Random Forest Proximities and Their Applications in Data Science

JAKE RHODES

BRIGHAM YOUNG UNIVERSITY

Outline

- Classification and Regression Trees
  - What are they?
  - How to optimize?
  - Benefits and Limitations
- Random Forests
  - Randomizations
  - Out-of-Bag Points
  - Predictions
  - Proximities




Decision Making

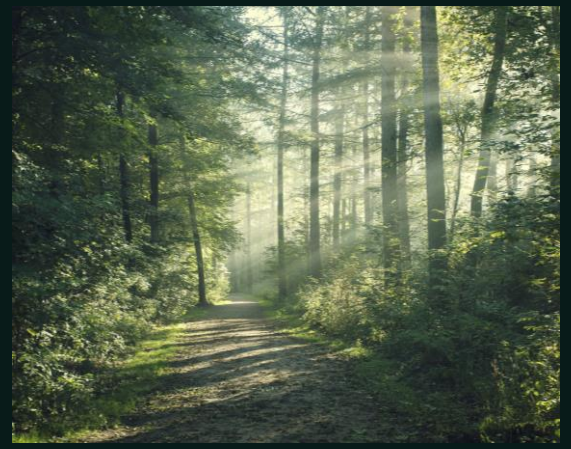
Suppose you would like to buy a car. What are some aspects you need to consider? What are the most important variables for your decision?

CART

Classification and Regression Trees

- Predictive models
- Sequences of binary questions (yes/no)
- Make predictions by following paths and voting/aggregating responses.






CART Terminology

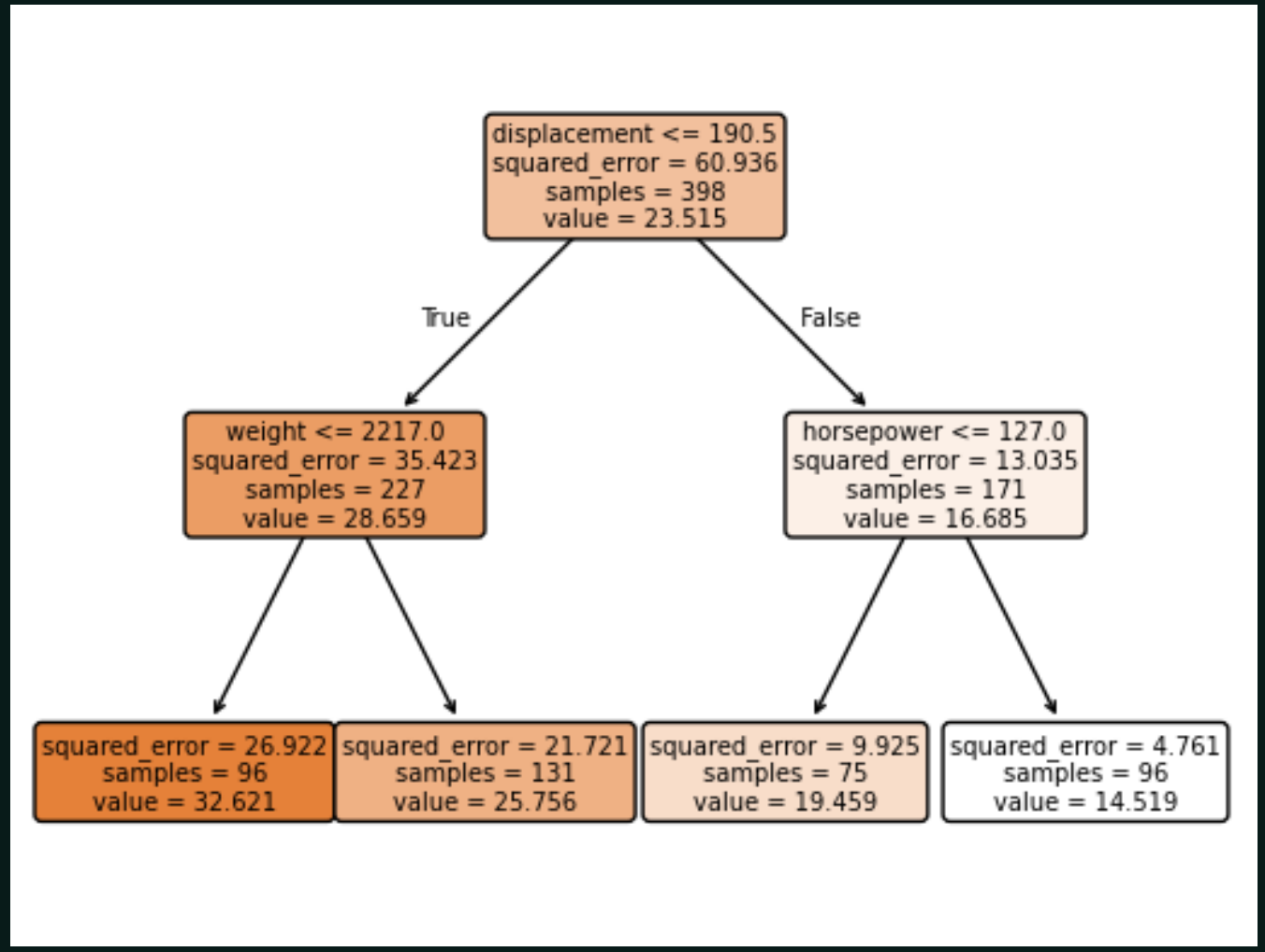
Nodes:

- Root (Beginning)
- Terminal or Leaf (End)
- Daughter/ (Internal)

Splits:

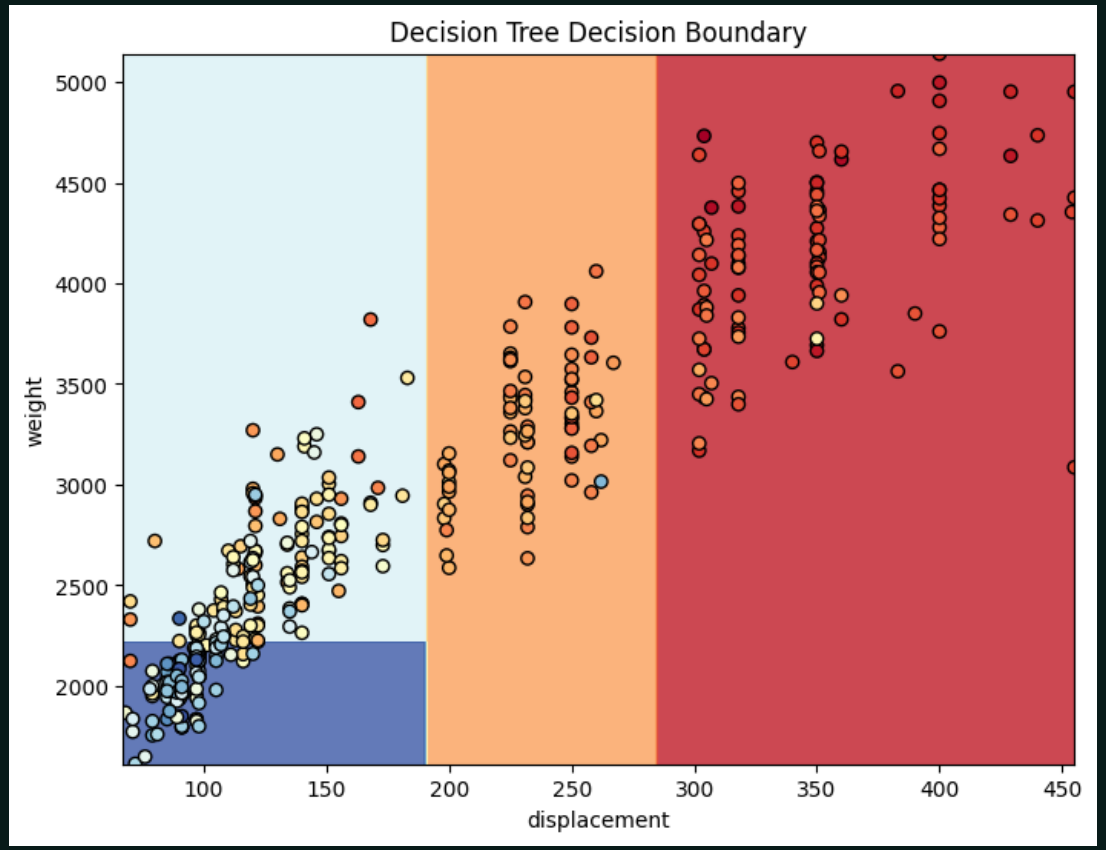
- Splitting Variables (What)
- Split Points (Where)
- Splitting Criteria (Why/How)

