Generalized Additive Models and Trees

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Overview

1. Preliminaries
2. Generalized Additive Models
3. Trees
4. Ensemble learning
   - Boosting
   - Loss functions and robustness
   - Bagging and Random Forests

Preliminaries

- We have covered two broad categories of methods for regression - the highly rigid linear methods and the very flexible local methods such as kNN.
- There exist an entire spectrum of methods that assuming some structured form for the unknown regression function in between these two extremes.

Generalized Additive Models

- A generalized additive model has the form:

$$E[Y|X_1, X_2, ..., X_p] = \alpha + \sum_{j=1}^{p} f_j(X_j)$$

- If f_j are expanded in terms of basis functions, this reduces to a least squares fit.
- For generalized additive models, we fit each function using a scatterplot smoother, e.g., cubic spline or kernel smoother.
- Penalized residual sum of squares is given as:

$$PRSS = \sum_{i=1}^{N} \left(y_i - \alpha - \sum_{j=1}^{p} f_j(X_j) \right)^2 + \sum_{j=1}^{p} \int f_j''(t_j)^2 dt_j$$

- First term is our standard sum squared error, and the right term is penalizes discontinuities (recall section on smoothing splines).

Fitting generalized additive models

- Each function f_j is a cubic spline of component X_j.
- To obtain unique solution, we impose a further convention that the functions average to zero over the data, i.e., $\sum_{i=1}^{N} f_j(x_{ij}) = 0 \forall j$
- Backfitting algorithm:
  1. Initialize $\hat{\alpha} = \frac{1}{N}\sum_{i=1}^{N} y_i, \hat{f}_j = 0$.
  2. Cycle through $1, 2, ...p, 1, 2, ..., p$

$$\hat{f}_j \longleftarrow S_j\left[\{y_i - \hat{\alpha} - \sum_{k\neq j}\hat{f}_k(x_{ik})\}_1^N\right]$$

$$\hat{f}_j \longleftarrow \hat{f}_j - \frac{1}{N}\sum_{i=1}^{N}\hat{f}_j(x_{ij})$$

- Conceptually, fitting a cubic smoothing spline S_j to the residual $y_i - \hat{\alpha} - \sum_{k\neq j}\hat{f}_k(x_{ik})$ for each f_j, and iterate until all $\hat{f}_j$s stabilize.

Extensions of Generalized Additive Models

- Note that we are not limited to cubic splines. E.g, local polynomial and kernel methods, linear regression, and surface smoothers etc. can be used with the appropriate choice of smoother S_j.
- GAMs can be used for classification as well, using the logit *link* function. For example, for binary classification:

$$\log \frac{P(Y=1|X)}{P(Y=0|X)} = \log \frac{P(Y=1|X)}{1-P(Y=1|X)} = \alpha + \sum_{j=1}^{p} f_j(X_j)$$

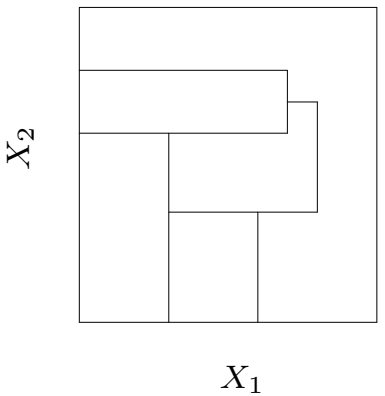
Very commonly used in medical research: outcomes encoded as 0 or 1 (e.g., death/relapse of disease).

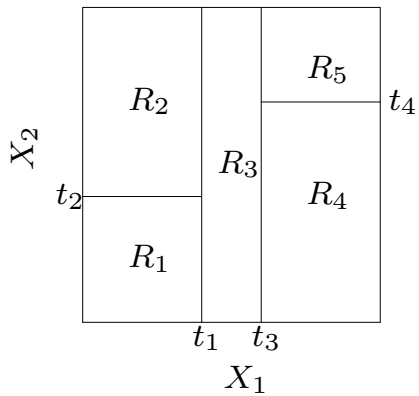
Tree-based methods

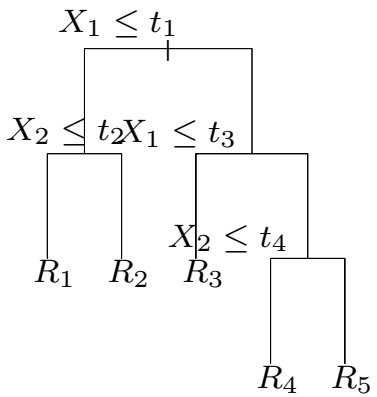
- Partition feature space into regions (e.g., rectangles for 2 features case), and simple model (e.g., constant) fitted into each rectangle.
- Classification And Regression Trees (CART)

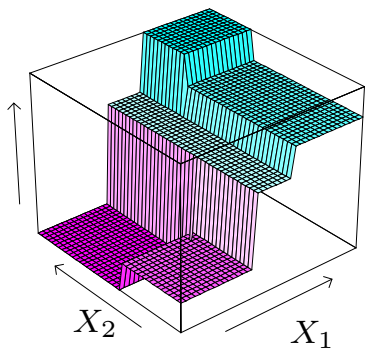
$$\hat{f}(X) = \sum_m c_m I\{(X_1, X_2) \in R_m\}$$

- Main question: How to decide on partitions/topology?









Regression tree fitting

- For CART, it is clear that each region should just be given by the average of the observations y_i in that region to minimize sum of squares.
- Best partition is usually not computationally tractable.
- Greedy algorithm: Start with all data, choose splitting variable X_j and split point s such that:

$$\min_{X_j, s} \left[\sum_{x_i \in R_1(X_j, s)} (y_i - c_1)^2 + \sum_{x_i \in R_2(X_j, s)} (y_i - c_2)^2 \right]$$

- For each X_j, splitting point s can be found quickly via scanning of the variables.
- This process is repeated for each region to grow the tree.
- Choice of tree size determines complexity of model - too large a tree results in overfitting, too small results in underfitting.

