Generalized Additive Models and Trees

Shyue Ping Ong

University of California, San Diego

NANO281

Overview

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 $\hat{f}_j$ 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).

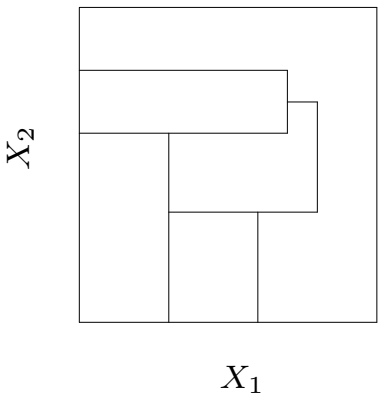
Example application of GAM

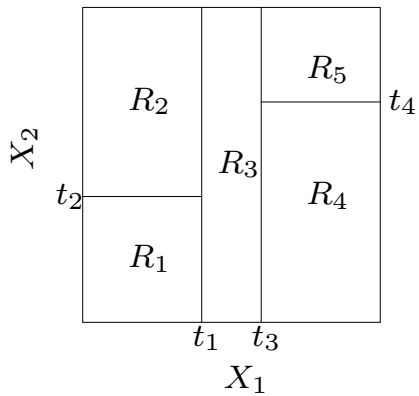
Tree-based methods

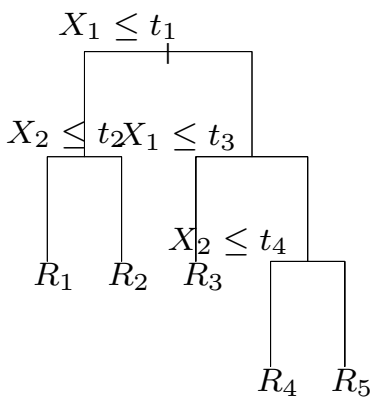
- Feature space partitioned into rectangles, and simple model (e.g., constant) fitted into each rectangle.
- CART

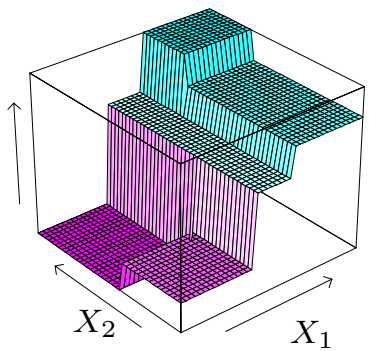
$$\hat{f}(X) = \sum_m c_m I\{(X_1, X_2) \in R_m\}$$

- 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 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 of the regions to grow the regression 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.
- 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 $\sum_{x_i \in R_m} (y_i - \hat{c_m})^2$.

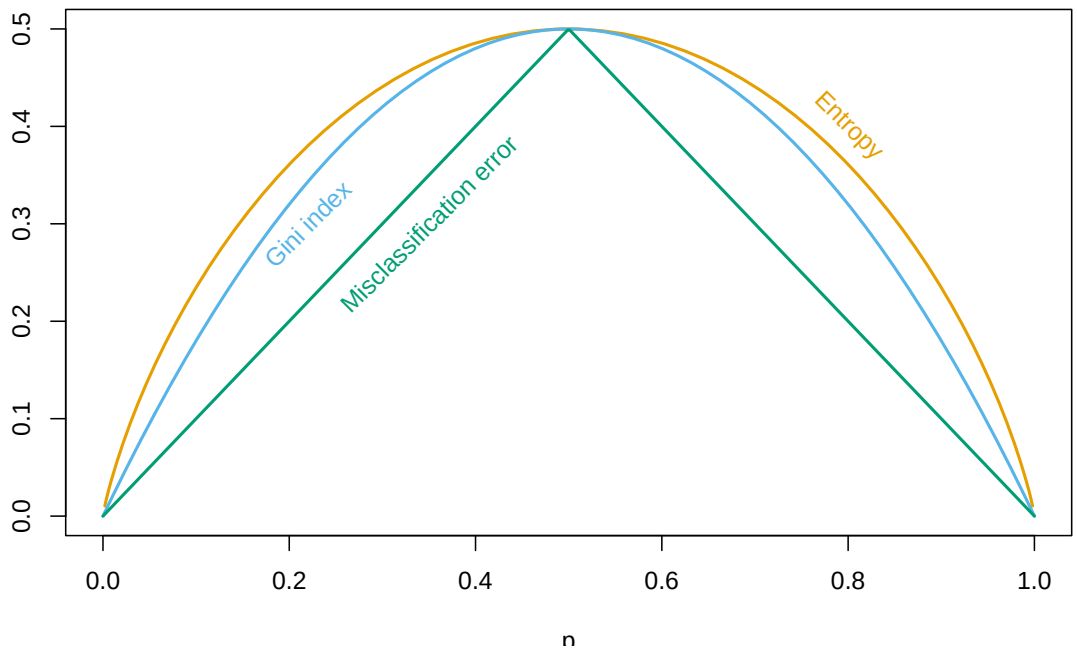
Classification Trees

- 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 $\sum_{k \neq k'} p_{\hat{m}k} p_{\hat{m}k'}$