- Decision Tree: Estimate MGP



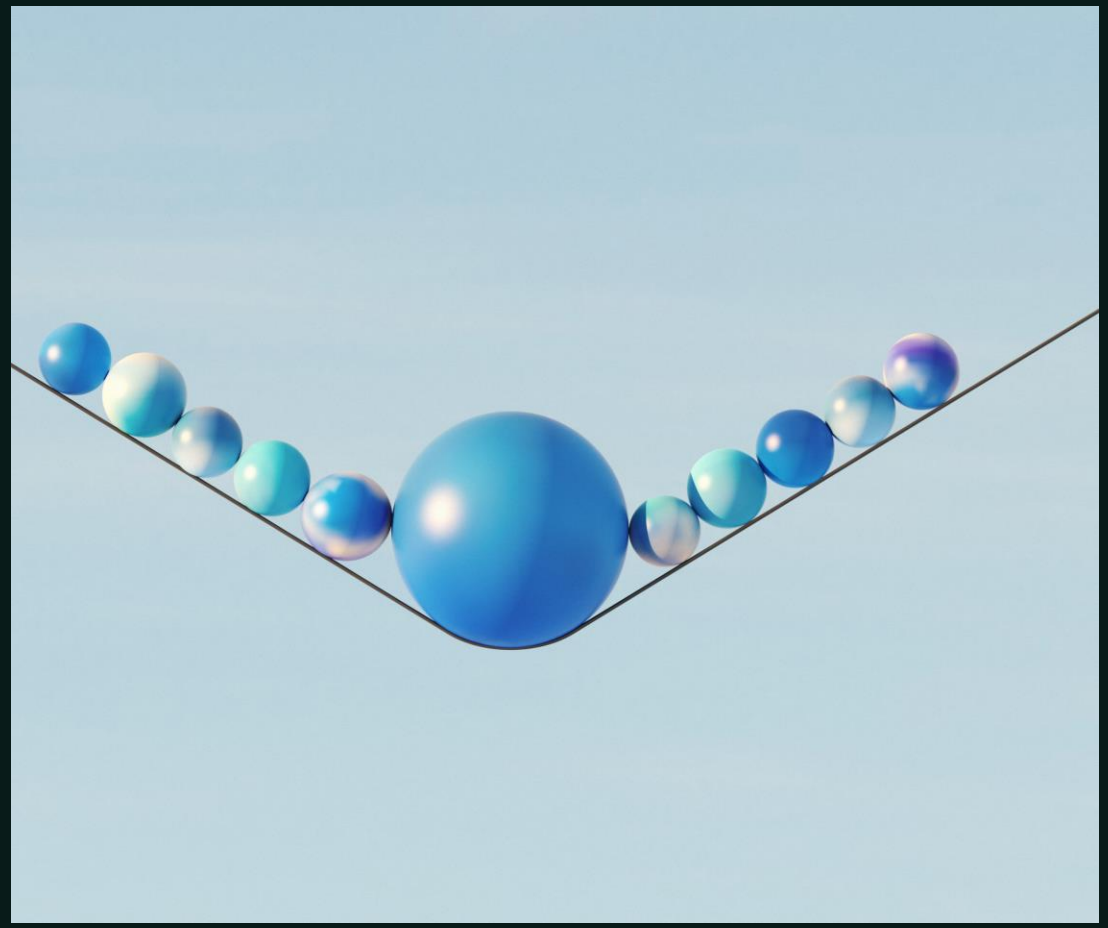
CART Decision Boundaries

- Splits form orthogonal decision regions.
- Splits spanning the space come first.
- Early variables → important



Mechanics of CART

- How to determine which variables?
- Which questions to ask first?
- How to determine split points?
- What process optimizes the decision-making?



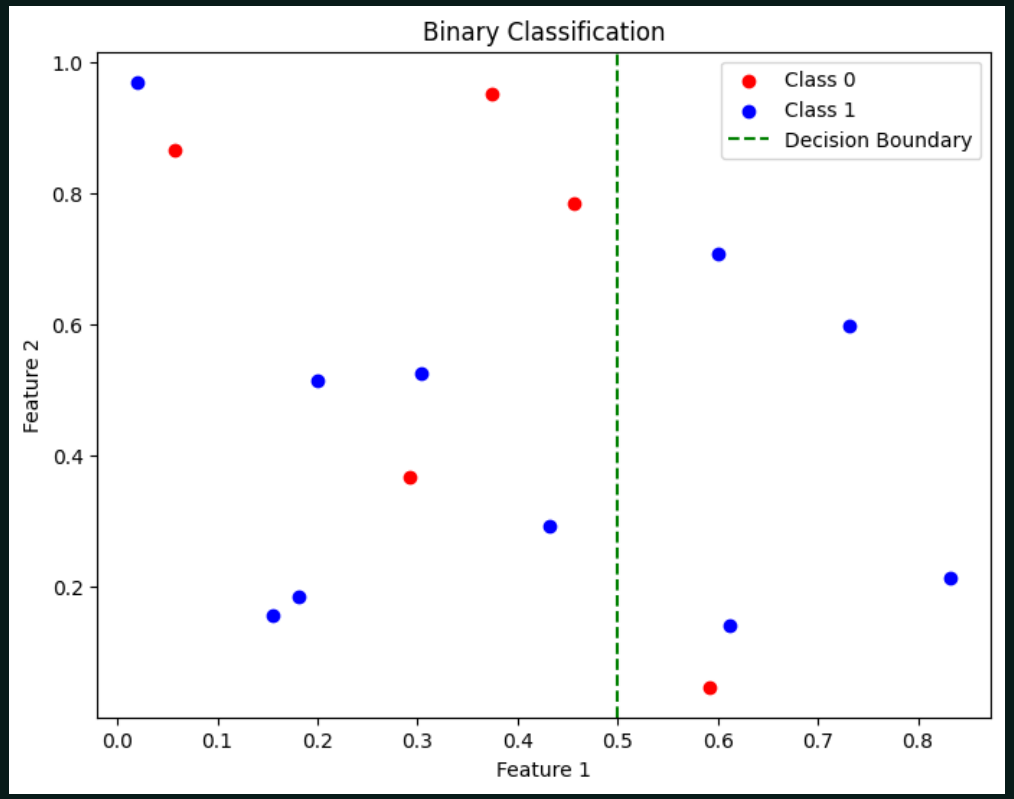
CART: Optimizing Splits (Classification)

GINI IMPURITY

- Quantifies the probability of misclassifying a randomly chosen data point if it's labeled according to the class distribution.
- A lower Gini Impurity (closer to 0) indicates a purer node (e.g., all one class)

$$G = 1 - \sum_{i=1}^{C} p_i^2$$

IMPURITY EXAMPLE



CART: Optimization Steps

$$G = 1 - \sum_{i=1}^{C} p_i^2$$

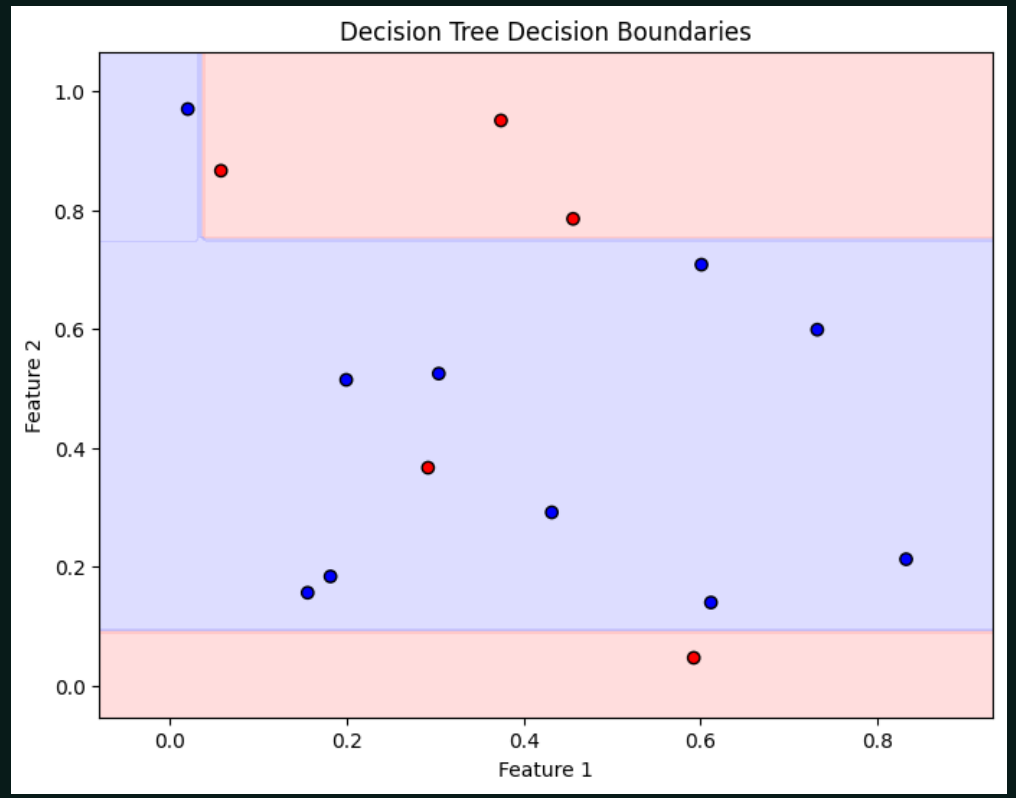
GINI OPTIMIZATION

1. Evaluate all possible splits
   a) Median between continuous values
   b) Subsets/groupings of categorical
2. Partition the data by split
3. Compute Gini impurity by branch
4. Calculate weighted impurity

$$G_{\text{split}} = \frac{n_L}{n} \cdot G_L + \frac{n_R}{n} \cdot G_R$$

5. Choose split by min. impurity

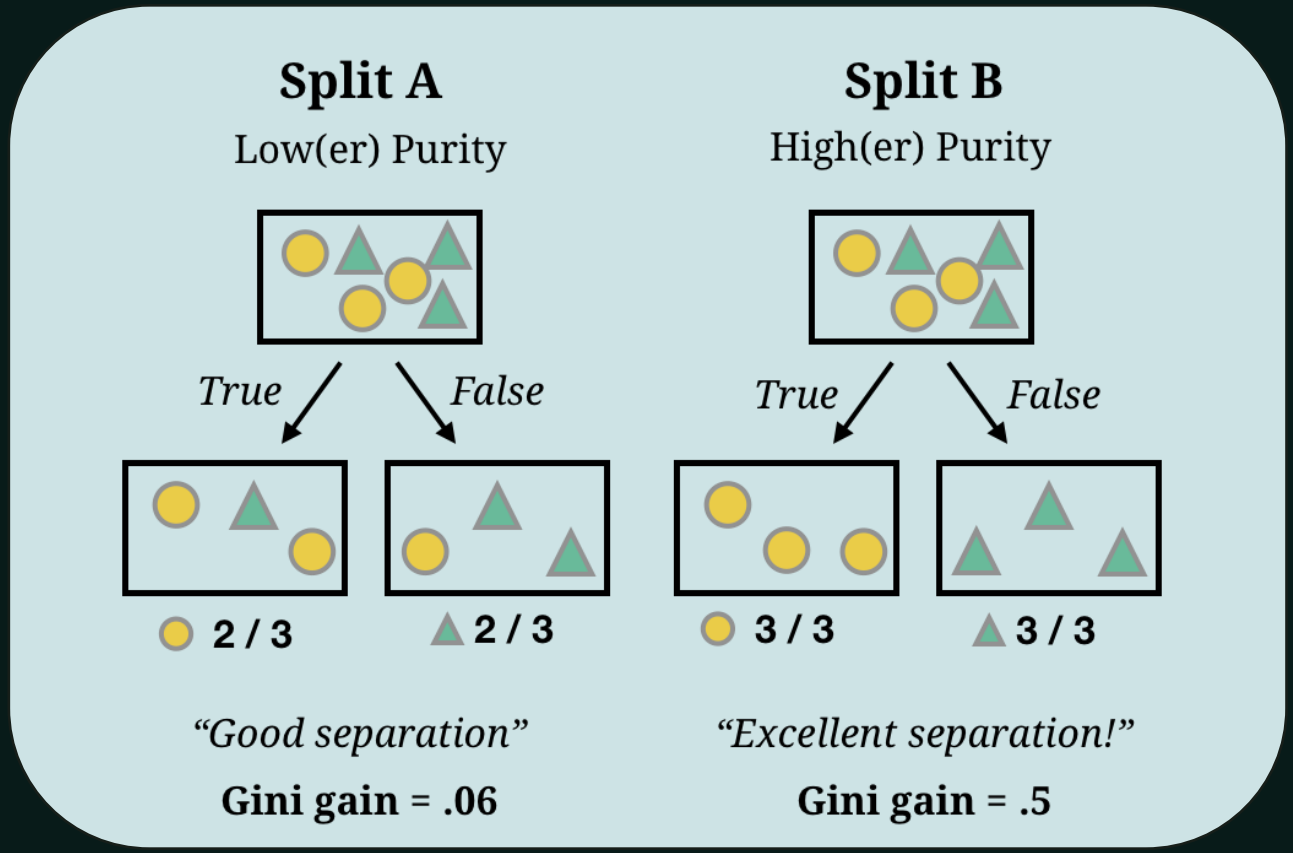
BINARY CLASSIFICATION



Other Considerations

PARAMETERS ET. AL

- When to stop splitting?
- Depth of the tree?
- Control for complexity.
- Data encoding.
- Data preparation.
- Feature selection.