Cost-Complexity Tree Pruning

- Generate the tree until a minimum node size is achieved.
- Note: perfect performance on training data can always be obtained with an arbitrarily large tree, e.g., when the final 'leaf' nodes each contain only one training observation.
- Number of samples in a node is therefore an indicator of tree complexity.
- Let subtree $T \subset T_0$ be any tree that can be obtained by pruning T_0.
- Cost-complexity criterion:

$$C_\alpha(T) = \sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{c_m})^2 + \alpha |T|$$

- Find the subtree T_α that minimizes $C_\alpha(T)$. α controls complexity. Large α results in smaller tree.
- Weakest link pruning: successively collapse each node that produces the smallest increase in $\sum_{x_i \in R_m} (y_i - \hat{c_m})^2$.

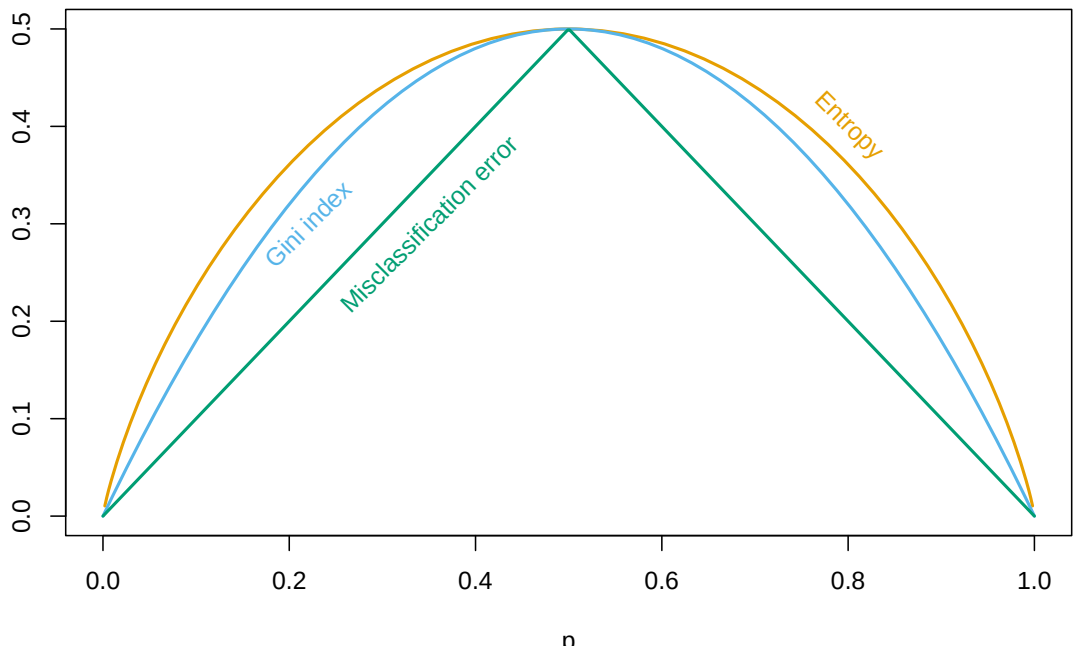
Classification Trees

- Instead of squared error, we need to use alternative *node impurity* measures:

  Misclassification error $1/N_m \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - p_{m\hat{k}(m)}$

  Gini index $\sum_{k \neq k'} p_{\hat{mk}} p_{\hat{mk'}}$

  Cross-entropy $-\sum_{k=1}^{K} p_{\hat{mk}} \log p_{\hat{mk}}$



Miscellaneous Issues with Trees

- Trees can be highly interpretable.
- Instability: small data changes can lead to very different splits.
- Lack of smoothness
- For some categorical problems, a misclassification in one category is more serious than another, e.g., it is better to have a false positive for a disease than a false negative. This can be handled by weighting the loss functions appropriately.

Example: Lab 2 revisited

- We will now play around with the metal/insulator classification problem in Lab 2.
- However, we will make a few changes. First, we will not bother with NaN values. Imputing values is ok for many other domains. In materials science, imputing arbitrary values is a recipe for disaster.
- Second, we will only select a smaller subset of elemental properties to construct our decision tree with. Namely, *'AtomicRadius'*, *'AtomicWeight'*, *'Column'*, *'Electronegativity'*, *'Row'*. These properties are available for most elements and we avoid obviously correlated features, e.g., AtomicRadius and AtomicVolume.

