ML_Chap.3Notes

Summary/Review - Week1_Logistic Regression (2021.12.28)

Classification Problems

The two main types of supervised learning models are:

- Regression models, which predict a continuous outcome
- Classification models, which predict a categorical outcome.

The most common models used in supervised learning are:

- Logistic Regression
- K-Nearest Neighbors
- Support Vector Machines
- Decision Tree
- Neural Networks
- Random Forests
- Boosting
- Ensemble Models

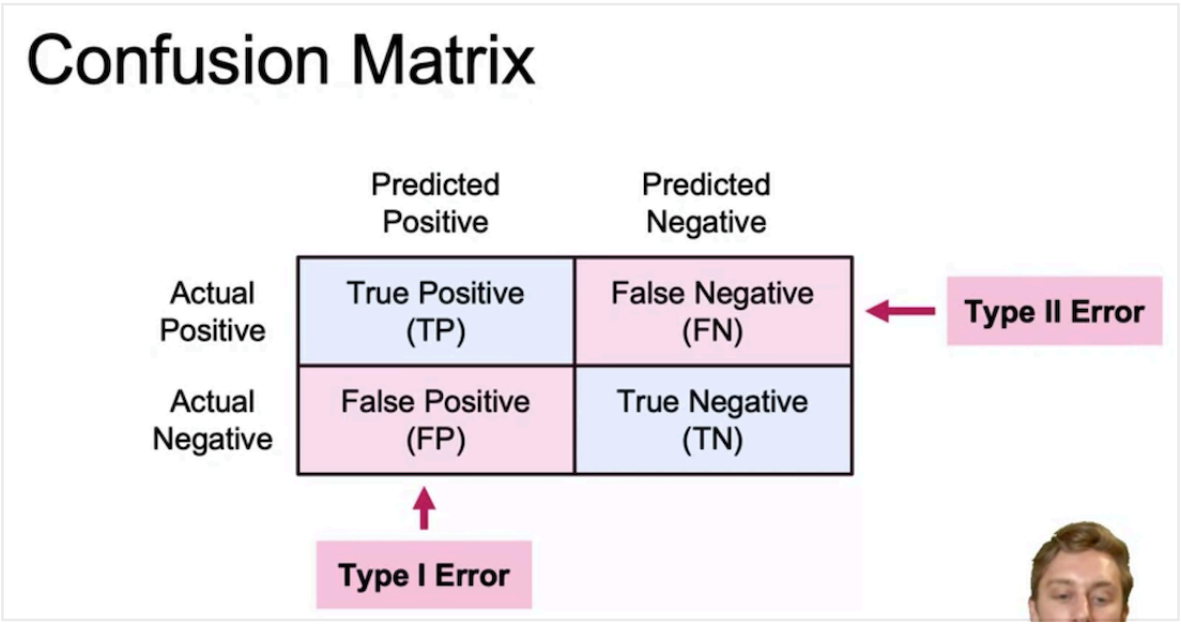
With the exception of logistic regression, these models are commonly used for both regression and classification.
Logistic regression is most common for dichotomous and nominal dependent variables.

Logistic Regression

Logistic regression is a type of regression that models the probability of a certain class occurring given other independent variables.It uses a logistic or logit function to model a dependent variable. It is a very common predictive model because of its high interpretability.

Classification Error Metrics

A confusion matrix tabulates true positives, false negatives, false positives and true negatives.



Remember that the false positive rate is also known as a type I error.
The false negatives are also known as a type II error.
Accuracy is defined as the ratio of true positives and true negatives divided by the total number of observations. It is a measure related to predicting correctly positive and negative instances.

$$\text{Accuracy} = \frac{TP + TN}{TP + FN + FP + TN}$$

Recall or sensitivity identifies the ratio of true positives divided by the total number of actual positives.
It quantifies the percentage of positive instances correctly identified.