CART: Benefits and Limitations

BENEFITS

- Both Classification and Regression
- Scale Invariant (rank-based)
- Learns Non-Linear Relationships
- Interpretable
- Mixed Variable Types

LIMITATIONS

- Low Performing
- High Variance
- Easily Overfit

Random Forests

Overcoming CART's Limitations

But first.. a little game!

Ensemble Methods

- Combine predictions from multiple models to produce more accurate / more stable results.
- Typically, a collection of “weak” learners

Random Forest

- An ensemble of randomized CART decision trees.
- Combining trees beneficial if uncorrelated.
- Two-part randomization.

Recall: CART Limitations

CART

- High variance
- Easy to overfit.

RANDOM FORESTS

- Decreased variance (ensembling)
- Less sensitive to outliers

Random Forest Randomizations

BOOTSTRAPPING

- For each tree, data is sampled with replacement
- Sampled data: In-bag
- Otherwise: Out-of-bag
- P(In-Bag) -->

$$1 - (1 - \frac{1}{n})^n \to 1 - \frac{1}{e} \approx 0.632$$

RANDOM FEATURE SELECTION

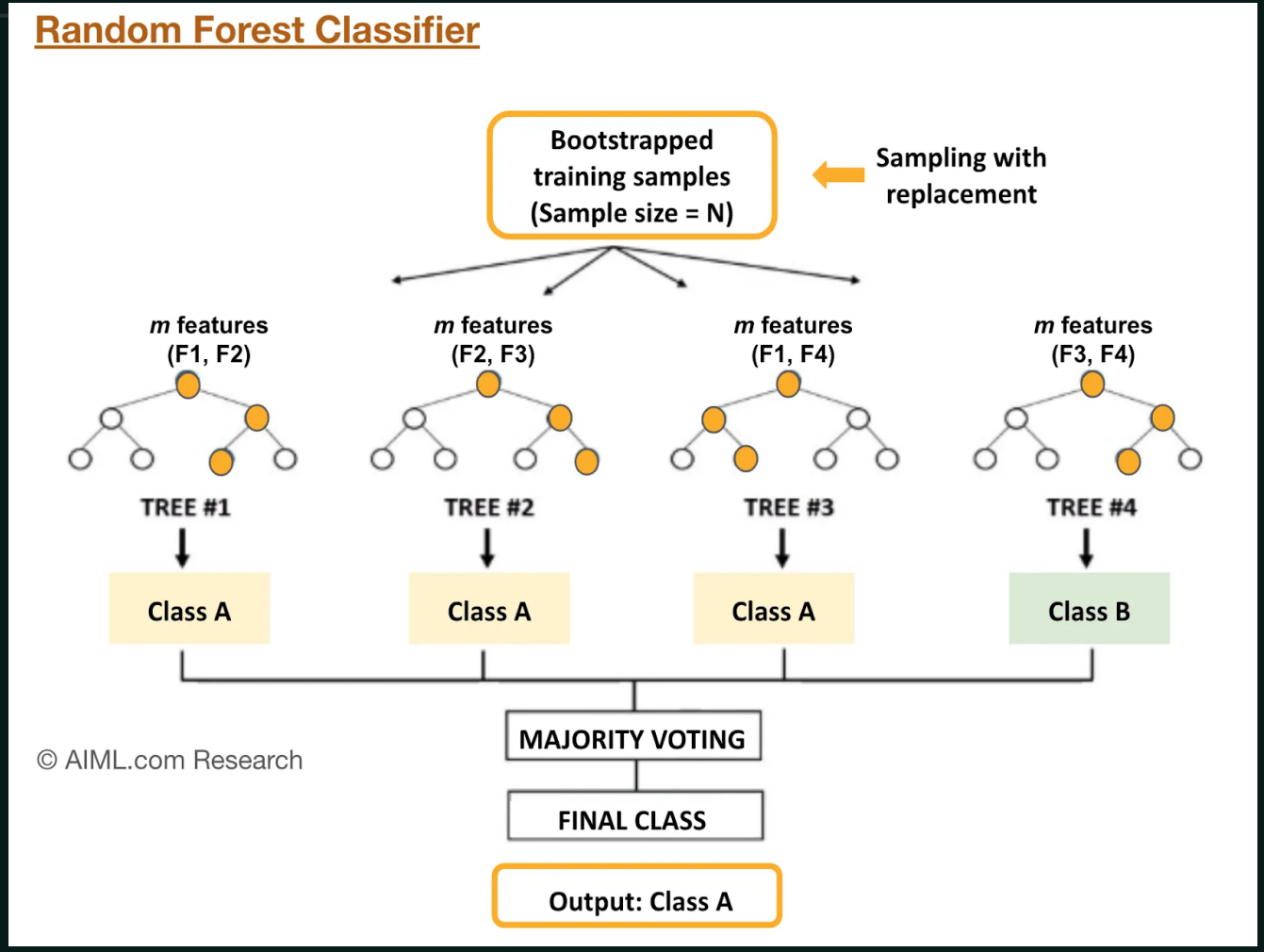
- At each split, *m* variables considered
- For classification: *m = sqrt(d)*
- For regression: *m = (1/3)d*

Out-of-Bag Points

- OOB pts. unseen by about 37% of trees
- Serval as an internal validation set.
- Used to estimate generalization error.
- Can serve as cross-validation for hyperparameter tuning

Random Forest Predictions

- Each tree provides one vote
- Unweighted majority voting
  - Weights implicitly defined in trees
- Averaging for regression



Benefits of Random Forests

- Classification and regression
- Mixed variable types
- Estimate of generalization error
- Trivially parallelizable
- Scale invariant
- Insensitive to outliers in predictor space
- Model non-linear relationships
- Natural produce a measure of similarity

Random Forest Proximities

"[Proximities] are one of the most useful tools in random forests."

--Leo Breiman

Original description:

"The proximities originally formed a NxN matrix. After a tree is grown, put all of the data, both training and oob, down the tree. If cases k and n are in the same terminal node increase their proximity by one. At the end, normalize the proximities by dividing by the number of trees."

https://www.stat.berkeley.edu/~breiman/RandomForests/cc_home.htm#:~:text=few%20data%20sets.-,Proximities,by%20the%20number%20of%20trees.

Proximities in a Nutshell

"Proximities don't just measure the similarity of the variables---they also take into account the importance of the variables."

"Two cases that have quite different predictor variables might have large proximity if they differ only on variables that are not important."

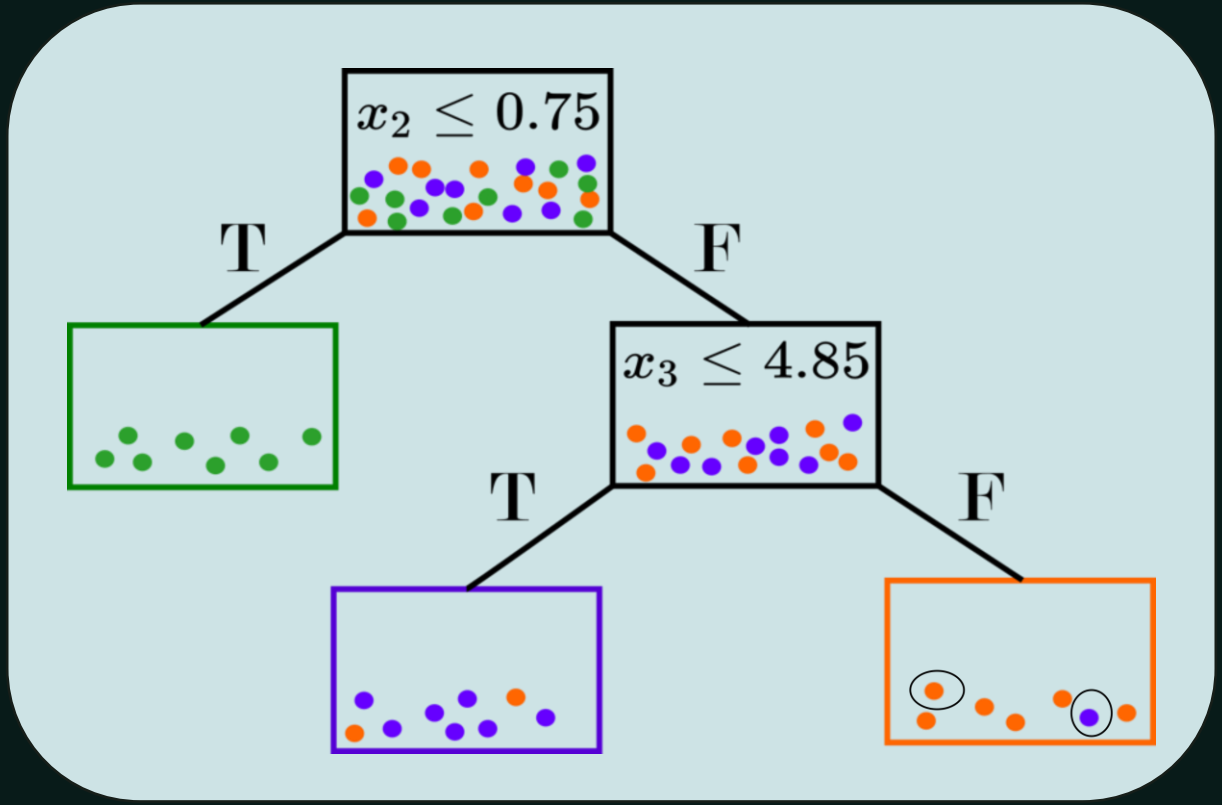
"Two cases that have quite similar values of the predictor variables might have small proximity if they differ on inputs that are important."