Decision Tree Regressor and Classifier in scikit-learn

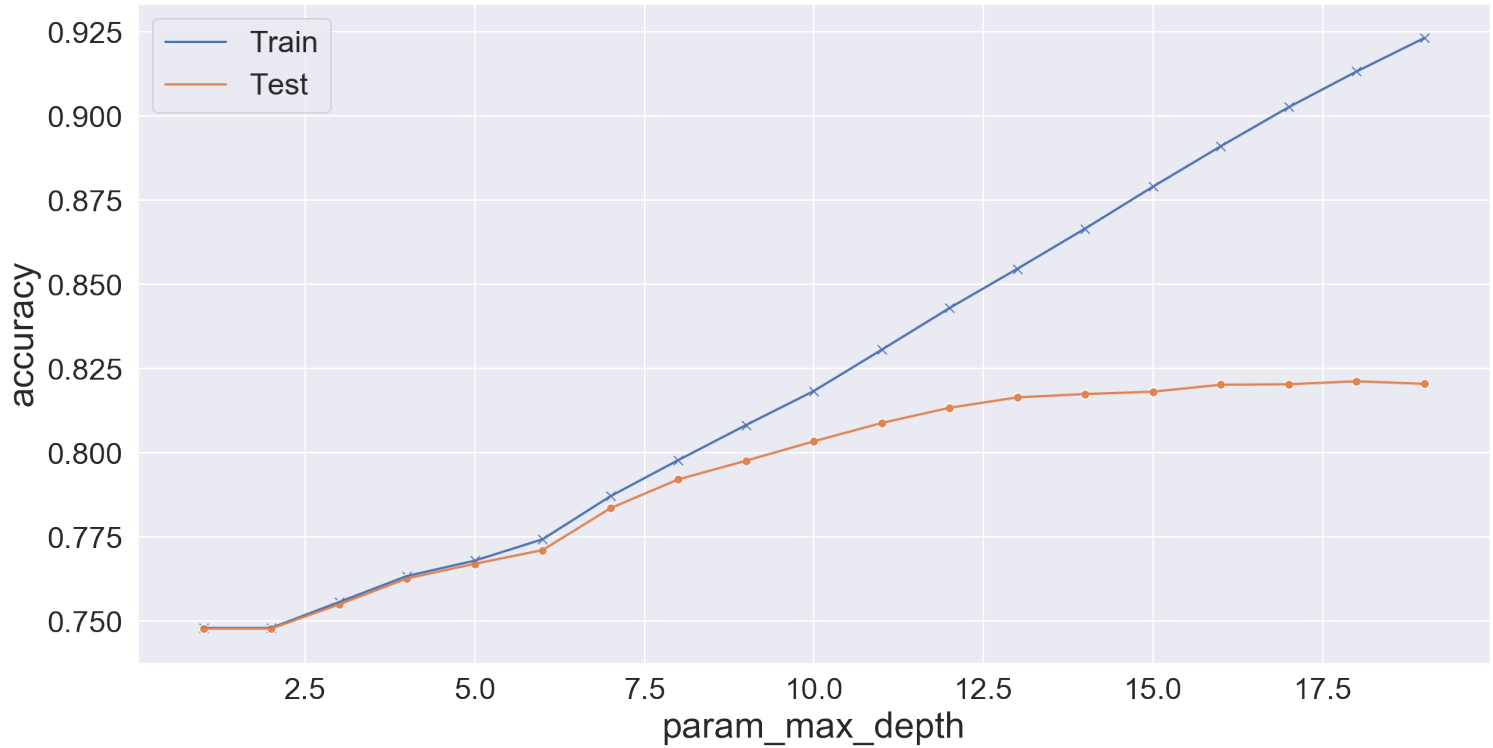
```
from sklearn.tree import DecisionTreeClassifier, DecisionTreeRegressor
from sklearn.model_selection import train_test_split
from sklearn.tree import export_text

x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=0.1)

decision_tree = DecisionTreeClassifier(criterion="entropy", random_state=0,
                                       max_depth=5)
decision_tree = decision_tree.fit(x_train, y_train)
train_accuracy = decision_tree.score(x_train, y_train)
test_accuracy = decision_tree.score(x_test, y_test)
r = export_text(decision_tree, feature_names=list(x.columns))
print("Train accuracy = %.3f; test accuracy: %.3f" % (train_accuracy, test_accuracy
print(r)

decision_tree = DecisionTreeRegressor(criterion="mse",
                                      random_state=0, max_depth=10)
decision_tree = decision_tree.fit(x_train, y_train)
y_pred = decision_tree.predict(x_test)
```

