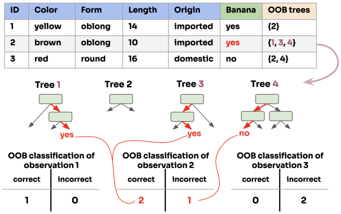
Introduction to Machine Learning

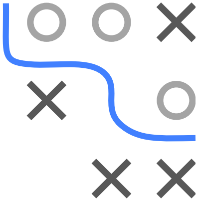
Random Forest
Out-of-Bag Error Estimate



Learning goals

- Understand the concept of out-of-bag and in-bag observations
- Learn how out-of-bag error provides an estimate of the generalization error during training

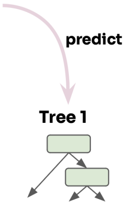
OUT-OF-BAG VS IN-BAG OBSERVATIONS



ID	Color	Form	Length	Origin	Banana
1	yellow	oblong	14	imported	yes
2	brown	oblong	10	imported	yes
3	red	round	16	domestic	no

OOB

IB



Bootstrapping to train tree 1

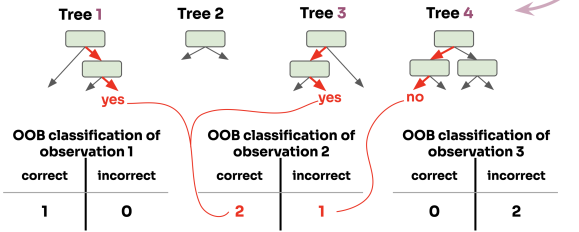
ID	Color	Form	Length	Origin	Banana
1	yellow	oblong	14	imported	yes
3	red	round	16	domestic	no
3	red	round	16	domestic	no

- IB observations for m-th bootstrap:
  $$\mathrm{IB}^{[m]} = \{i \in \{1, \ldots, n\} | \left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{D}^{[m]}\}$$
- OOB observations for m-th bootstrap:
  $$\mathrm{OOB}^{[m]} = \{i \in \{1, \ldots, n\} | \left(\mathbf{x}^{(i)}, y^{(i)}\right) \notin \mathcal{D}^{[m]}\}$$
- Nr. of trees where i-th observation is OOB:
  $$S_{\mathrm{OOB}}^{(i)} = \sum_{m=1}^{M} \mathbb{I}(i \in \mathrm{OOB}^{[m]}).$$

OUT-OF-BAG ERROR ESTIMATE

Predict i-th observation with all trees $\hat{b}^{[m]}$ for which it is OOB:

ID	Color	Form	Length	Origin	Banana	OOB trees
1	yellow	oblong	14	imported	yes	{2}
2	brown	oblong	10	imported	yes	{1, 3, 4}
3	red	round	16	domestic	no	{2, 4}



OOB prediction $\hat{\pi}^{(2)}_{\mathrm{OOB}} = 2/3$. Evaluating all OOB predictions with some loss function L or set-based metric ρ estimates the GE.
As we do not violate the **untouched test set principle**, $\widehat{\mathrm{GE}}$ is not *optimistically* biased.

OUT-OF-BAG ERROR PSEUDO CODE

Out-Of-Bag error estimation

Input: $\mathrm{OOB}^{[m]}, \hat{b}^{[m]} \forall m \in \{1, \dots, M\}$

for $i = 1 \to n$ **do**

  Compute the ensemble OOB prediction for observation i, e.g., for regression:

$$\hat{f}^{(i)}_{\mathrm{OOB}} = \frac{1}{S^{(i)}_{\mathrm{OOB}}} \sum_{m=1}^{M} \mathbb{I}(i \in \mathrm{OOB}^{[m]}) \cdot \hat{f}^{[m]}(\mathbf{x}^{(i)})$$

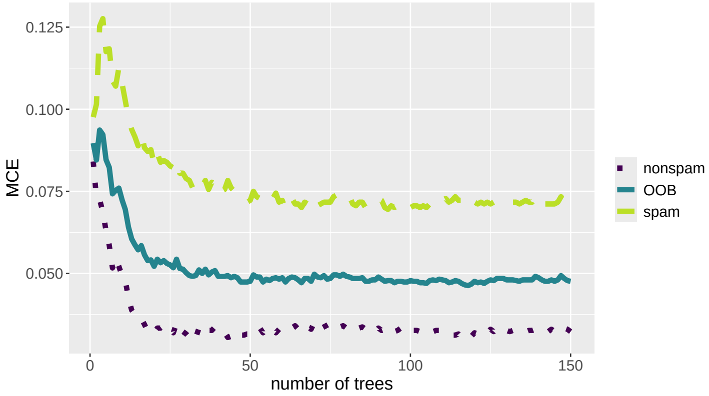
end for

Average losses over all observations:

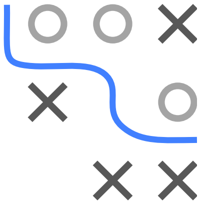
$$\widehat{\mathrm{GE}}_{\mathrm{OOB}} = \frac{1}{n} \sum_{i=1}^{n} L(y^{(i)}, \hat{f}^{(i)}_{\mathrm{OOB}})$$

USING THE OUT-OF-BAG ERROR ESTIMATE

- Gives us a (proper) estimator of GE, computable during training
- Can even compute this for all smaller ensemble sizes
  (after we fitted M models)



OOB ERROR: COMPARABILITY, BEST PRACTICE



OOB Size: The probability that an observation is out-of-bag (OOB) is:

$$\mathbb{P}\left(i \in \mathrm{OOB}^{[m]}\right) = \left(1 - \frac{1}{n}\right)^n \stackrel{n\to\infty}{\longrightarrow} \frac{1}{e} \approx 0.37$$

$\Rightarrow$ similar to holdout or 3-fold CV (1/3 validation, 2/3 training)

Comparability Issues:

- **OOB error** rather unique to RFs / bagging
- To compare models, we often still use CV, etc., to be consistent

Use the OOB Error for:

- Get first impression of RF performance
- Select ensemble size
- Efficiently evaluate different RF hyperparameter configurations