--Adele Cutler

What are Random Forest Proximities

PROXIMITIES AS A METRIC

- A measure of "closeness"
- Supervised, but not class-conditional
- Based on splits (optimized over responses)
- Natural incorporation of variable importance



Applications of Proximities

Visualization

Imputation

Outlier Detection

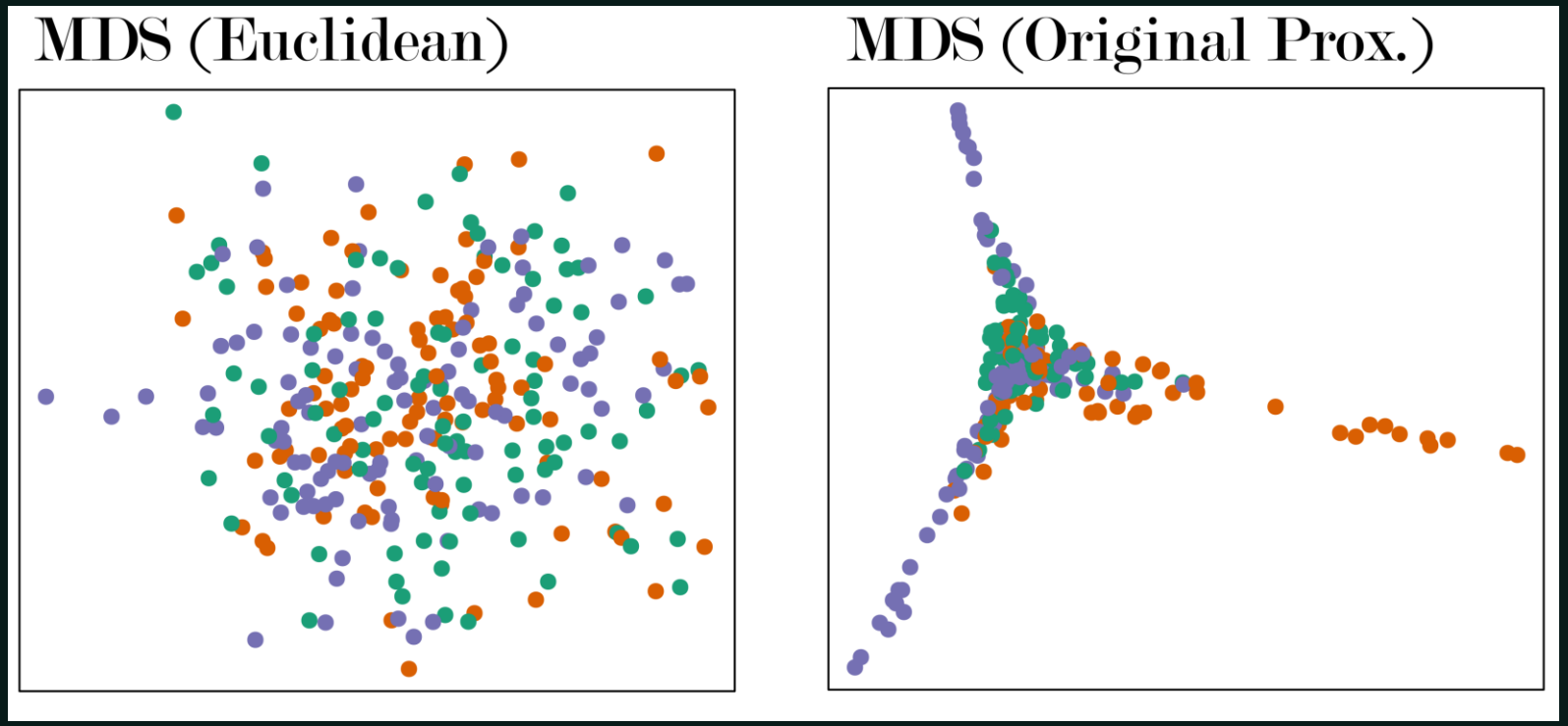
Uncertainty Quantification

Manifold Learning / Alignment




Other Proximity Considerations

- Overfit if use all training data
  - Trees grown until pure (typically)
  - In-bag points of different classes always in different nodes
  - Exaggerate class separation



A random sample of 300 points generated from a bivariate normal distribution was randomly assigned one of three classes. MDS was applied to 1 – proximities.

Proximities as Neighbor-based Predictor

What do we want?

- The similarity measure to encapsulate the supervised learning from the random forest!
- E.g., we want a proximity-weighted predictor to match the RF OOB predictions.
- This is **not the case** with the original definition, even when limiting it to OOB points only.

Why does this not work?

- The voting mechanism in random forests considers all training instances, not just pairwise relationships.

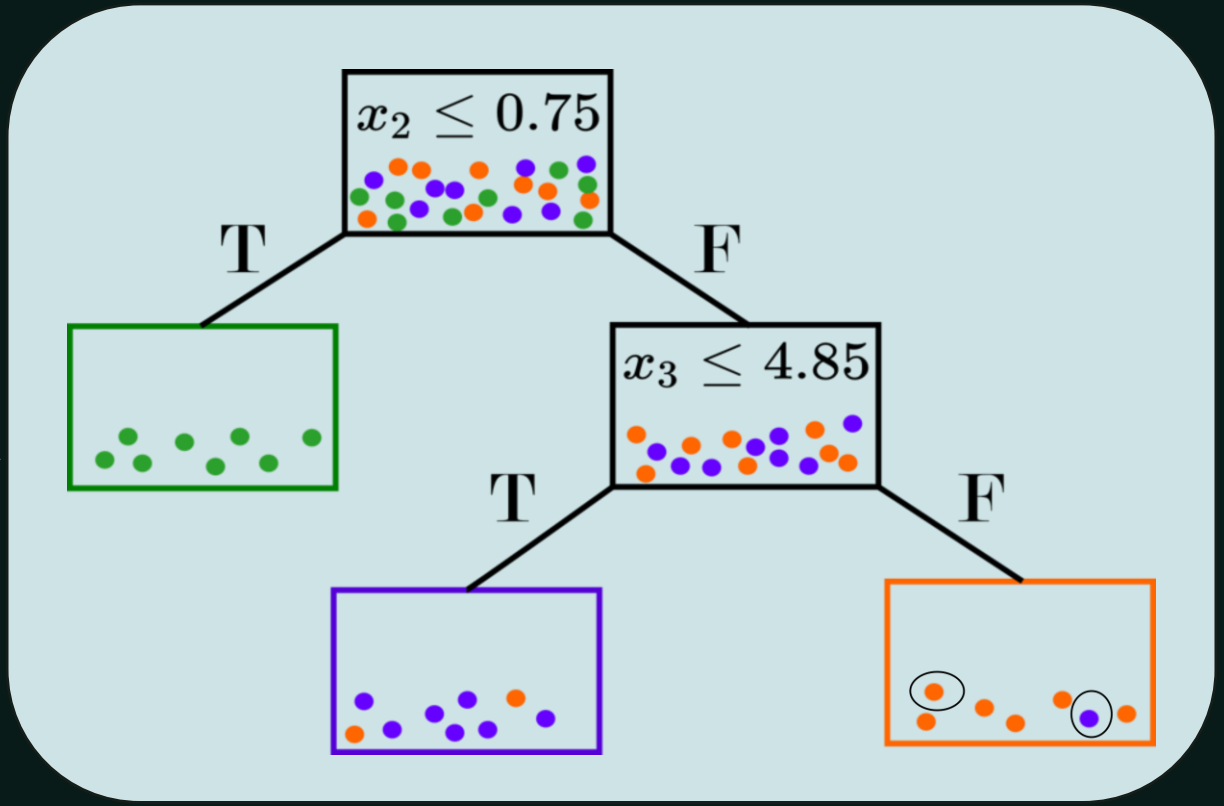
Similar to SVM Predictions:

$$\hat{y}_i(p) = \sum_{j=1}^{n} p(i,j) y_j$$

Accuracy Preserving Proximities

ACCOUNT FOR PREDICTION

- Proximities to be defined between an OOB point and all “similar” training points.
- Tree-wise proximities proportionate to size of terminal node.
- Proximity weighted predictor matches OOB or test predictions.