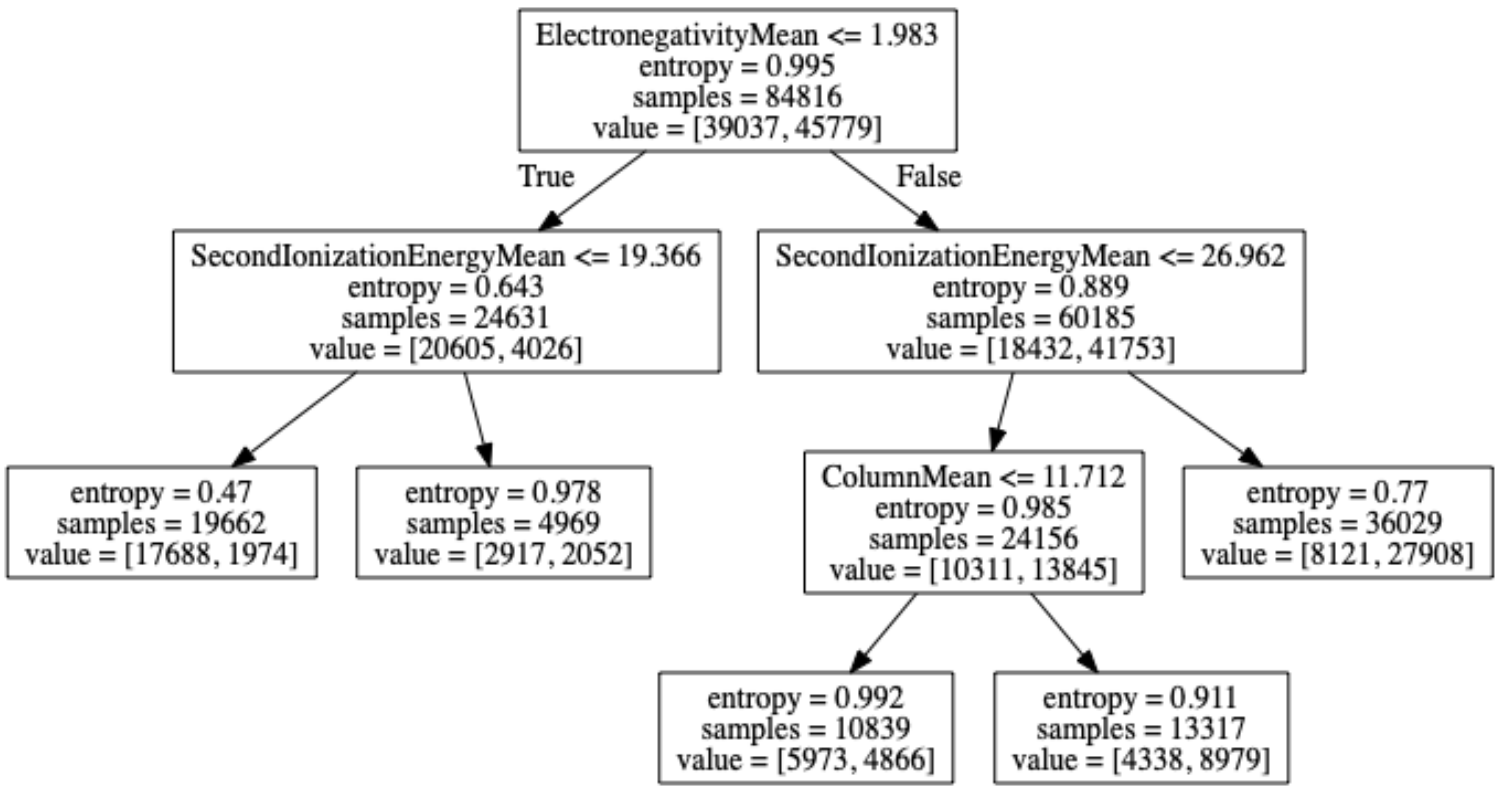
Classification accuracy



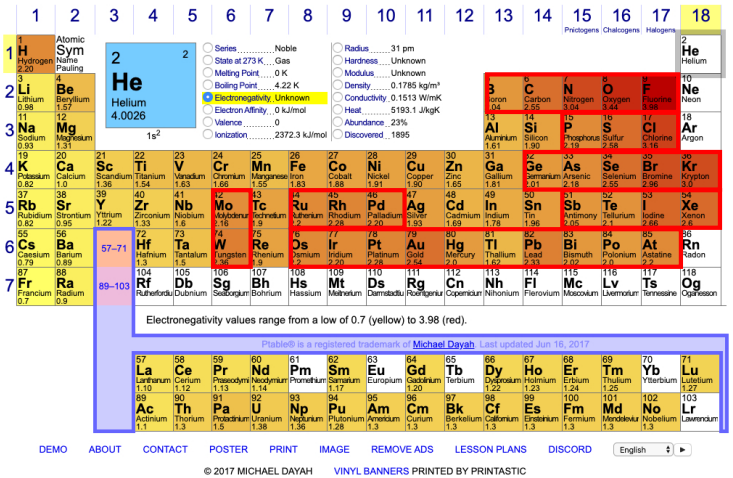
- Quite clearly, we cannot do much better than a $\sim 82\%$ accuracy (test misclassification rate of about 18%) with a tree-depth of around 15.
- Also, the training and test errors diverge significantly after a depth of around 8, which indicates overfitting.

Interpreting the tree

- A 8-deep tree is not very easy to read. Here, we will use cost-complexity pruning with a parameter $\alpha = 0.01$ to prune the tree. The resulting tree has an accuracy of around 74%. Let's see how the decision is being made at the first few levels.



Interpreting the tree, contd.

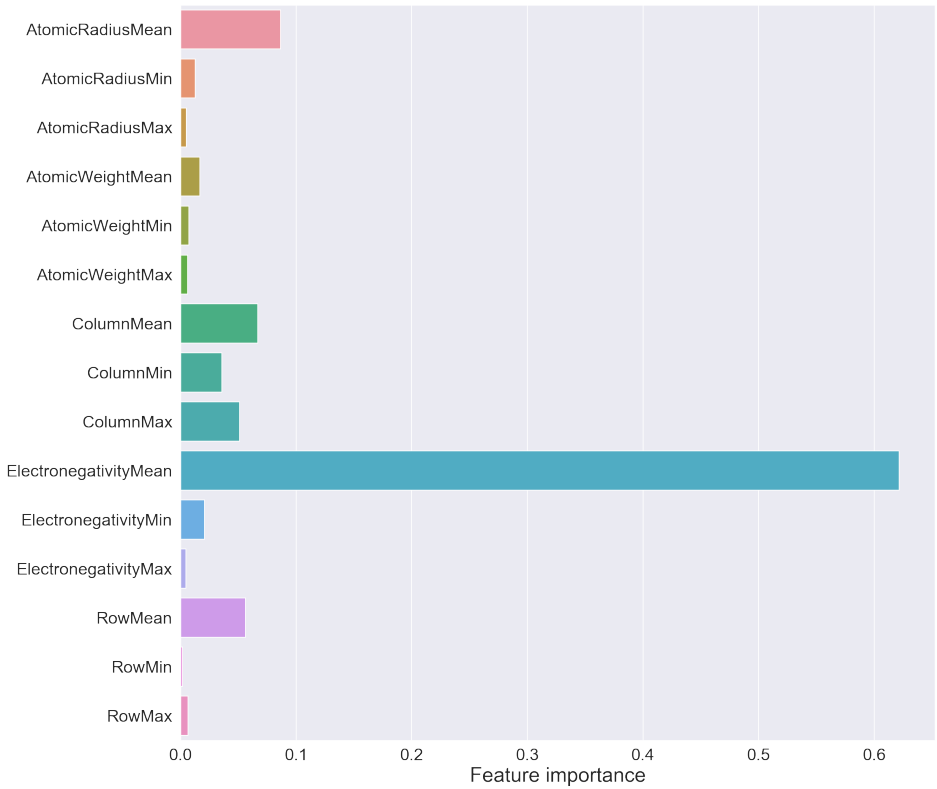


- Compounds with mean $\chi \leq 2.03$ are mostly classified as metals.
- Compounds with mean $\chi > 2.03$ are classified as insulators, i.e., mostly ionic compounds containing chalcogenides and halides with high χ.

```
|--- ElectronegativityMean <= 2.03
|    |--- ColumnMin <= 2.50
|    |    |--- ElectronegativityMax <= 5.09
|    |    |    |--- class: 0
|    |    |--- ElectronegativityMax >  5.09
|    |    |    |--- class: 1
|    |--- ColumnMin >  2.50
|    |    |--- ColumnMax <= 44.50
|    |    |    |--- class: 0
|    |    |--- ColumnMax >  44.50
|    |    |    |--- class: 0
|--- ElectronegativityMean >  2.03
|    |--- AtomicRadiusMean <= 0.98
|    |    |--- AtomicWeightMean <= 22.98
|    |    |    |--- class: 1
|    |    |--- AtomicWeightMean >  22.98
|    |    |    |--- class: 1
|    |--- AtomicRadiusMean >  0.98
|    |    |--- ColumnMax <= 31.00
|    |    |    |--- class: 0
|    |    |--- ColumnMax >  31.00
|    |    |    |--- class: 1
```

Feature importance

- Another way of interpreting trees is using the feature importance.
- The importance of a feature is the (normalized) total reduction of the criterion brought by that feature.