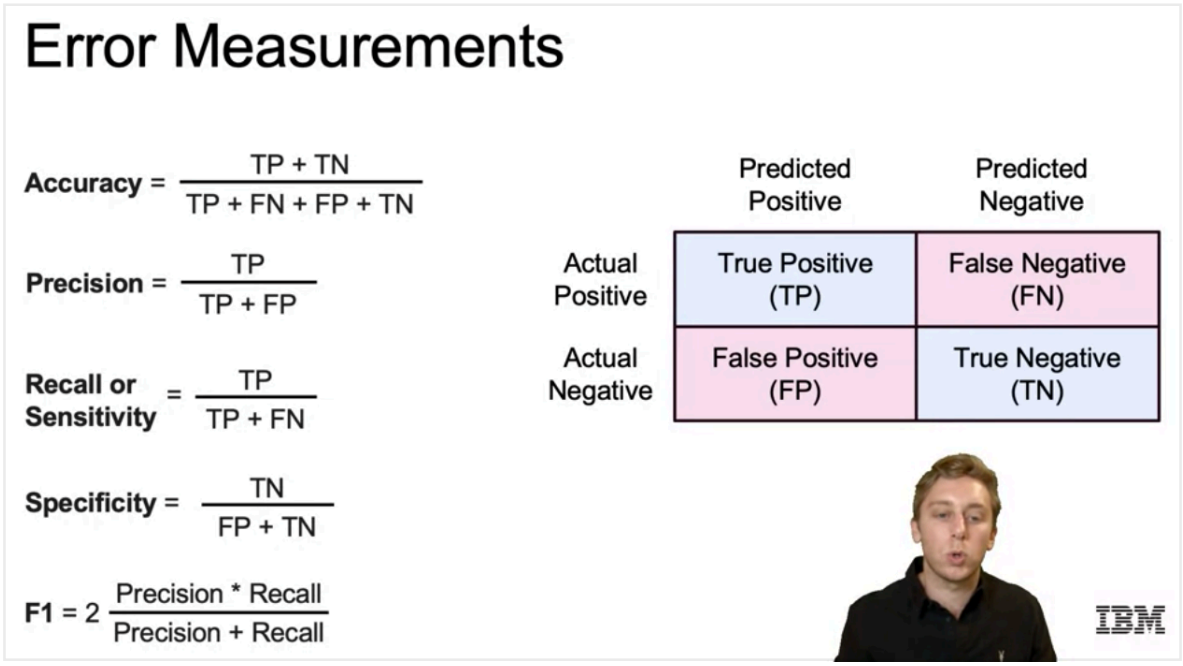
$$\text{Recall or Sensitivity} = \frac{TP}{TP + FN}$$

Precision is the ratio of true positive divided by total of predicted positives. The closer this value is to 1.0, the better job this model does at identifying only positive instances.

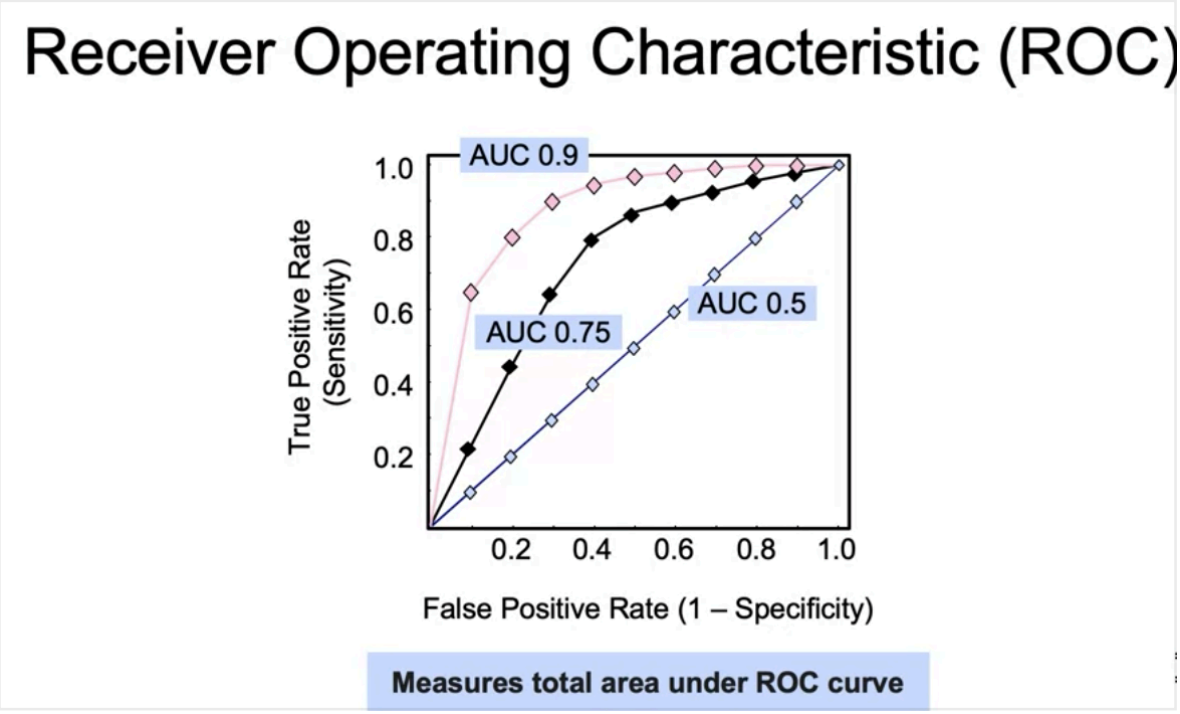
	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
Actual Negative	False Positive (FP)	True Negative (TN)

