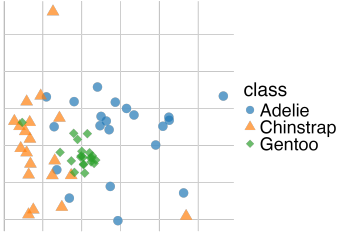
Introduction to Machine Learning

Random Forest Proximities

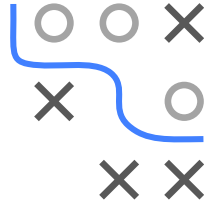


Learning goals

- Understand how RF can be used to define proximities of observations
- Know how proximities can be used for visualization, outlier detection and imputation

PROXIMITIES

RFs have built-in similarity measure for pairs of observations:

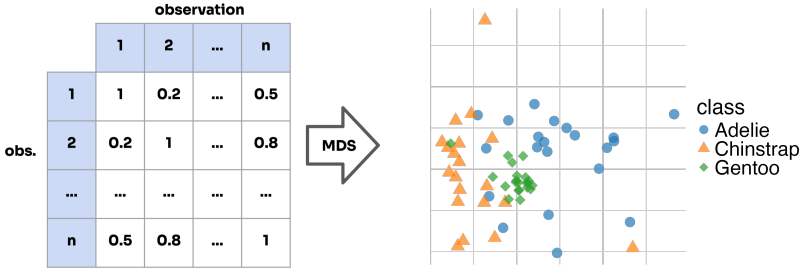


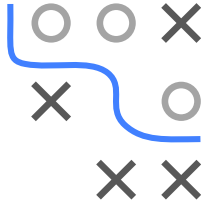
ID	Color	Form	Length
1	yellow	oblong	14

ID	Color	Form	Length
2	brown	oblong	10

- After training, push all observations through each tree
- To calculate prox $\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)$: Percentage of how often both points are placed in **same terminal node of a tree**
- Here: prox $\left(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}\right) = 2/3$
- All proximities are arranged in symmetric $n \times n$ matrix

VISUALIZING PROXIMITIES



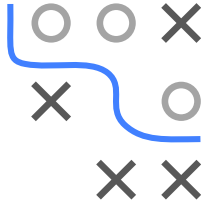


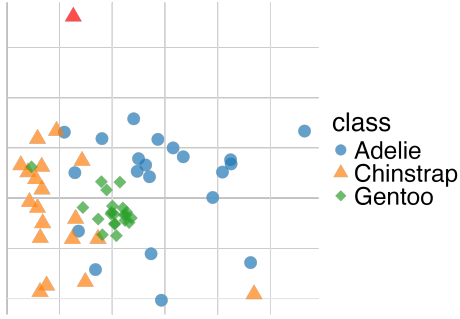
Can visualize the proximity matrix by projecting it into lower-dim. space, e.g., via multidim. scaling (might have to turn proximities into distances)

- Samples from same class usually form **identifiable clusters**
- **Offers some error-inspection**, e.g., Adelie has high within-class variance and has overlaps with other classes

OUTLIER DETECTION

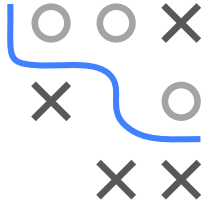
- Can also be used to **locate outliers**
- Or mislabeled points, especially in manually labeled data sets





IMPUTING MISSING DATA

ID	Color	Form	Origin	Length
1	yellow	round	domestic	14
2	brown	oblong	imported	???
3	brown	oblong	imported	19
4	???	round	domestic	14



1. Replace missings per feature by median (of available values)
2. Compute proximities (NB: data has changed)
3. Replace missings in $\mathbf{x}^{(i)}$ by weighted average of non-missings; weights proportional to proximities

Steps 2 and 3 are iterated a few times.

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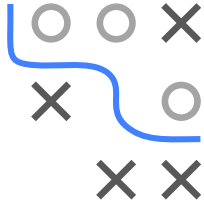

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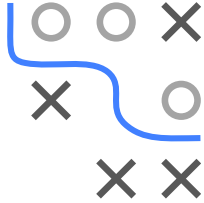
weighted average
using proximities



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