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



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, ElectronAffinity, Electronegativity, FirstIonizationEnergy, Row, SecondIonizationEnergy. 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

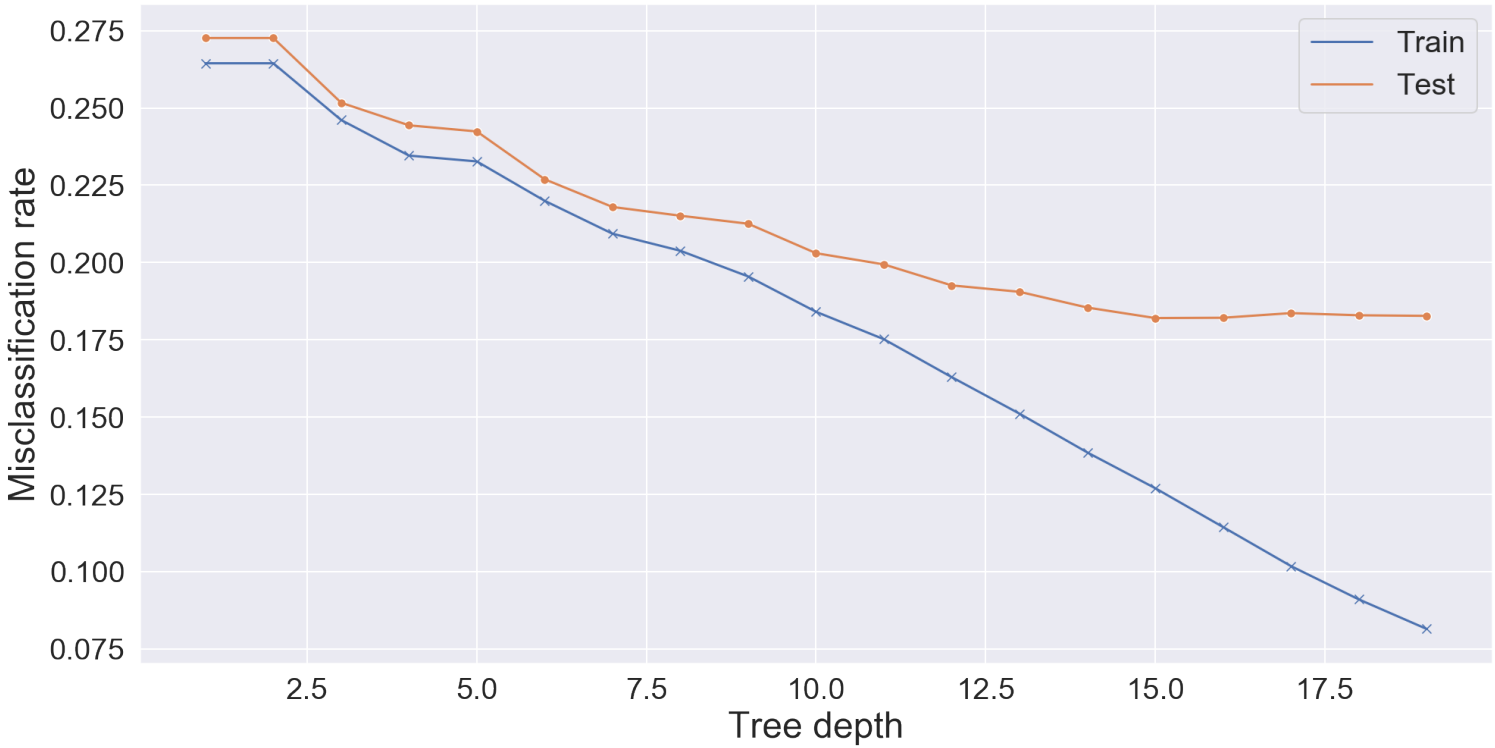
```
from sklearn.tree import DecisionTreeClassifier, DecisionTreeRegressor
from sklearn.model_selection import train_test_split
from sklearn.tree import export_text

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)
```