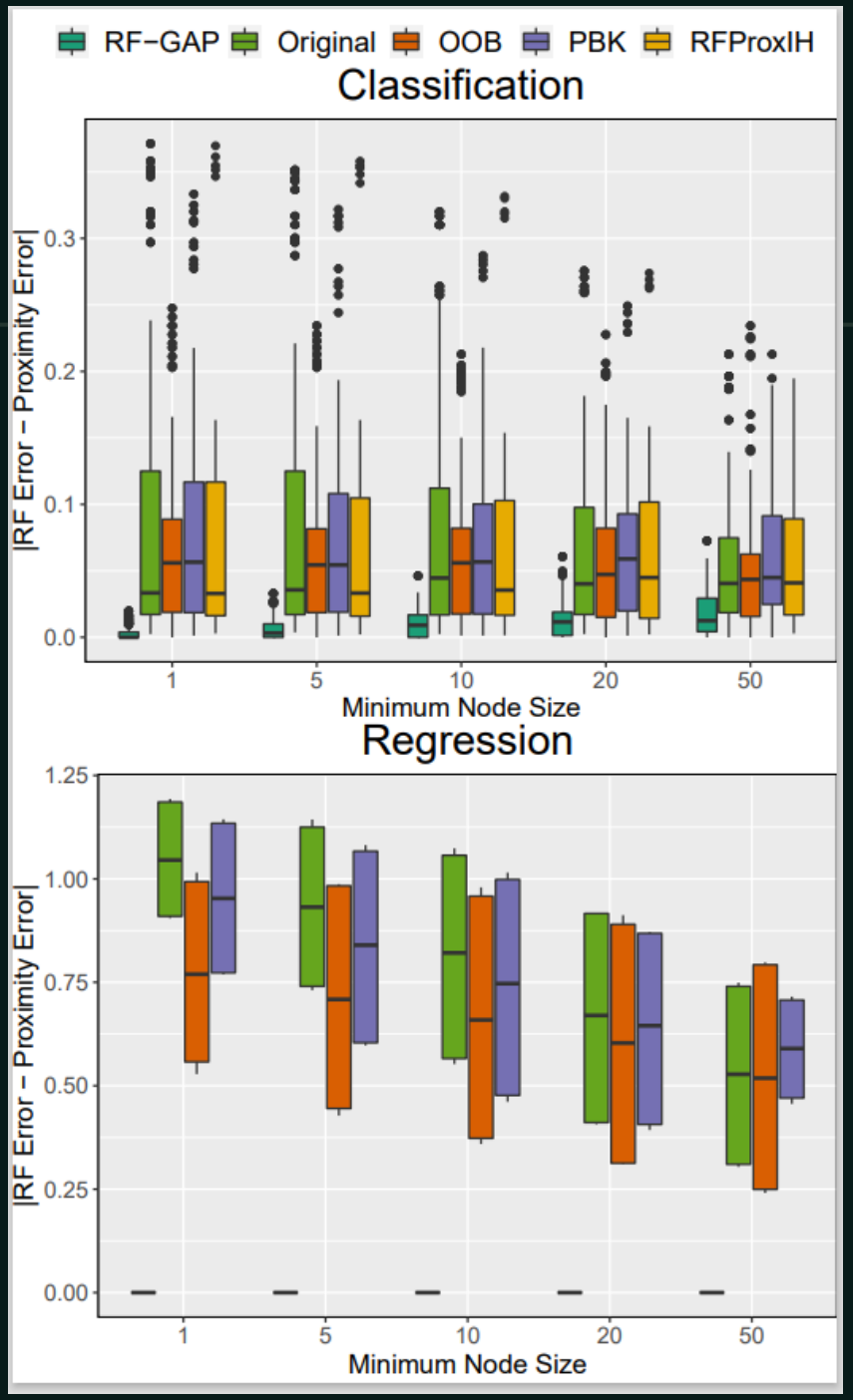
Random Forest Geometry- and Accuracy-Preserving Proximities

- **T**: Set of trees in the forest ($|T| = T$)
- **S_i**: Trees where obs. *i* is OOB
- **$J_i(t)$**: In-bag indices in node with *i* in tree *t*
- **$M_i(t)$**: Multiset of in-bag indices in *i*'s terminal node
- **$c_j(t)$**: In-bag count of obs. J in tree t.

$$p_{GAP}(i,j) = \frac{1}{|S_i|} \sum_{t \in S_i} \frac{c_j(t) \cdot I\left(j \in J_i(t)\right)}{|M_i(t)|}.$$

Proximity-Weighted Errors

- As desired, RF predictions match proximity predictions
- (Results aggregated across 24 datasets / 10 repetitions)



RF-GAP Proximities Notes

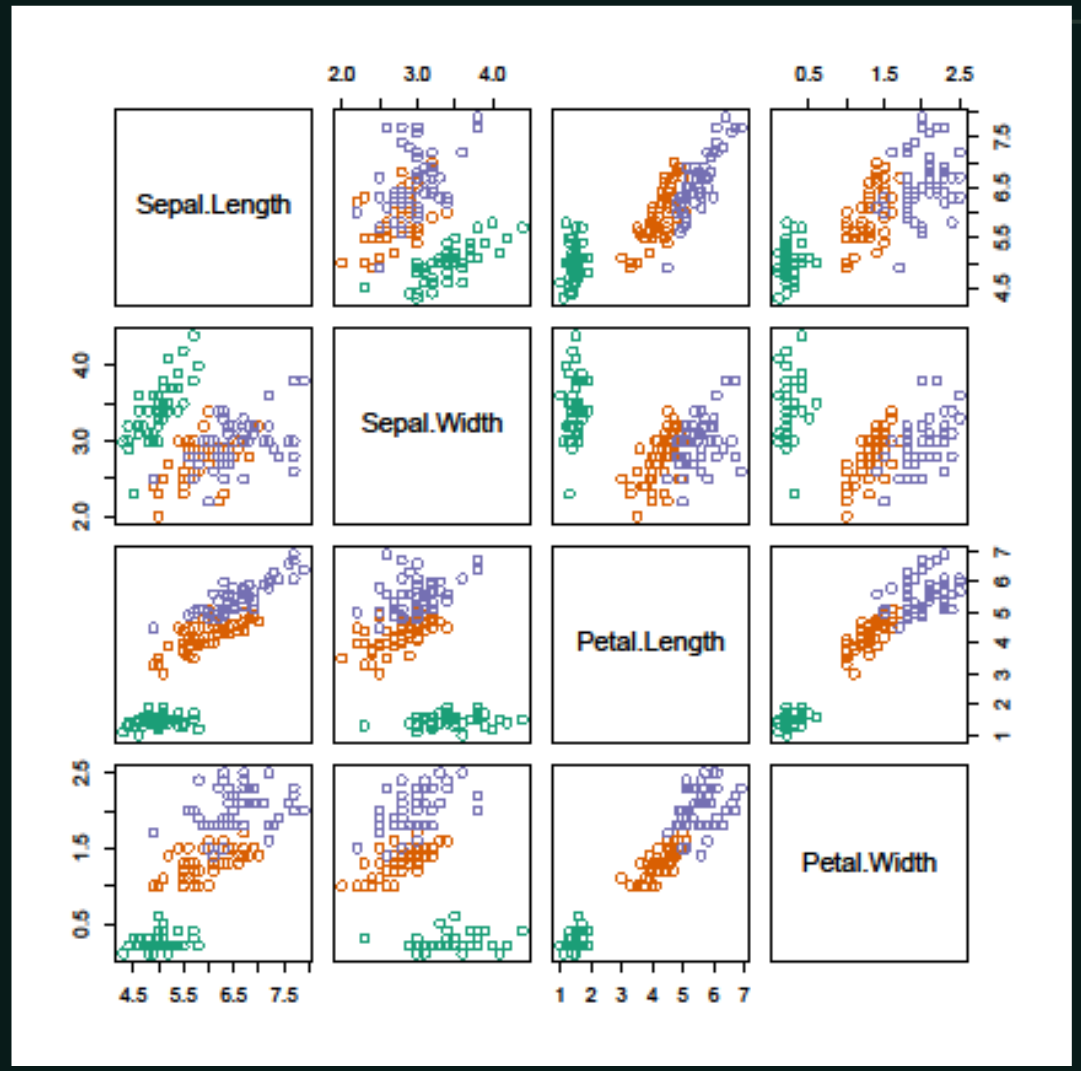
- RF-GAP proximities are not symmetric!
- By design, p(i, i) = 0 to serve as proper weights for RF predictions.
- For some applications, we must reassign self-similarity and symmetrize.

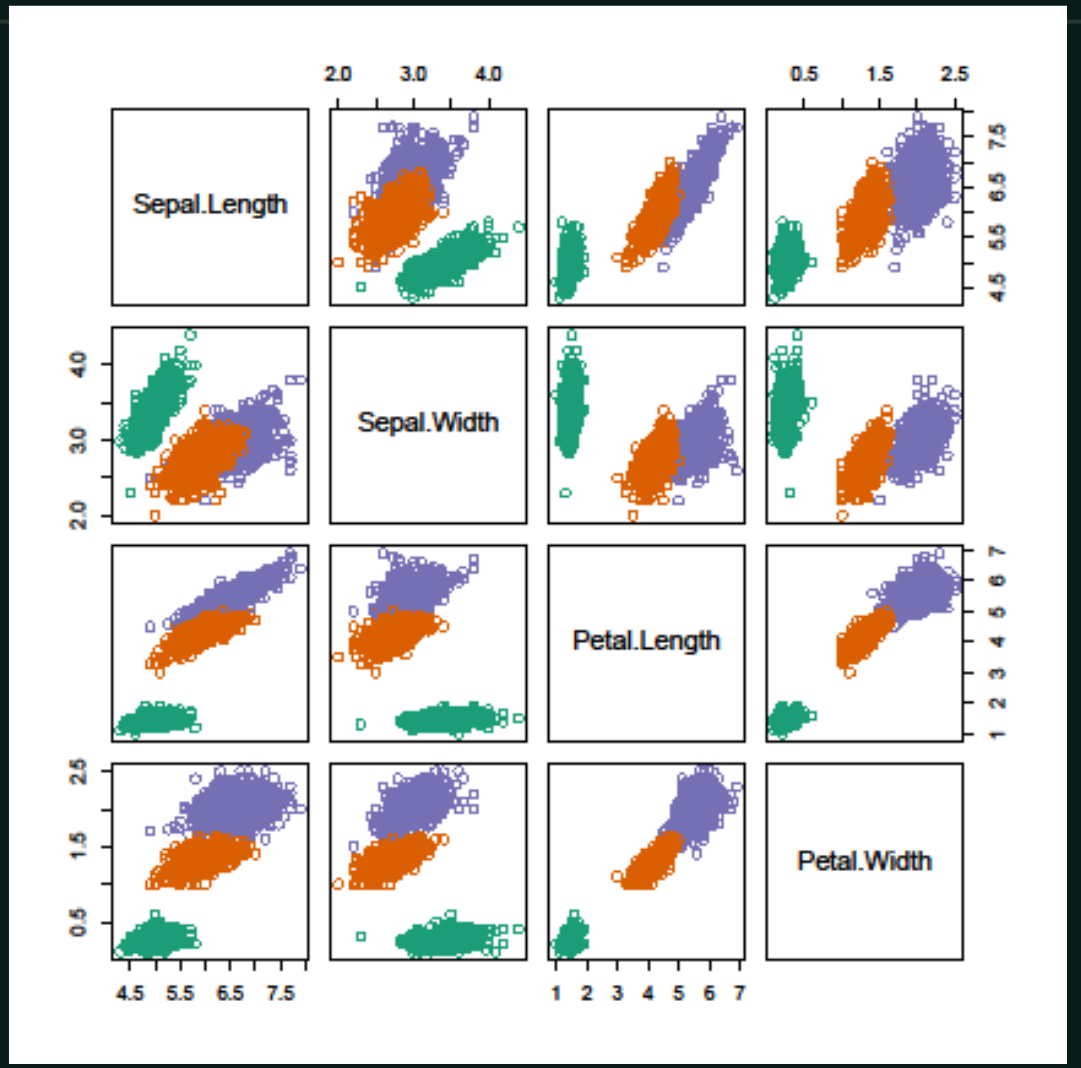
$$\begin{cases} \dfrac{1}{|\bar{S}_i|} \displaystyle\sum_{t \in \bar{S}_i} \dfrac{c_i(t)}{|M_i(t)|}, & j = i, \\ \dfrac{1}{|S_i|} \displaystyle\sum_{t \in S_i} \dfrac{c_j(t)\, I\left(j \in J_i(t)\right)}{|M_i(t)|}, & j \neq i, \end{cases}$$

- This guarantees that self-similarity is maximal but on the same scale.