$$\text{Precision} = \frac{TP}{TP + FP}$$

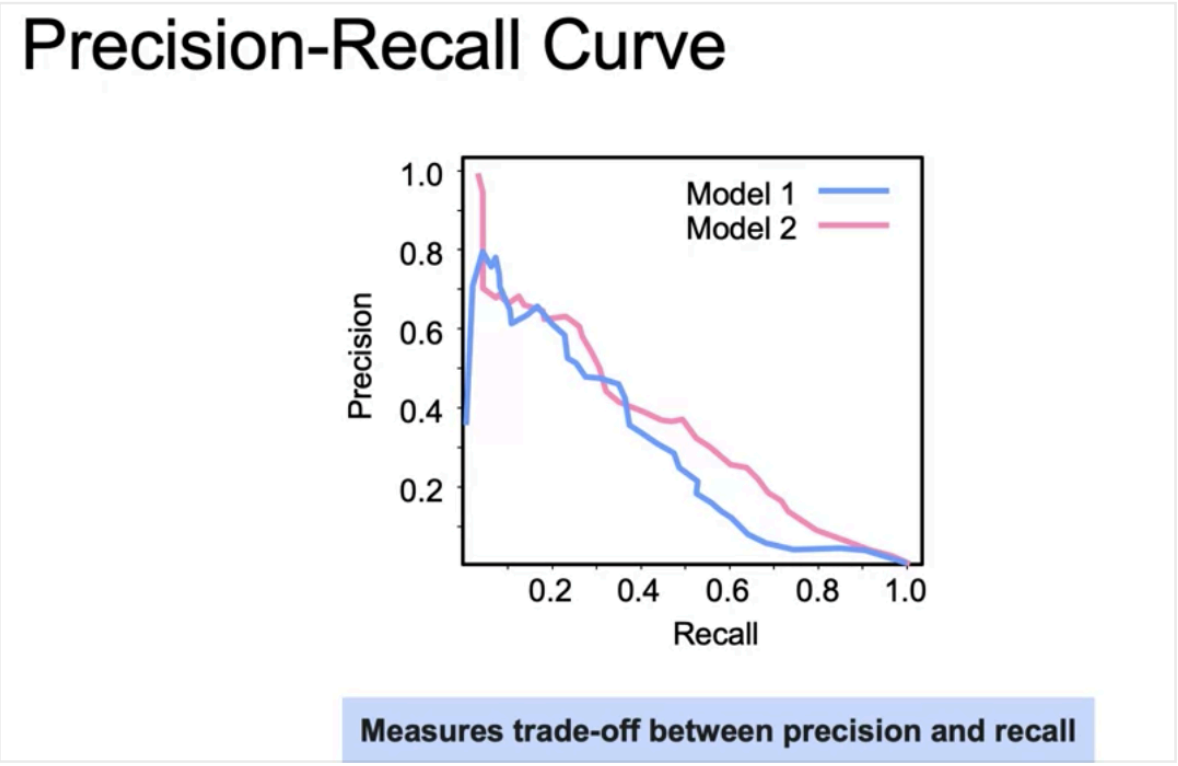
Specificity is the ratio of true negatives divided by the total number of actual negatives. The closer this value is to 1.0, the better job this model does at avoiding false alarms.



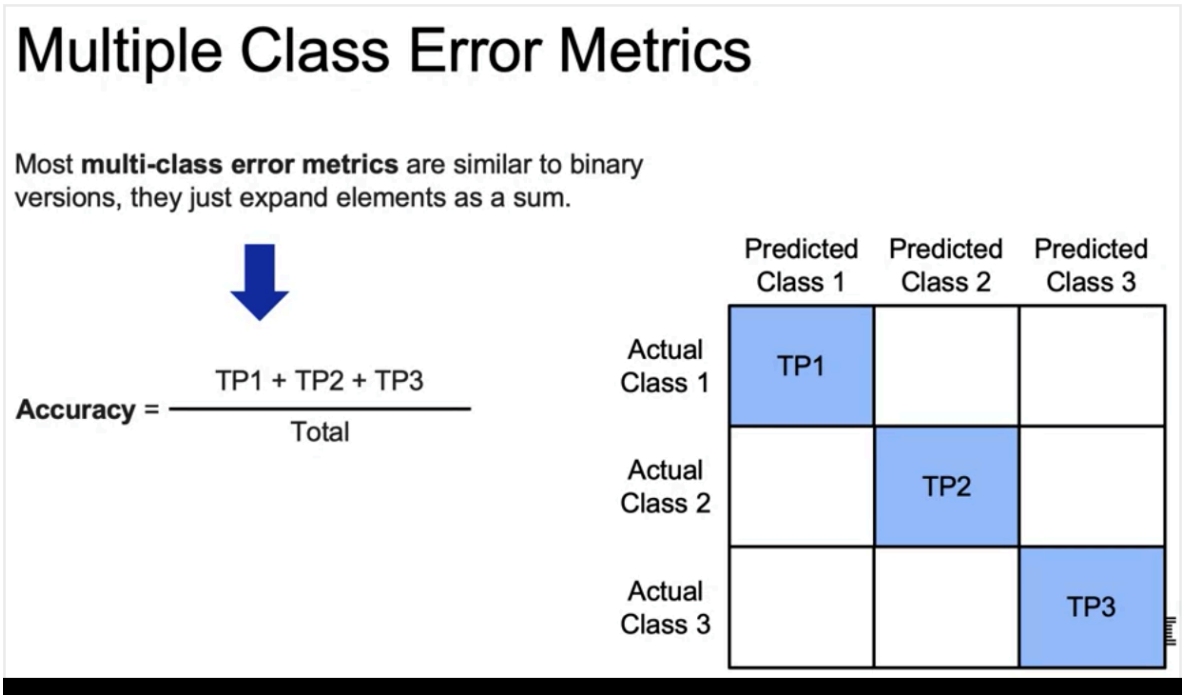
The receiver operating characteristic (ROC) plots the true positive rate (sensitivity) of a model vs. its false positive rate (1-sensitivity).