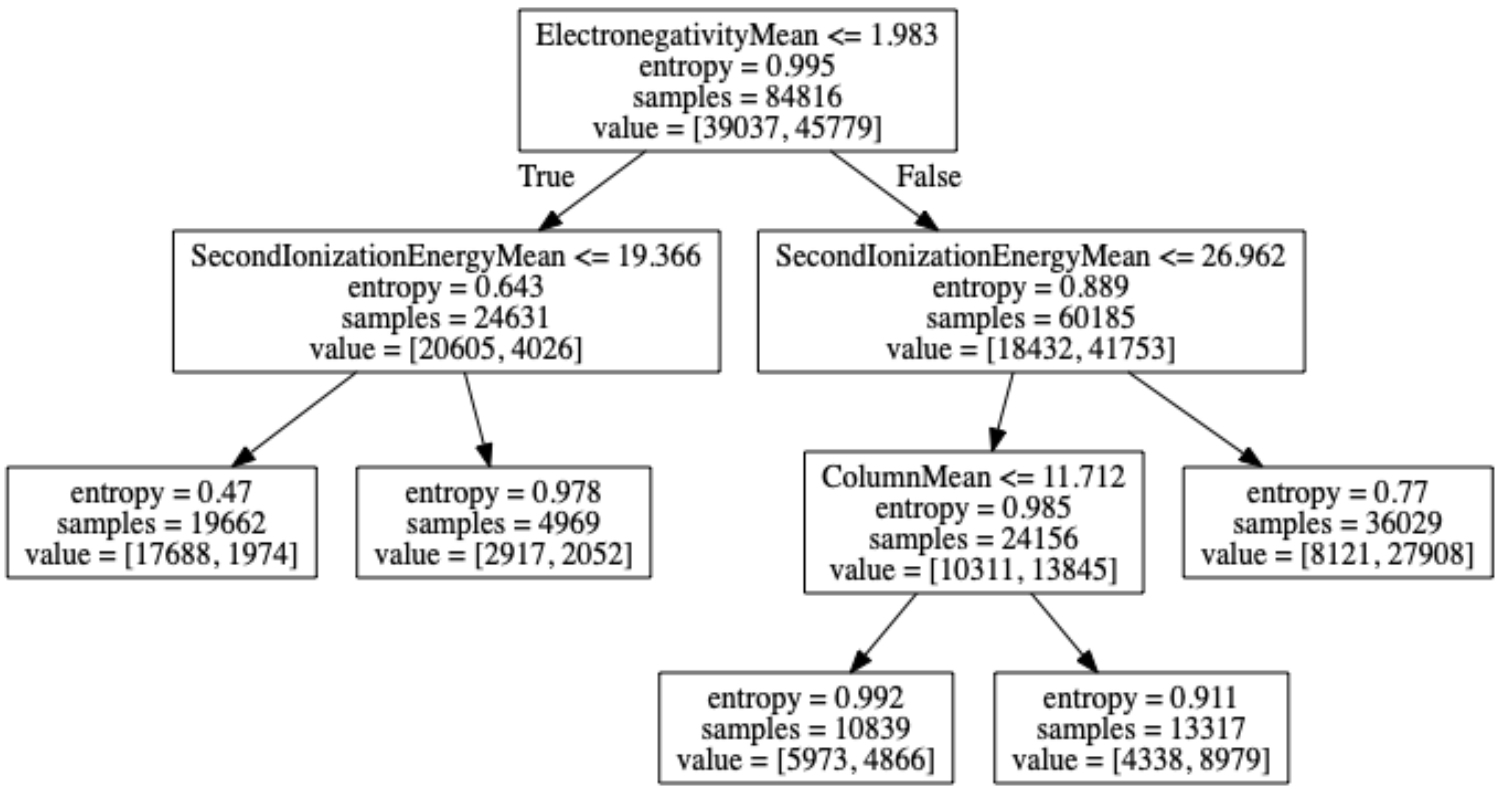
Misclassification rate



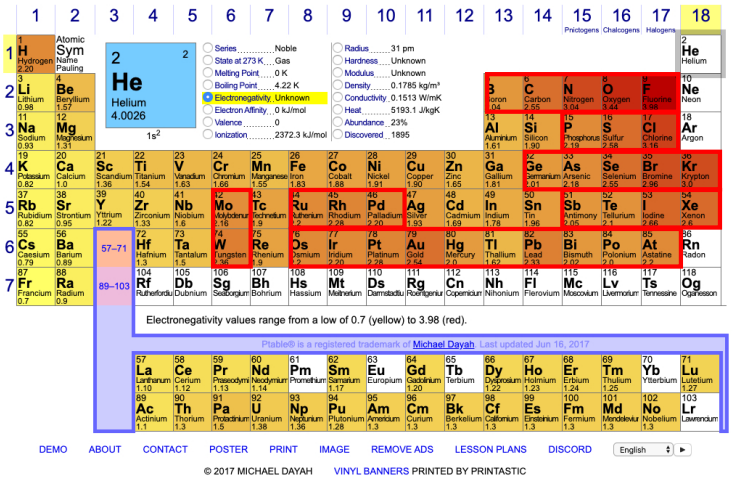
- Quite clearly, we cannot do much better than a $\sim 82\%$ accuracy (test misclassification rate of about 18%) with a tree-depth of around 15.
- Also, the training and test errors diverge significantly after a depth of around 8, which indicates overfitting.

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.