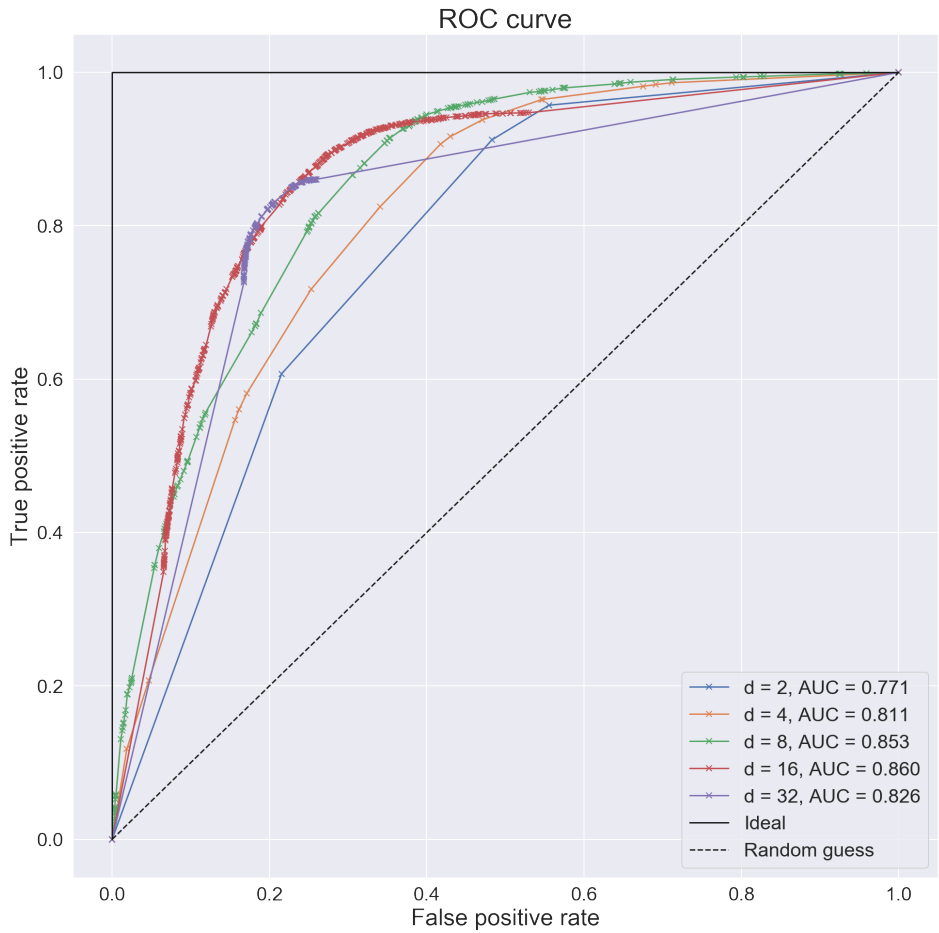


Receiver Operating Characteristic (ROC) Curve

$$TPR = \frac{TP}{P} = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{N} = \frac{FP}{TN + FP}$$

- Plot of the TPR (*sensitivity*) vs FPR (1-*selectivity*).
- $y = x$ line denotes random guessing (TPR = FPR).
- The greater the area under curve (AUC), better the performance.



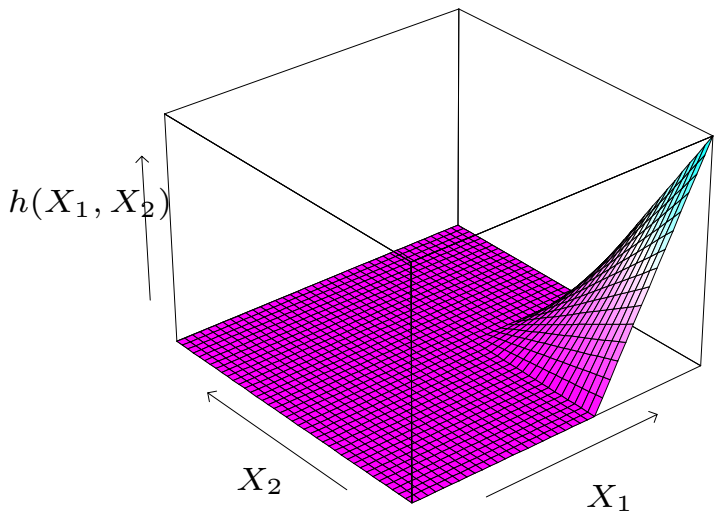
Multivariate Adaptive Regression Splines (MARS)

- Essentially a modification of CART to use step-wise linear regression.
- MARS uses piece-wise linear basis functions:

$$(x-t)_+ = \begin{cases} x-t & ,x > t \\ 0 & ,otherwise \end{cases}$$

$$(t-x)_+ = \begin{cases} t-x & ,x < t \\ 0 & ,otherwise \end{cases}$$

- Implementation available in the py-earth package.



Ensemble learning

- So far, we have covered the basics of using a single model (linear, kernel, tree) to perform an ML prediction.
- In *ensemble learning*, we use multiple models and average the results to improve prediction performance.
- Advantage: lower variance and in many cases, dramatically improved prediction performance.
- Disadvantage: some of the interpretability is lost in the process.
- Here, we will cover two of the most popular ensemble learning approaches - *boosting* and *bagging*.
- While ensemble learning can be applied to any of the previous ML methods, we will focus here on their application to decision trees.