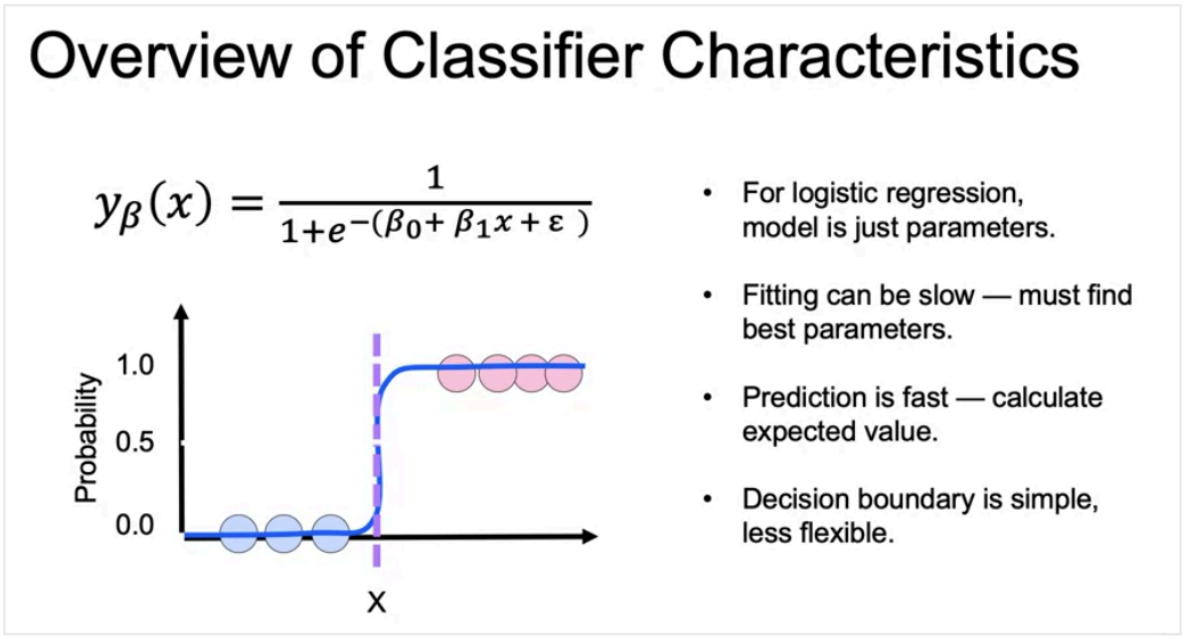


The area under the curve of a ROC plot is a very common method of selecting a classification methods.
The precision-recall curve measures the trade-off between precision and recall.



The ROC curve generally works better for data with balanced classes, while the precision-recall curve generally works better for data with unbalanced classes.





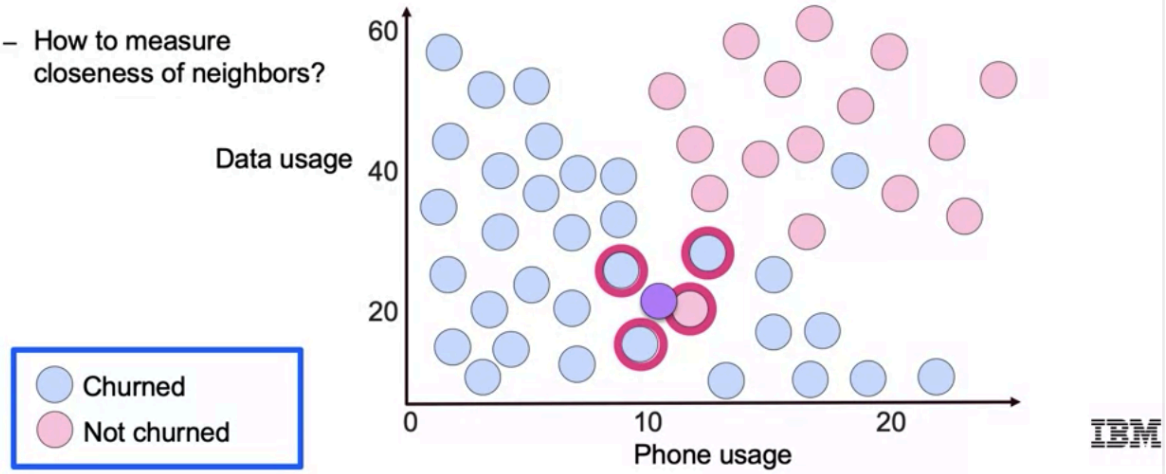
Week2

_K Nearest Neighbor Methods for Classification (2021.12.29)

K nearest neighbor methods are useful for classification.
The elbow method is frequently used to identify a model with low K and low error rate.
These methods are popular due to their easy computation and interpretability, although it might take time scoring new observations, it lacks estimators, and might not be suited for large data sets.

What is Needed to Select a KNN Model?

