} = k)}{S^{(i)}_{\text{OOB}}} & \text{in classification.} \end{cases}$$

- Then, take the average of the resulting point-wise losses to estimate the OOB error of the forest:

$$\widehat{\text{err}}_{\text{OOB}} = \frac{1}{n} \sum_{i=1}^{n} L(y^{(i)}, \hat{y}^{(i)}_{\text{OOB}})$$

- Note that the use of class labels commands the use of 0-1 loss in classification (alternative formulations for other losses are possible).
- OOB size: $\mathbb{P}(i \in \text{OOB}^{[m]}) = \left(1 - \frac{1}{n}\right)^n \overset{n \to \infty}{\longrightarrow} \frac{1}{e} \approx 0.37$ for $i \in \{1, \ldots, n\}$.
- Similar to 3-CV, can be used for a quick model selection.