Boosting

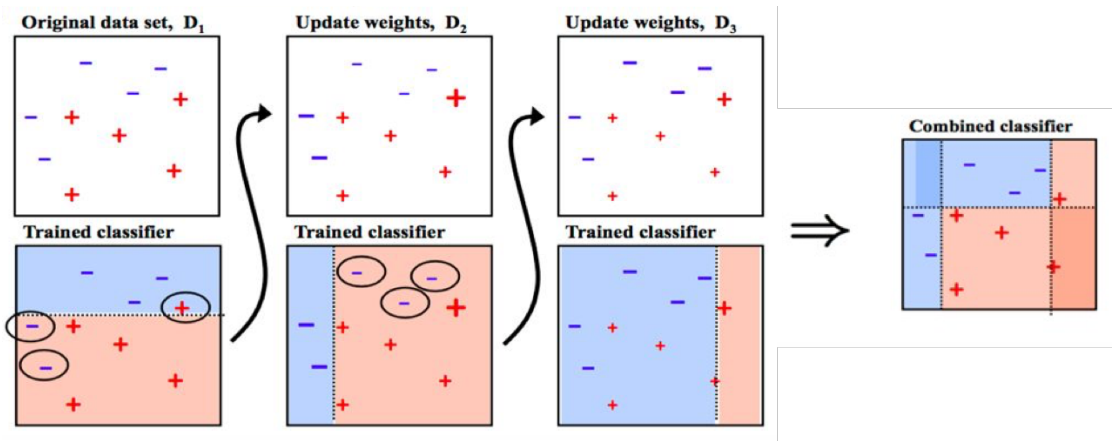
- One of the most successful ML approaches in the past few decades.
- Concept: combine many "weak" learners in a "committee".
- Can be used for either classification or regression.
- Weak classifier: One whose error rate is slightly better than random guessing.
- Apply weak classifier to repeatedly modified versions of data to produce a sequence of weak classifiers.
- Predictions from sequence are combined using weighted majority vote:

$$G(x) = sign\left(\sum_{m=1}^{M} \alpha_m G_m(x)\right)$$

- Weights α_m are computed by boosting algorithm and is the contribution of each weak learner $G_m(x)$.
- While $G(x)$ can be any classifier, we will focus here on using decision trees as the base classifier.

AdaBoost.M1 Algorithm (Classification)

1. Initialize observation weights as $w_i = 1/N$.
2. For $m = 1$ to M:
   1. Fit classifier $G_m(x)$ to training data using weights w_i.
   2. Compute $err_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$
   3. Compute $\alpha_m = \log \frac{1-err_m}{err_m}$.
   4. Set $w_i = w_i \exp[\alpha_m I(y_i \neq G_m(x_i))]$, $i = 1, 2, ...N$. Conceptually, increase weights in step m for observations that are misclassified in step $m-1$.
3. Output $G(x) = sign\left(\sum_{m=1}^{M} \alpha_m G_m(x)\right)$



AdaBoost in scikit-learn

```
from sklearn.ensemble import AdaBoostClassifier

x_train, x_test, y_train, y_test = train_test_split(x, y_class, test_size=0.2)

decision_tree = AdaBoostClassifier(DecisionTreeClassifier(criterion="entropy", rand
                                   n_estimators=20)
decision_tree = decision_tree.fit(x_train, y_train)
train_accuracy = decision_tree.score(x_train, y_train)
test_accuracy = decision_tree.score(x_test, y_test)
```

Gradient Boosting

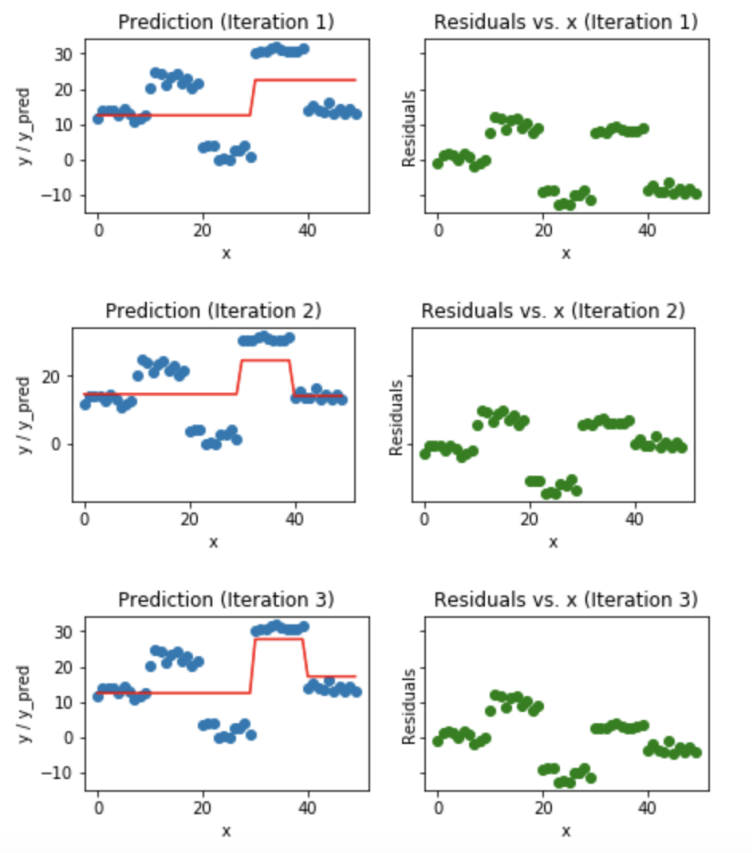


Figure: Source: Gradient Boosting from Scratch

- We can think of the algorithm in Slide 22 as essentially a forward stage-wise fit of an additive model $f(x) = \sum_{m=1}^{M} \alpha_m G_m(x)$ (refer to [1] for details).
- Greedy approach in that it seeks to maximally reduce the loss at each step, i.e., steepest descent, by adjusting the weights iteratively.
- In contrast, *gradient boosting* attempts to fit a new learner to the residuals of the errors from the previous step.