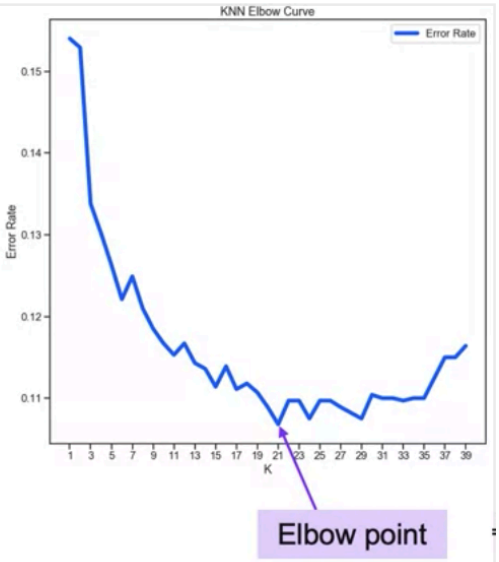
- Correct value for 'K'
- How to measure closeness of neighbors?



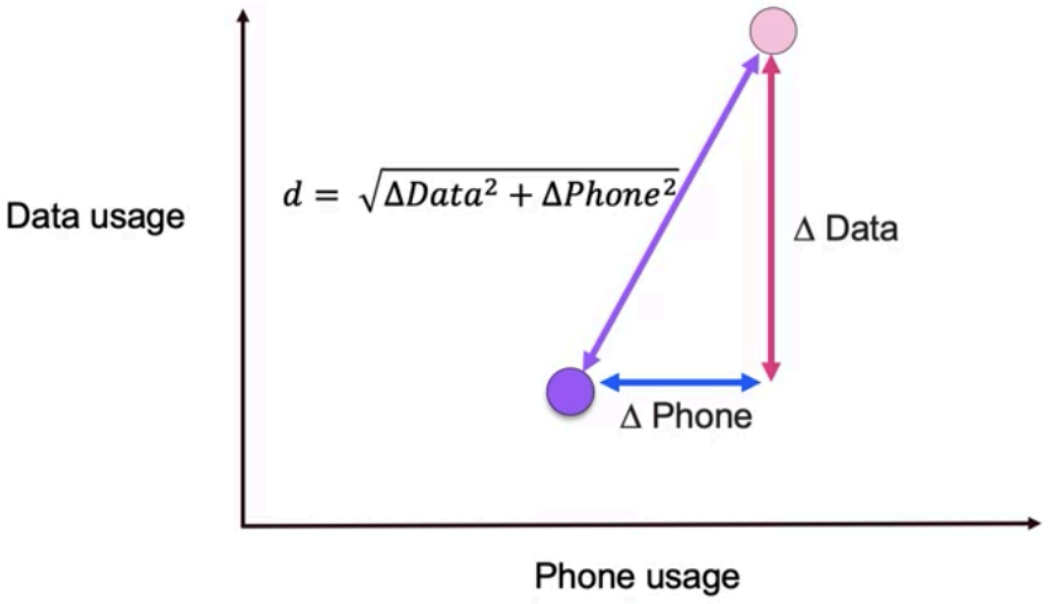
IBM

Choosing the right value for K

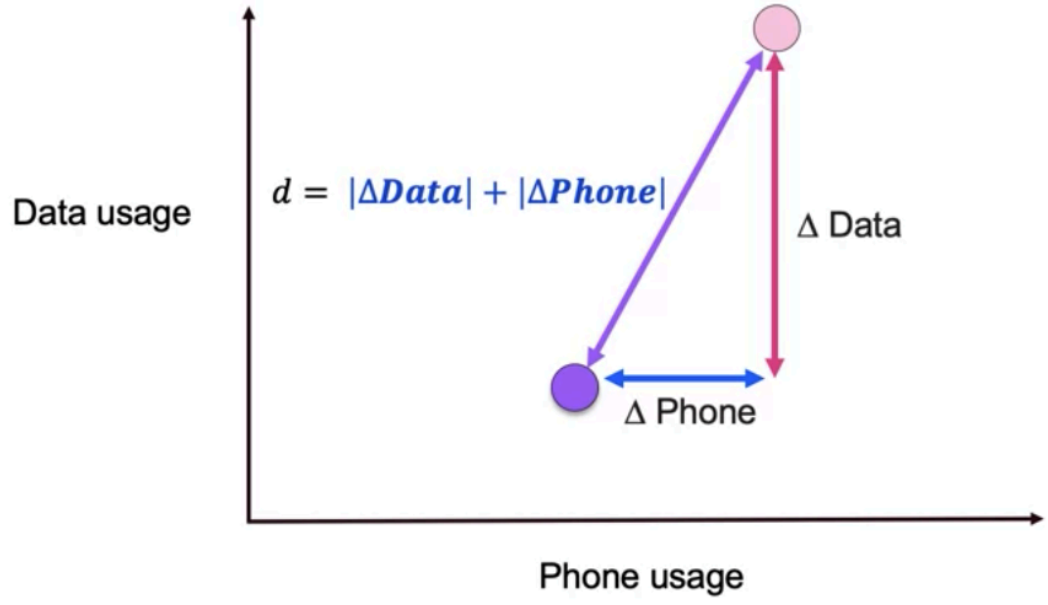
- KNN does not provide a 'correct' *K*
- The right value depends on which error metric is most important
- A common approach is to use an 'elbow method' approach
- This emphasizes kinks in a curve of the error rate as a function of K
- Beyond this point, the rate of improvement slows or stops