Bonus Applications

Oversampling

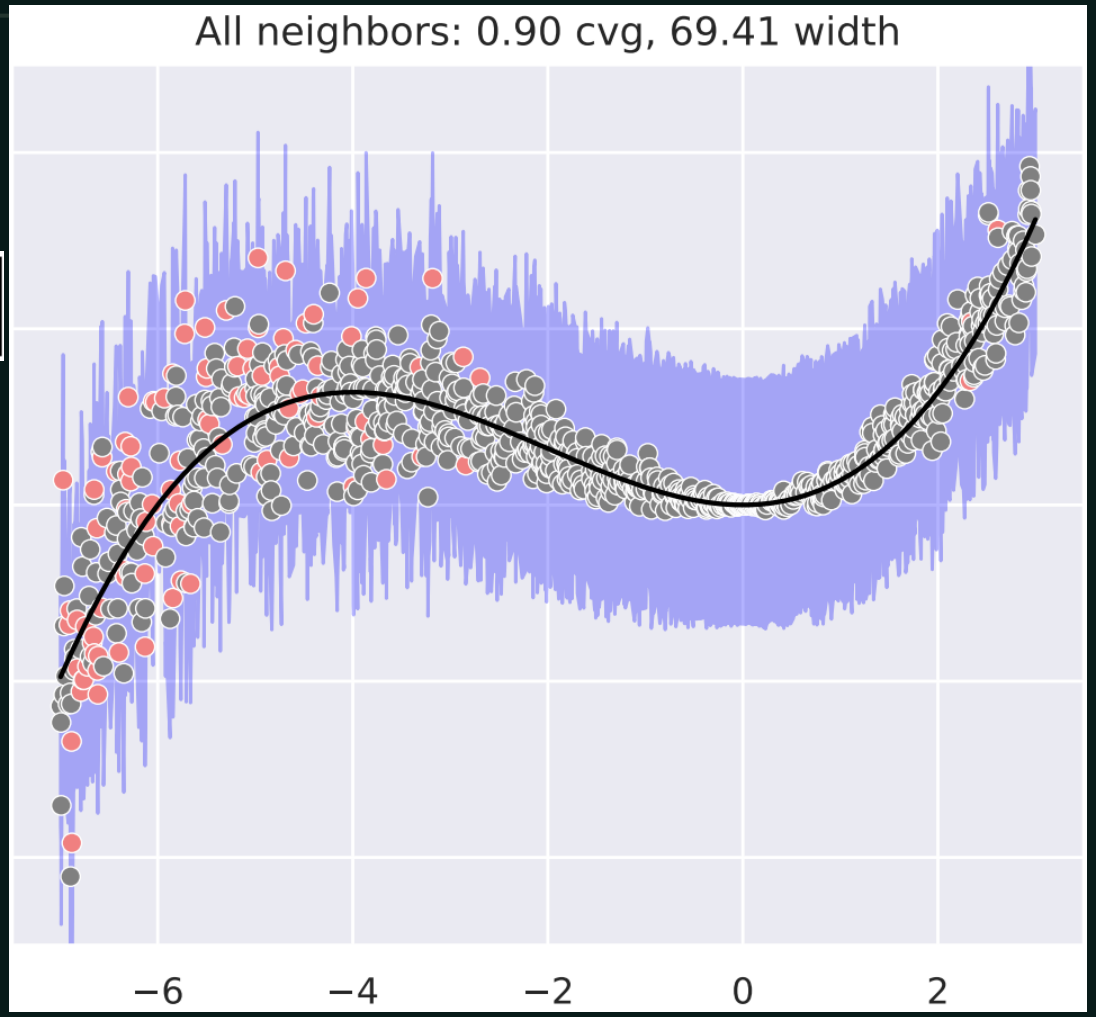




Intervals from Out-of-Bag Error Distribution (Haozhe Zhang and Nordman, 2020)

$$1 - \alpha \approx \mathbb{P}\left[D_{[n,\alpha/2]} \leq D \leq D_{[n,1-\alpha/2]}\right]$$

$$= \mathbb{P}\left[\widehat{Y} + D_{[n,\alpha/2]} \leq Y \leq \widehat{Y} + D_{[n,1-\alpha/2]}\right]$$

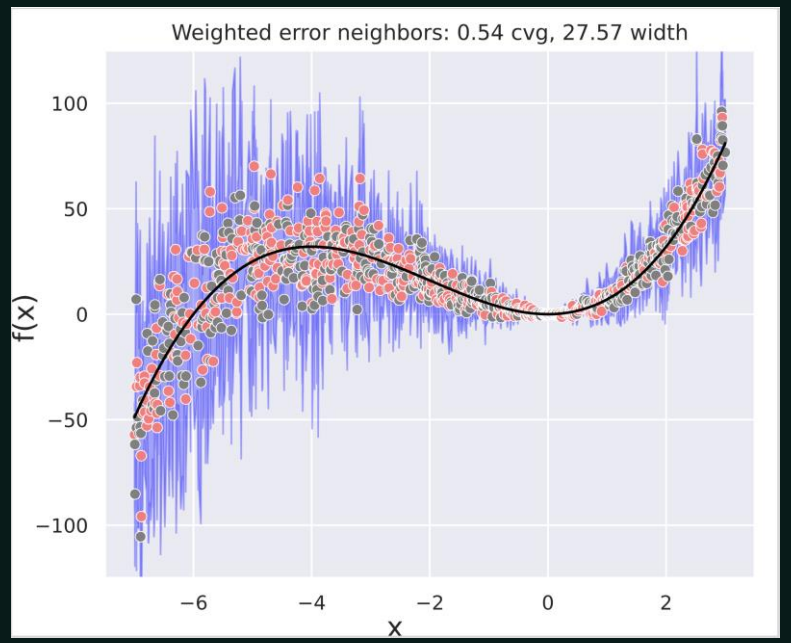


Regression – Prediction Intervals

Random Forest Interval Residual Estimation (RF-FIRE)

(1) Weighted out-of-bag errors:

$$\hat{y}_0 \pm \sum_{i=1}^{n} w_{0i} L(y_i, \hat{y}_i)$$



(2) Localized error distribution:

$$\left[\hat{y}_i - \mathcal{D}^{k_i}_{\alpha/2}, \quad \hat{y}_i + \mathcal{D}^{k_i}_{1-\alpha/2}\right]$$

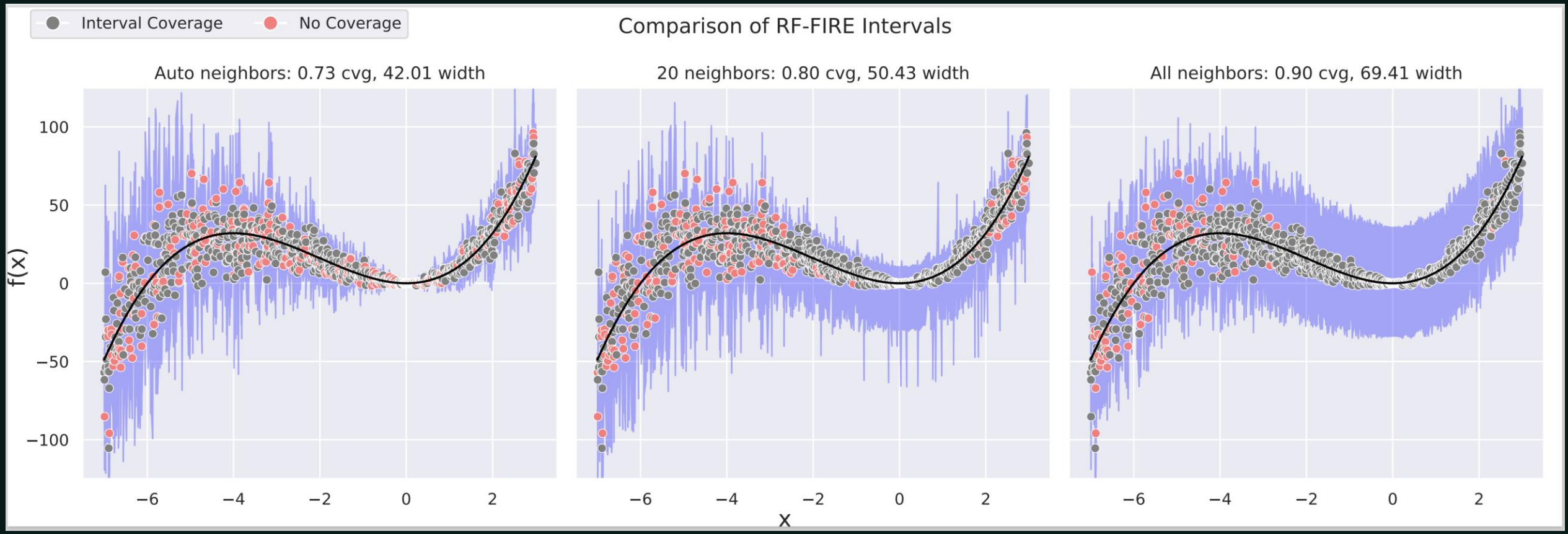
Where:

- $\mathcal{D}^{k_i}$ is the distribution of OOB errors limited to the k_i nearest* neighbors of x_i .