Gradient Boosting in Scikit-Learn

```
from sklearn.ensemble import GradientBoostingClassifier, GradientBoostingRegressor

model = GradientBoostingClassifier(n_estimators=50)
model.fit(x, y_class)
model.predict(x)

model = GradientBoostingRegressor(n_estimators=50)
model.fit(x, y_reg)
model.predict(x)
```

Loss functions for regression

- We have thus far focused on the squared error loss $L(y, f(x)) = (y - f(x))^2$
- Another common loss function is the absolute error $L(y, f(x)) = |y - f(x)|$
- MSE penalizes outliers with large observed residuals severely, and hence is less robust in data with long-tailed distributions.
- MAE is more robust against outliers.
- Other criteria include the Huber loss:

$$L(y, f(x)) = \begin{cases} (y - f(x))^2 & |y - f(x)| \leq \delta \\ 2\delta(y - f(x) - \delta^2 & \textit{otherwise} \end{cases}$$

Loss functions for binary classification

- Consider a simple binary classification with two levels (-1, 1). The decision boundary is at 0.
- Using the square error does not make sense, since we only care about whether it is > 0 or < 0.
- *Margin* $yf(x)$ is positive when prediction and actual value is in the same class, and negative if they are in opposite classes.
- Need a loss that penalizes negative values much more than positive values for margins, i.e., monotone decreasing function.
- Exponential loss: $L(y, f(x)) = e^{-yf(x)}$
- Binomial/multinomial loss (can be used for K-classes):

$$L(y, p(x)) = -\sum_{k=1}^{K} I(y = G_k) f_k(x) + \log\left(\sum_{l=1}^{K} e^{f_l(x)}\right)$$

Loss functions for binary classification

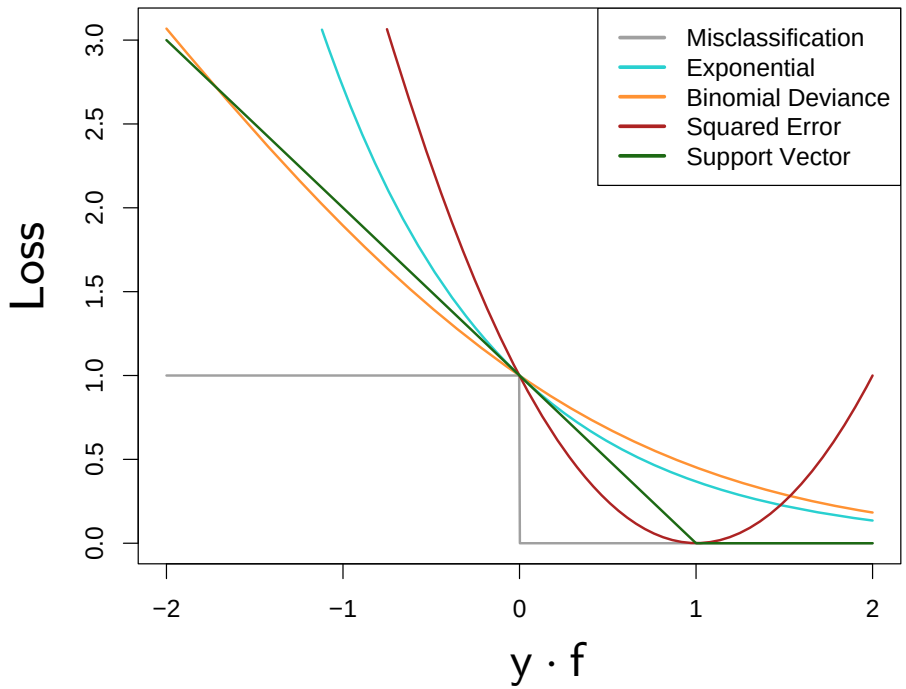
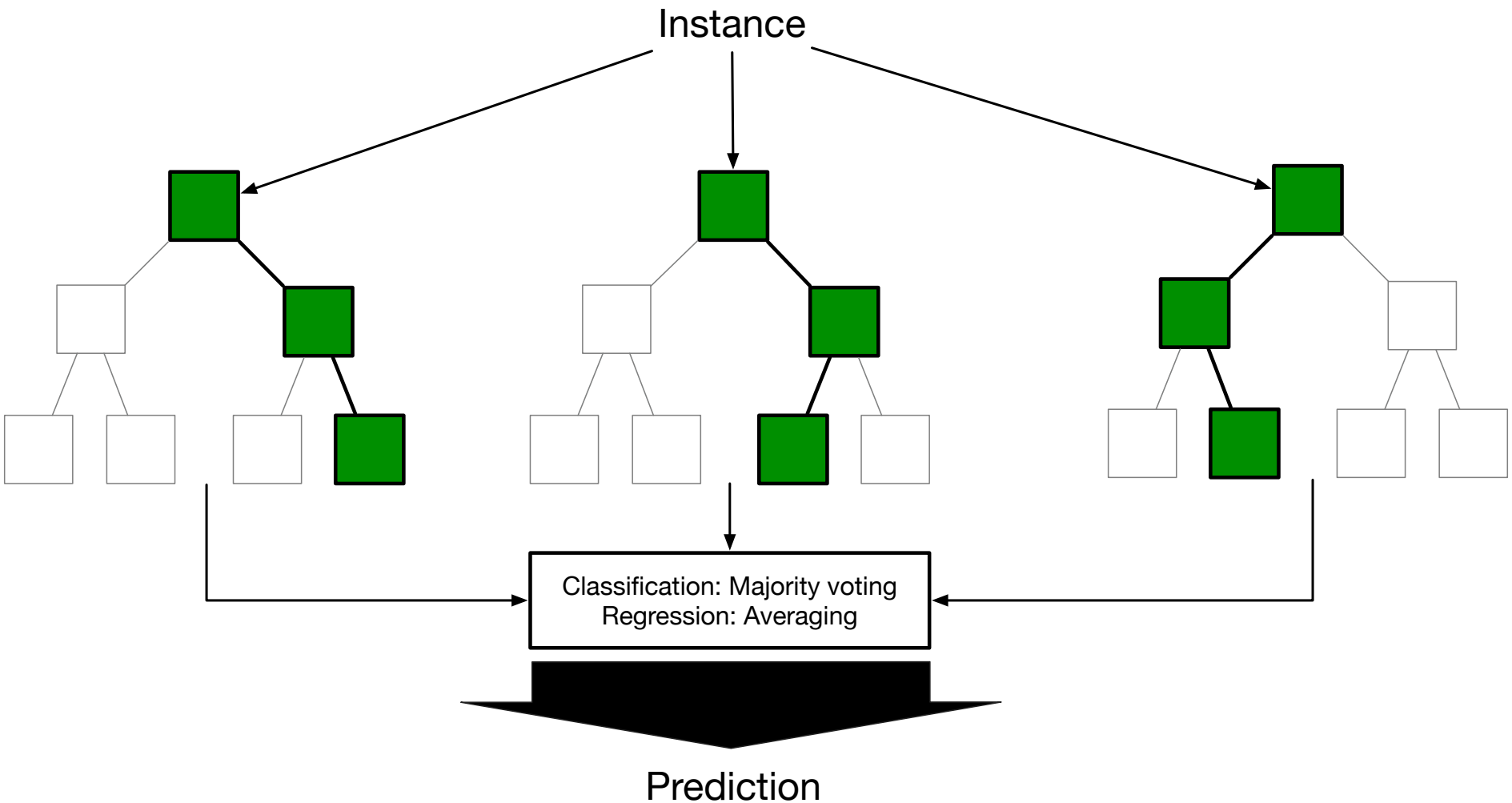