Euclidean Distance (L2)



Manhattan Distance (L1)



KNN Overview

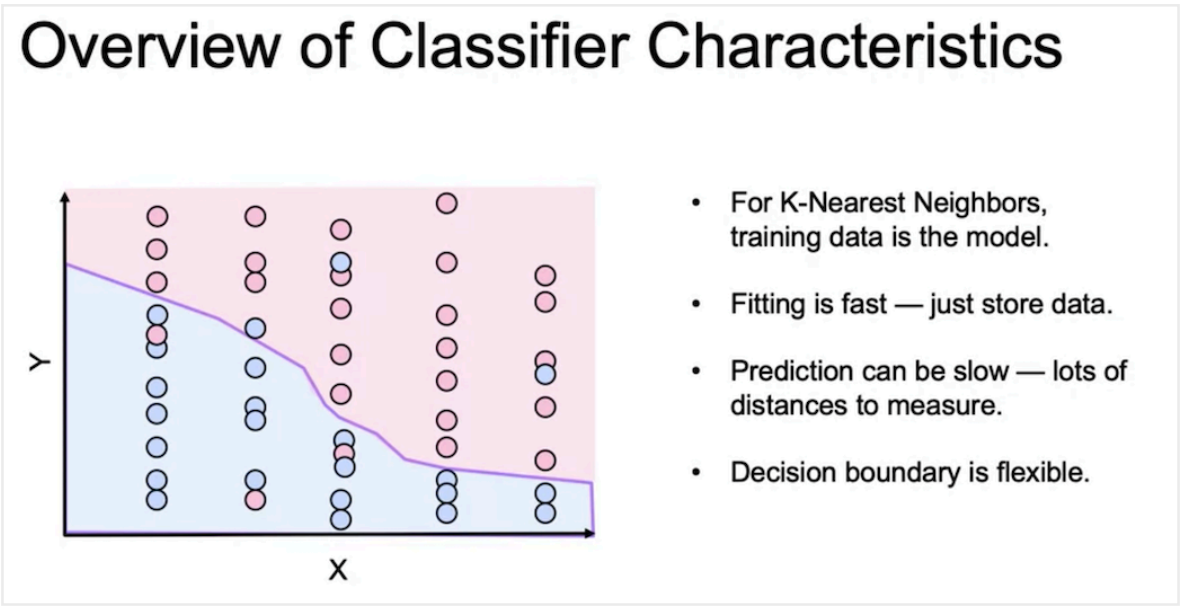
Pros:
- Simple to implement (does not require estimation)
- Adapts well as new training data
- Easy to interpret

Cons:
- Slow to predict because many distance calculations
- Does not generate insight into data generating process (no model)
- Can require lots of memory if data set is large (or as it grows)
- When there are many predictors, KNN accuracy can break down due to curse of dimensionality

Linear Regression	K Nearest Neighbors
– Fitting involves minimizing cost function (slow)	– Fitting involves storing training data (fast)
– Model has few parameters (memory efficient)	– Model has many parameters (memory intensive)
– Prediction involves calculation (fast)	– Prediction involves finding closest neighbors (slow)

Code

```
# Import the class containing the classification method
from sklearn.neighbors import KNeighborsClassifier

# Create an instance of the class
KNN = KNeighborsClassifier(n_neighbors=3)

# Fit the instance on the data and then predict the expected value
KNN = KNN.fit(X_train, y_train)
y_predict = KNN.predict(X_test)

Regression can be done with KNeighborsRegressor.
```



_SVM (2021.12.30)

The main idea behind support vector machines is to find a hyperplane that separates classes by determining decision boundaries that maximize the distance between classes.

When comparing logistic regression and SVMs, one of the main differences is that the cost function for logistic regression has a cost function that decreases to zero, but rarely reaches zero. SVMs use the Hinge Loss function as a cost function to penalize misclassification. This tends to lead to better accuracy at the cost of having less sensitivity on the predicted probabilities.

Regularization can help SVMs generalize better with future data.

By using gaussian kernels, you transform your data space vectors into a different coordinate system, and may have better chances of finding a hyperplane that classifies well your data. SVMs with RBFs Kernels are slow to train with data sets that are large or have many features.

SVMs with Kernels: The Syntax

Code

```
# Import the class containing the classification method
from sklearn.svm import SVC

# Create an instance of the class
rbfSVC = SVC(kernel='rbf', gamma=1.0, C=10.0)

# Fit the instance on the data and then predict the expected value
rbfSVC = rbfSVC.fit((X_train, y_train)
y_predict = rbfSVC.predict(X_test)

Tune kernel and associated parameters with cross-validation.
```