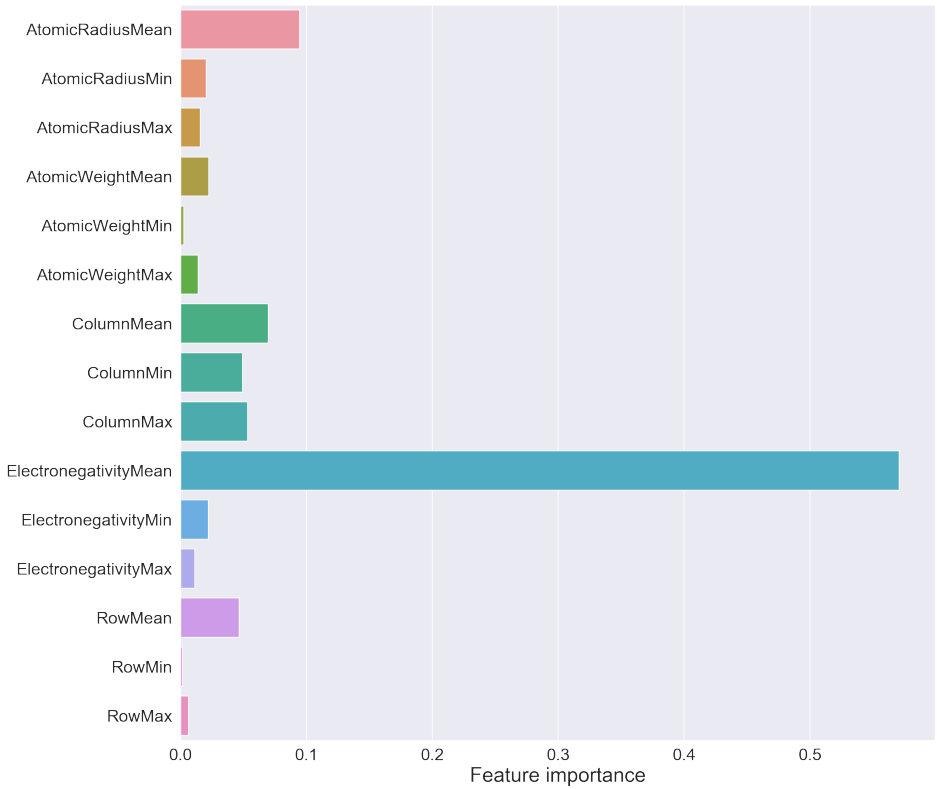


- Compounds with mean $\chi \leq 1.92$ are classified as metals.
- Compounds with mean $1.92 \leq \chi \leq 2.05$ are classified as metals, unless they contain elements in groups I and II, i.e., ionic compounds.
- Compounds with mean $\chi > 2.05$ are insulators unless "AtomicRadiusMean" $>$ 0.97, i.e., metals in group 6, 8, 9, 10, 11.

```
|--- ElectronegativityMean <= 2.05
|    |--- ElectronegativityMean <= 1.92
|    |    |--- ColumnMin <= 2.50
|    |    |    |--- class: 0
|    |    |--- ColumnMin >  2.50
|    |    |    |--- class: 0
|    |--- ElectronegativityMean >  1.92
|    |    |--- ColumnMin <= 2.50
|    |    |    |--- class: 1
|    |    |--- ColumnMin >  2.50
|    |    |    |--- class: 0
|--- ElectronegativityMean >  2.05