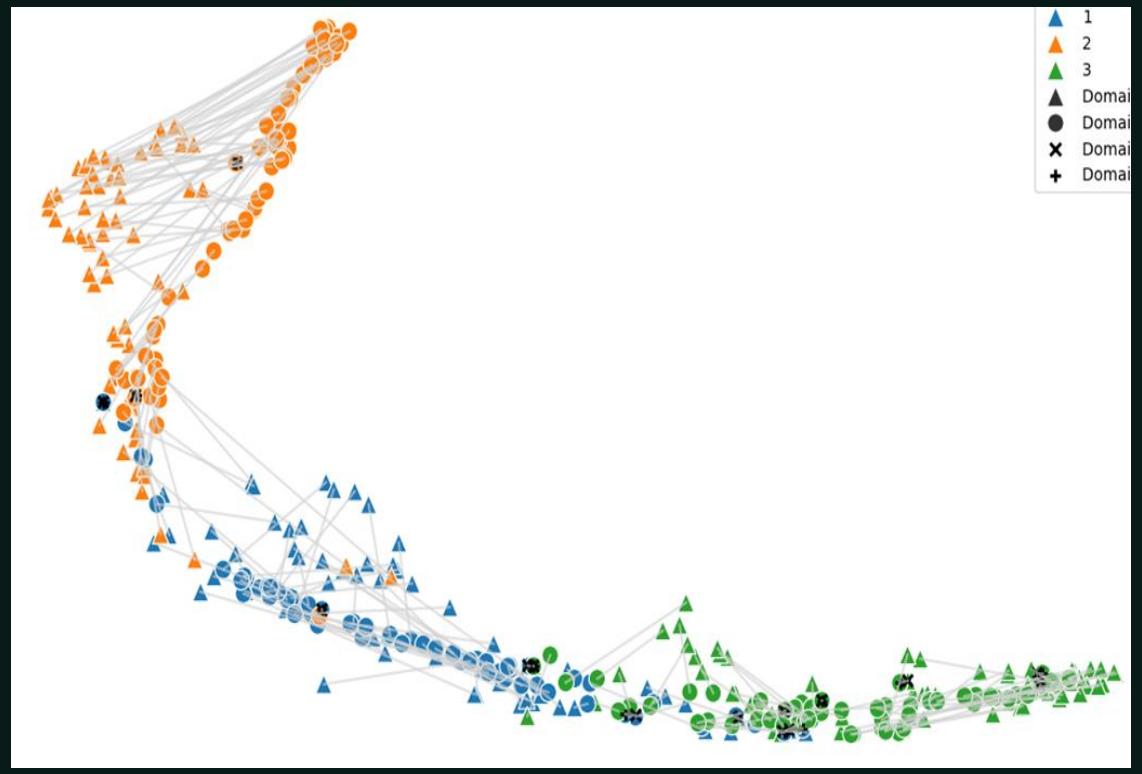
*Nearest based on RF-GAP proximity

BYU

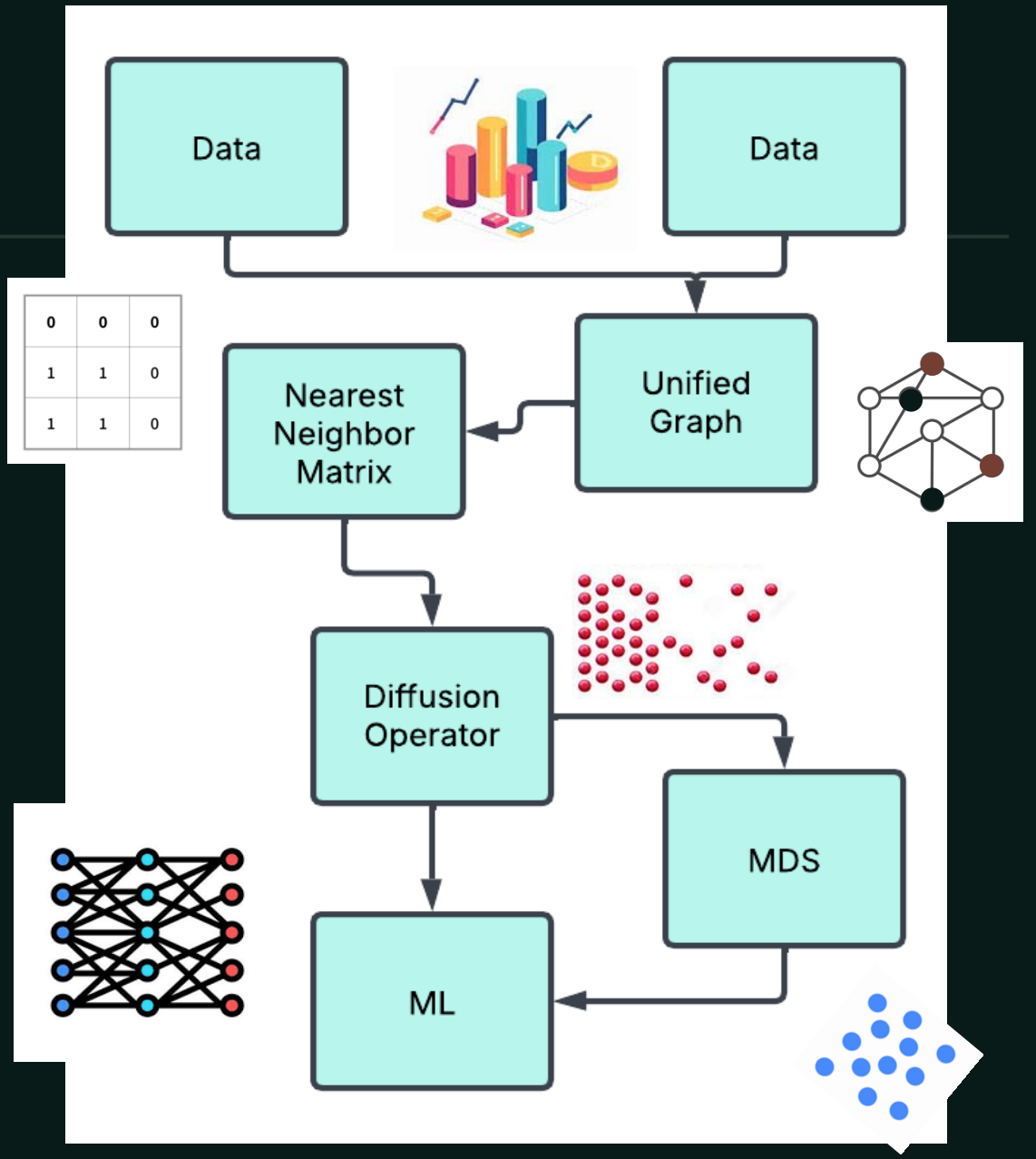
Regression – RF-FIRE (Localized Error Dist.)



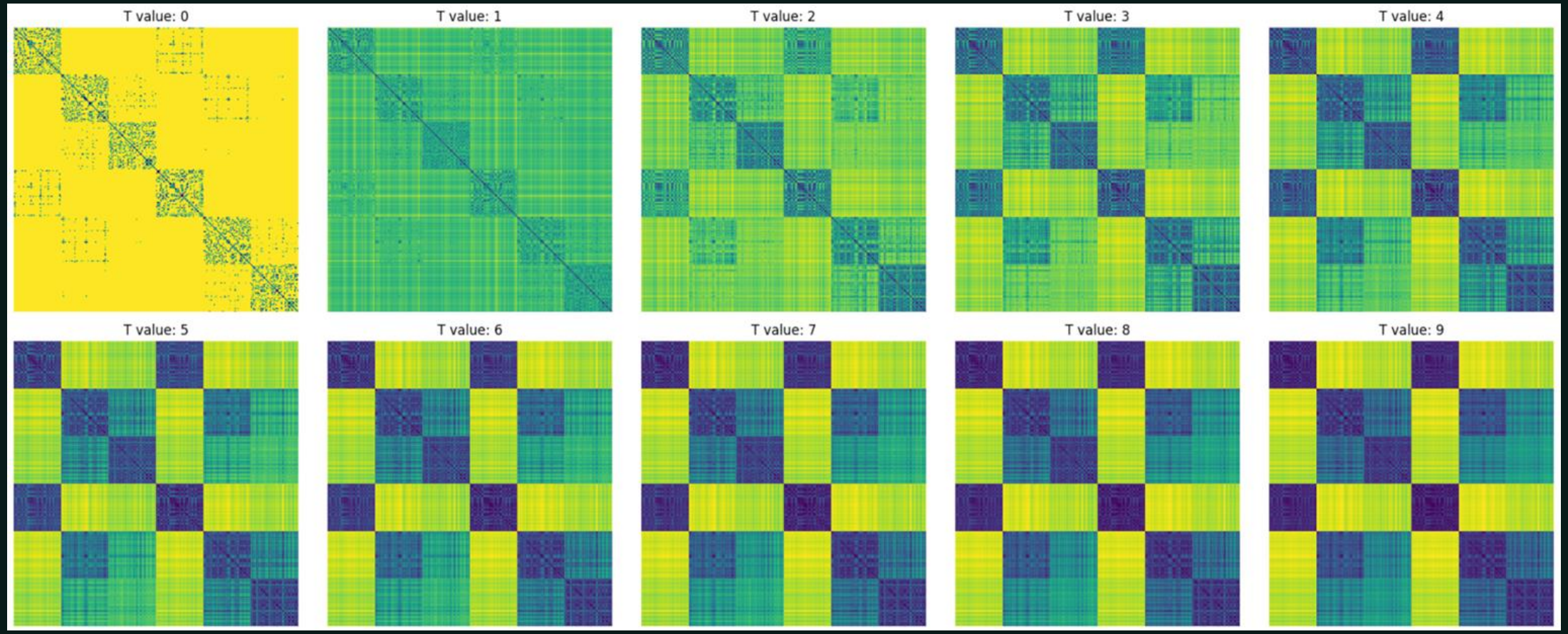
RF-Manifold Alignment



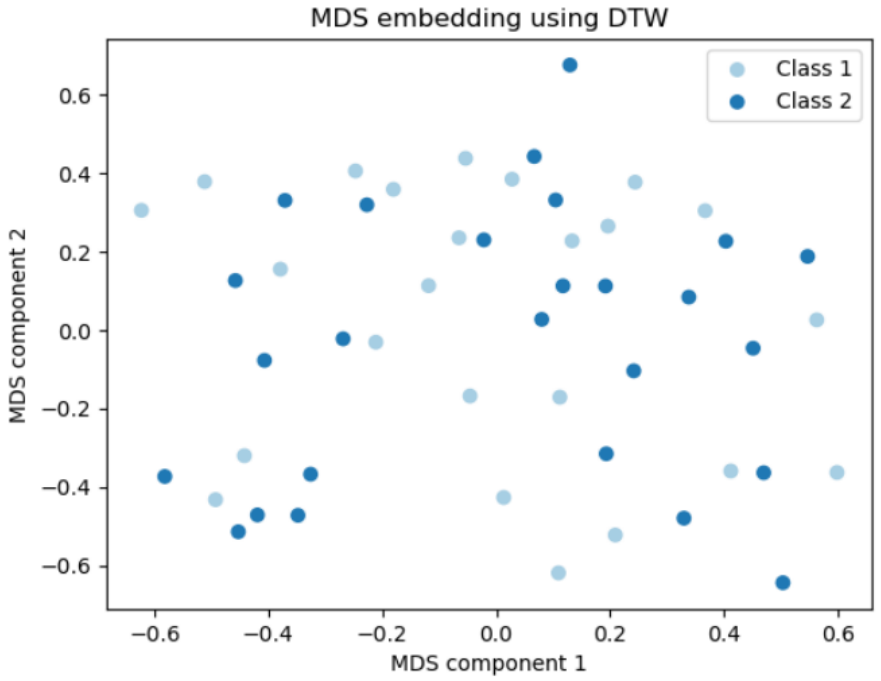
RF-MASH's resulting manifold on the seeds data set