"C" is penalty associated with the error term

Faster Kernel Transformations: The Syntax

Code

```
# Import the class containing the classification method
from sklearn.kernel_approximation import Nystroem

# Create an instance of the class
NystroemSVC = Nystroem (kernel='rbf', gamma=1.0,
n_components=100)

# Fit the instance on the data and transform
X_train = NystroemSVC.fit_transform(X_train)
X_test = NystroemSVC.transform(X_test)

Tune kernel and associated parameters with cross-validation.
```

n_components is number of samples

Machine Learning Workflow

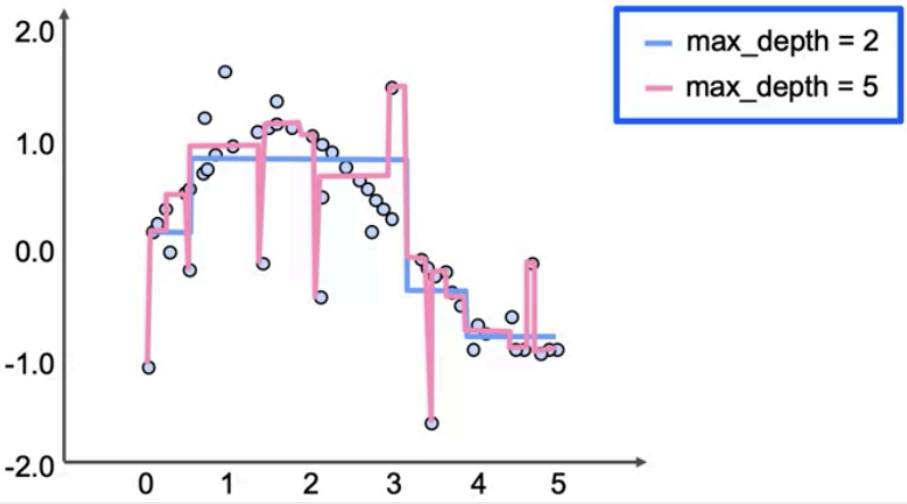
Features	Data	Model Choice
- Many (~10K Features)	- Small (1K rows)	- Simple, Logistic or LinearSVC
- Few (<100 Features)	- Medium (~10k rows)	- SVC with RBF
- Few (<100 Features)	- Many (>100K Points)	- Add features, Logistic, LinearSVC, or Kernel Approx.

Wk3_Decision Tress (2021.12.31)

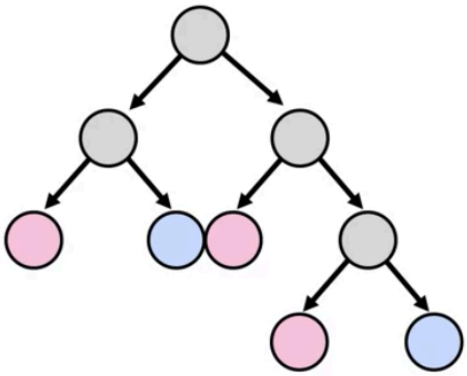
Decision trees split your data using impurity measures.
They are a greedy algorithm and are not based on statistical assumptions.

The most common splitting impurity measures are Entropy and Gini index.
Decision trees tend to overfit and to be very sensitive to different data.

Trees Predict Continuous Values



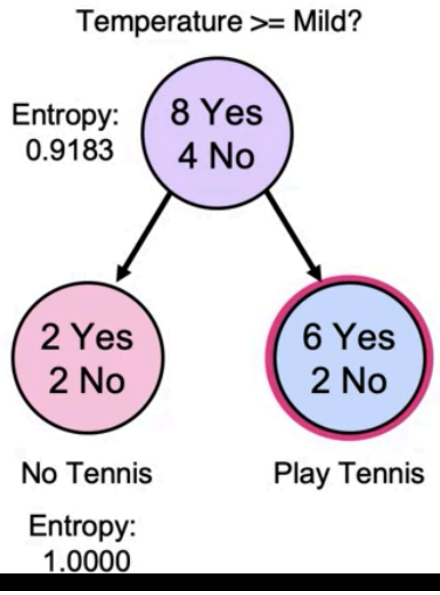
How Long to Keep Splitting?



Until:

- Leaf node(s) are **pure** (only **one class** remains).
- A **maximum depth** is reached.
- A **performance metric** is achieved.

Splitting Based on Entropy



- Entropy Equation

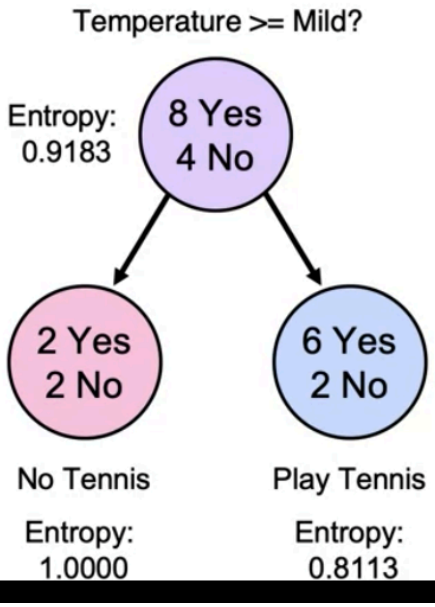
$$H(t) = -\sum_{i=1}^{n} p(i|t) log_2[p(i|t)]$$