Figure: Loss functions for binary classification. Response: $y = \pm 1$. X-axis is the margin $y \cdot f$. Misclassification : $I(\mathrm{sign}(f) \neq y)$; exponential: e^{-yf}; binomial deviance: $\log(1 + e^{-2yf})$; squared error: $(y - f)^2$; and support vector: $(1 - yf)_+$. Source: [1]

Random Forests

- Bagging: average many noisy, unbiased models to reduce variance.
- Random forest: Grow B trees at random and average the results. Classification: majority vote (mode), regression: mean.
- Tree growing:
  1. At each branch, select m variables at random from p variables.
  2. Determine best split among the m.
  3. Split node into two daughter nodes.
  4. Repeat until minimum node size is reached.

Random Forest Algorithm



Example: Identification of Local Environments from K-edge XANES

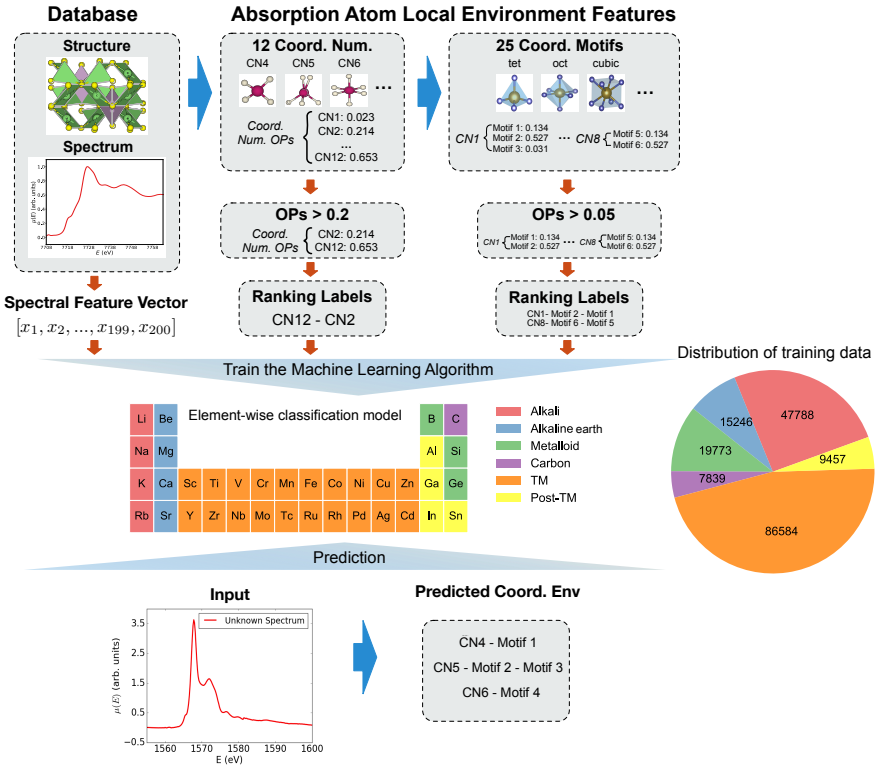


Figure: Workflow for classification of K-edge XANES spectra into one of 25 coordination environments.[2]

Example: Identification of Local Environments from K-edge XANES

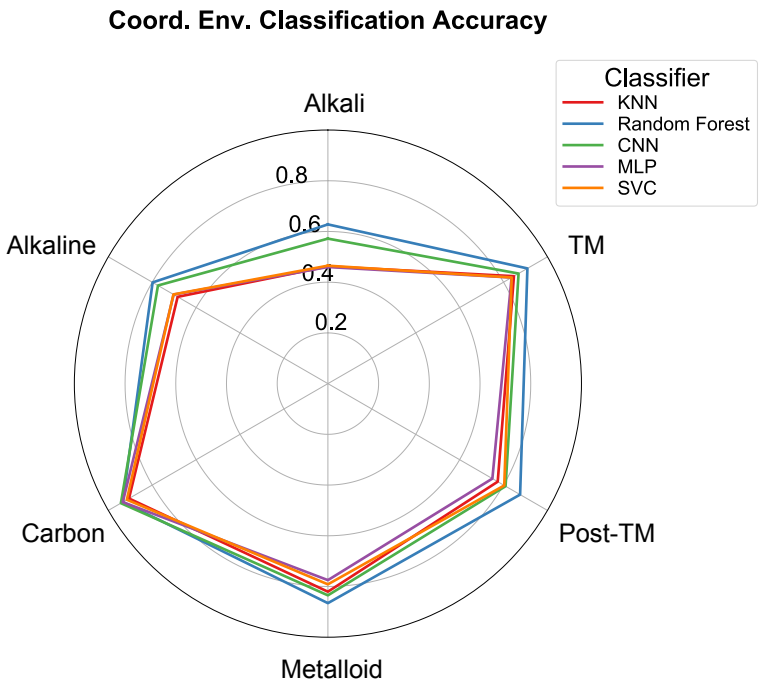


Figure: Comparison of different ML methods for K-edge XANAES classification.[2]

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The End