|    |--- AtomicRadiusMean <= 0.97
|    |    |--- RowMean <= 2.48
|    |    |    |--- class: 1
|    |    |--- RowMean >  2.48
|    |    |    |--- class: 1
|    |--- AtomicRadiusMean >  0.97
|    |    |--- 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.

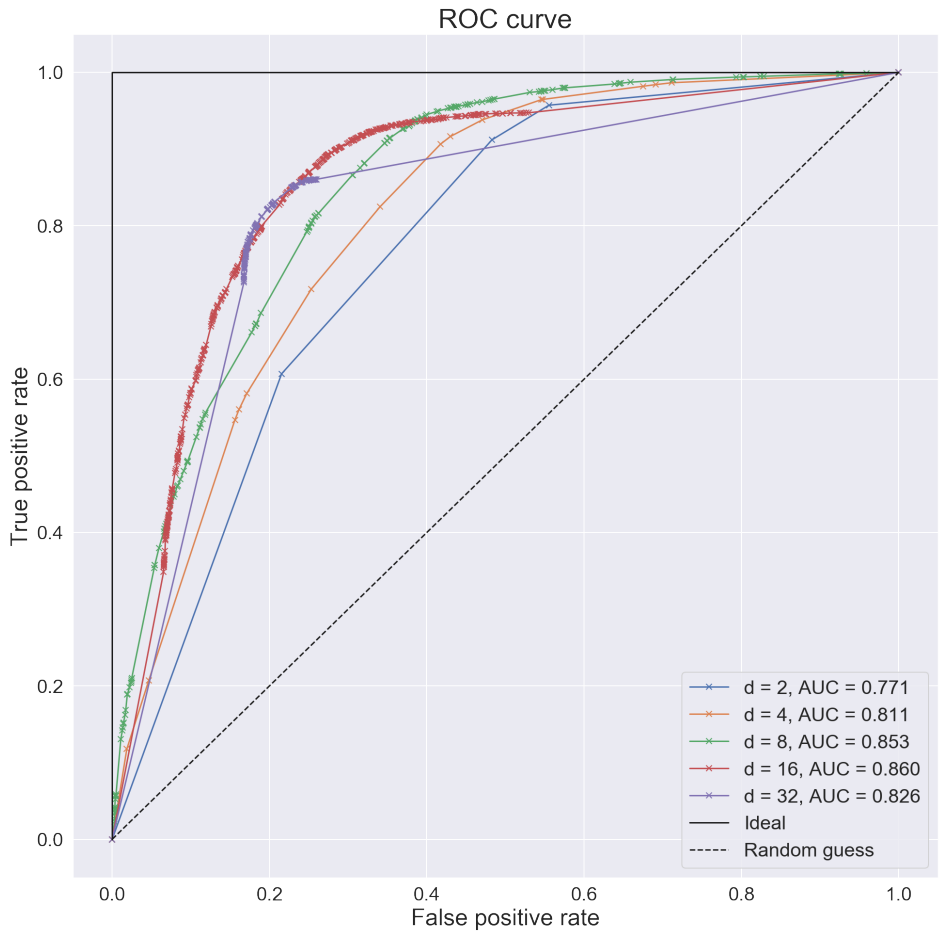


Receiver Operating Characteristic (ROC) Curve

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

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

- 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.



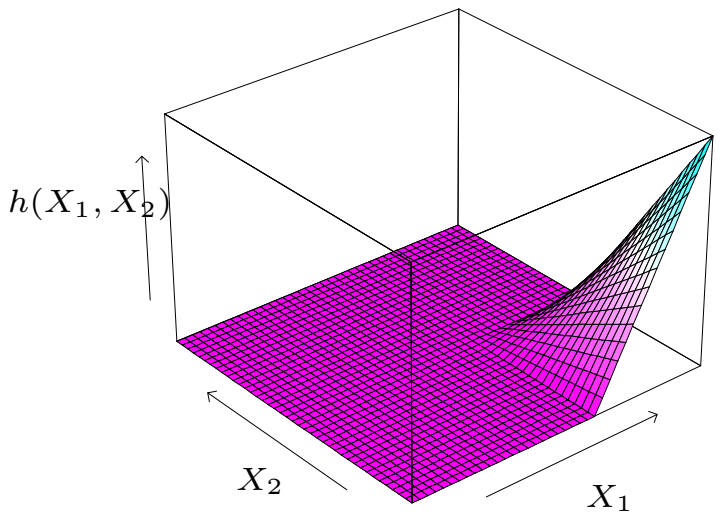
Multivariate Adaptive Regression Splines (MARS)

- 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.



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)
```

Bibliography

The End