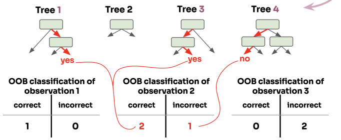
# Introduction to Machine Learning

# Random Forest
# Out-of-Bag Error Estimate

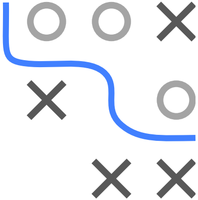
| ID | Color | Form | Length | Origin | Banana | OOB trees |
|---|---|---|---|---|---|---|
| 1 | yellow | oblong | 14 | imported | yes | {2} |
| 2 | brown | oblong | 10 | imported | yes | {1, 3, 4} |
| 3 | red | round | 16 | domestic | no | {2, 4} |




## 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



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Bootstrapping to train tree 1

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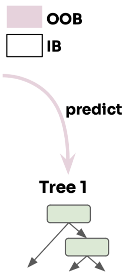
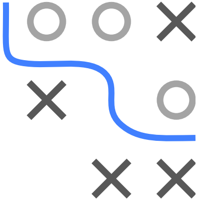



- IB observations for $m$-th bootstrap:
  $\mathrm{IB}^{[m]} = \{i \in \{1, \ldots, n\} | \left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{D}^{[m]}\}$
- OOB observations for $m$-th bootstrap:
  $\mathrm{OOB}^{[m]} = \{i \in \{1, \ldots, n\} | \left(\mathbf{x}^{(i)}, y^{(i)}\right) \notin \mathcal{D}^{[m]}\}$
- 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 |
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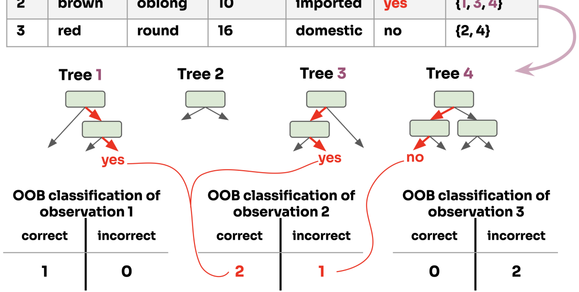
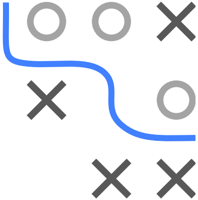



OOB prediction $\hat{\pi}^{(2)}_{\mathrm{OOB}} = 2/3$. Evaluating all OOB predictions with some loss function $L$ or set-based metric $\rho$ estimates the $\mathrm{GE}$.

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**

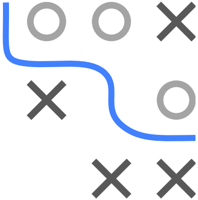
**Input:** $\mathrm{OOB}^{[m]}, \hat{b}^{[m]} \forall m \in \{1, \ldots, M\}$
**for** $i = 1 \to n$ **do**
    Compute the ensemble OOB prediction for observation $i$, e.g., for regression:

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

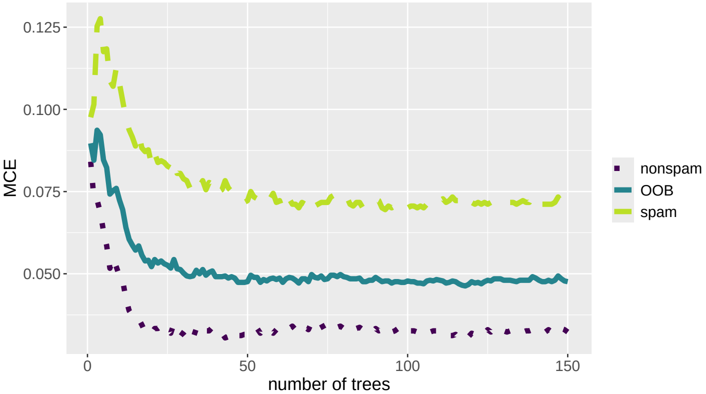
**end for**
Average losses over all observations:

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

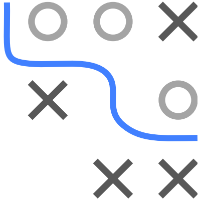
# USING THE OUT-OF-BAG ERROR ESTIMATE



- Gives us a (proper) estimator of $\mathrm{GE}$, 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