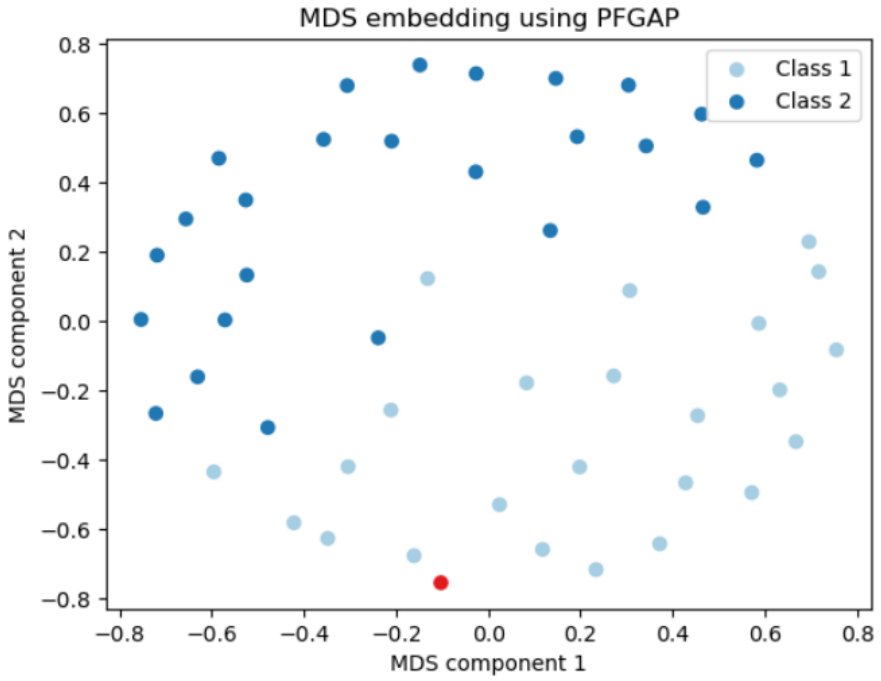
Diffusion over Combined Proximities



Time Series Classification – Proximity Forests

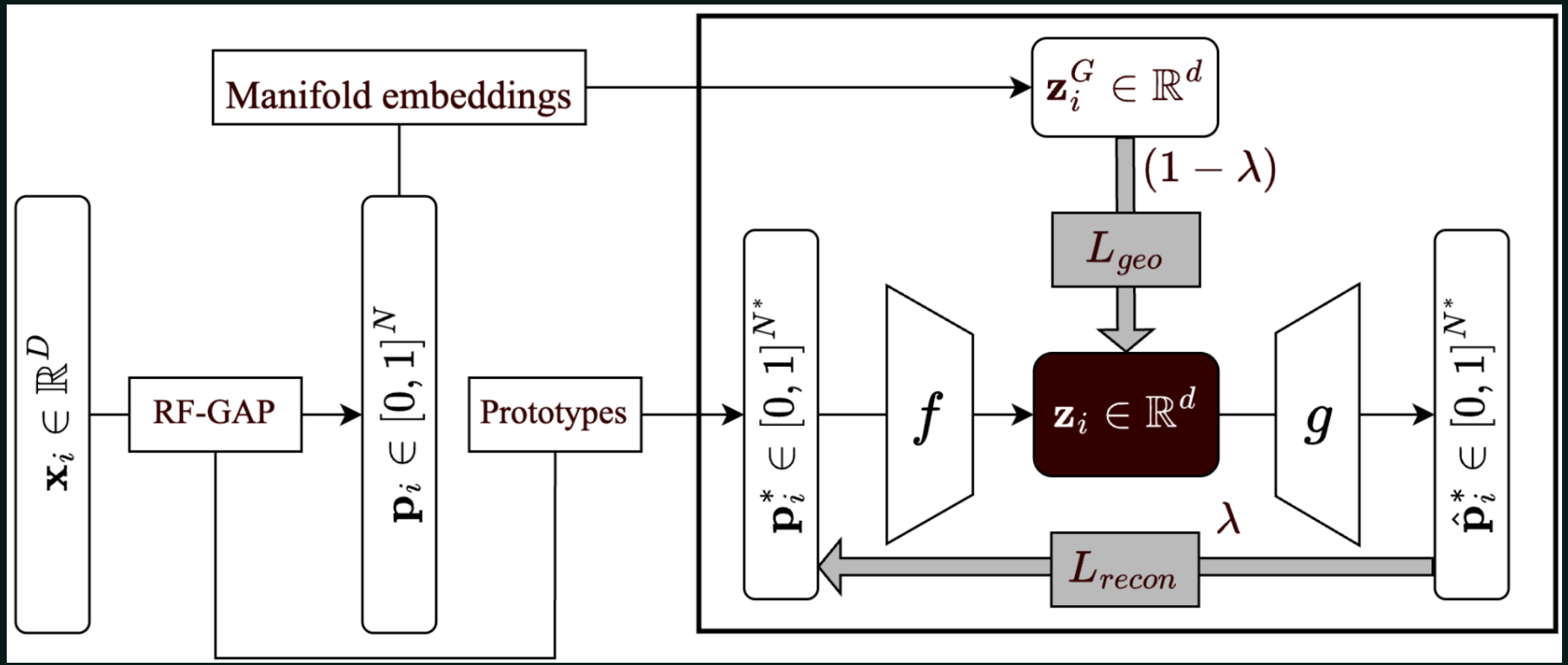


(a) MDS embedding of the *GunPoint* dataset using pairwise dissimilarity defined by dynamic time warping distances.

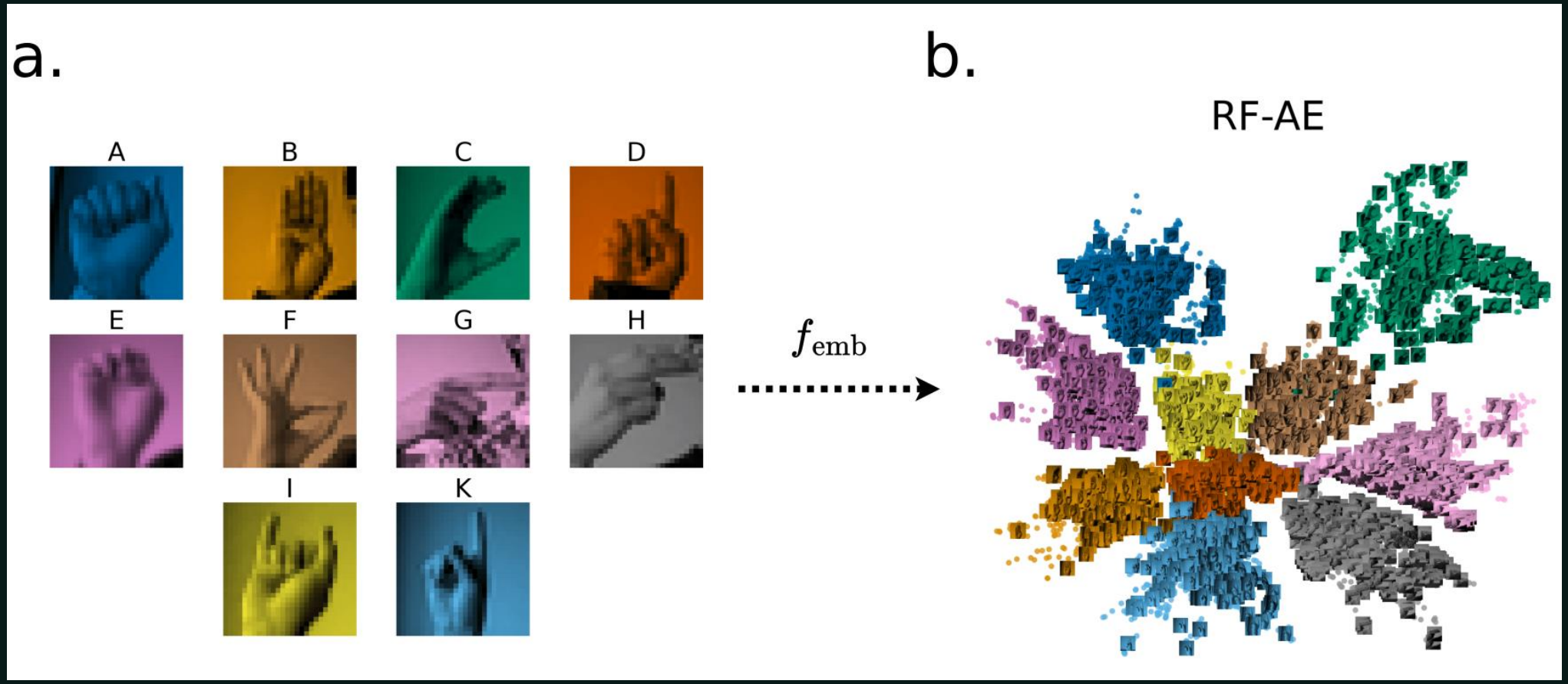


(b) MDS embedding of the *GunPoint* dataset using pairwise dissimilarities defined by PF-GAP. The point with the highest within-class outlier score is indicated in red and belongs to Class 2.

Random Forest Autoencoders



RF-AE Example



The way to get started is to quit talking and begin doing.

Walt Disney

Thank you

RF-GAP

RF-PHATE

Time Seres (PF-GAP)

RF-MA

RF-AE