- Entropy Right Side

$$-{}^{6}/_{8}\, log_2({}^{6}/_{8}) \; -{}^{2}/_{8}\, log_2({}^{2}/_{8})$$

$$= 0.8113$$

Splitting Based on Entropy



- Classification Error Equation

$$E(t) = 1 - \max_i [p(i|t)]$$

- Entropy Change

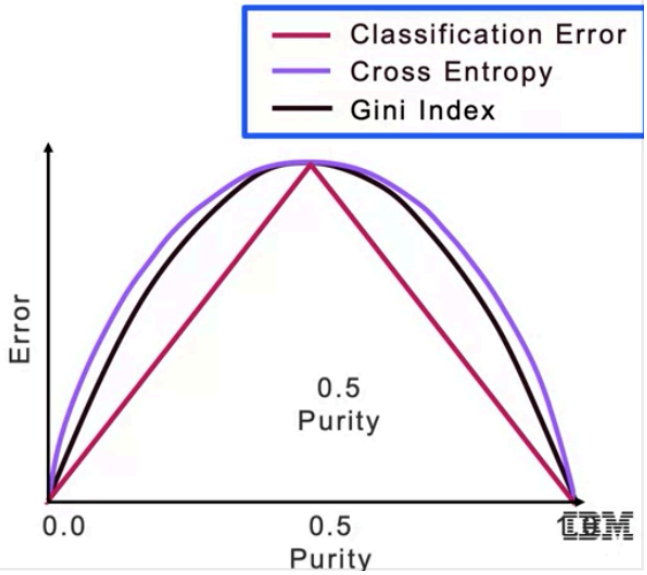
$$0.9183 - {}^{4}/_{12} * 1.0000$$
$$- {}^{8}/_{12} * 0.8113$$

$$= 0.0441$$

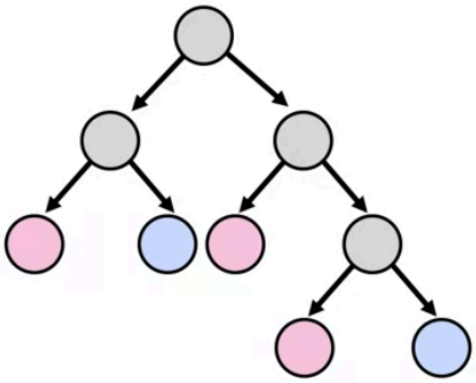
The Gini Index

- In practice, **Gini index** often used for splitting.
- Function is similar to entropy — has bulge.
- Does not contain logarithm.

$$G(t) = 1 - \sum_{i=1}^{n} p(i|t)^2$$

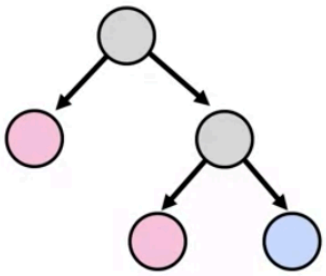


Decision Trees are High Variance



- Problem: decision trees tend to overfit.
- Small changes in data greatly affect prediction - high variance.
- Solution: Prune trees.

Pruning Decision Trees



- How to decide what leaves to prune?
- Solution: prune based on classification error threshold.

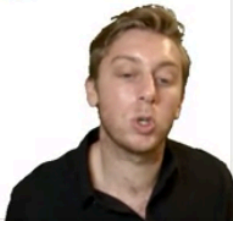
$$E(t) = 1 - \max_i [p(i|t)]$$

Cross validation and pruning sometimes help with some of this.
Great advantages of decision trees are that they are really easy to interpret and require no data preprocessing.

Code

```
# Import the class containing the classification method
from sklearn.tree import DecisionTreeClassifier

# Create an instance of the class
DTC = DecisionTreeClassifier (criterion='Gini',
max_features=10, max_depth=5)

# Fit the instance on the data and then predict the expected
value
DTC = DTC.fit(X_train, y_train)
y_predict = DTC.predict(X_test)

Tune parameters with cross-validation. Use
DecisionTreeRegressor for regression.
```

tree parameters



Stratified-Shuffle-Split Method

- Use `StratifiedShuffleSplit` to split data into train and test sets that are stratified by wine quality. If possible, preserve the indices of the split for question 5 below.
- Check the percent composition of each quality level for both the train and test data sets.

```
### BEGIN SOLUTION
# All data columns except for color
feature_cols = [x for x in data.columns if x not in 'color']
```

```
from sklearn.model_selection import StratifiedShuffleSplit

# Split the data into two parts with 1000 points in the test data
# This creates a generator
strat_shuff_split = StratifiedShuffleSplit(n_splits=1, test_size=1000, random_state=42)

# Get the index values from the generator
train_idx, test_idx = next(strat_shuff_split.split(data[feature_cols], data['color']))

# Create the data sets
X_train = data.loc[train_idx, feature_cols]
y_train = data.loc[train_idx, 'color']

X_test = data.loc[test_idx, feature_cols]
y_test = data.loc[test_idx, 'color']
```

Now check the percent composition of each quality level in the train and test data sets. The data set is mostly white wine, as can be seen below.

```
y_train.value_counts(normalize=True).sort_index()
```

```
0    0.753866
1    0.246134
Name: color, dtype: float64
```

remarks

n_splits=1 (only split once on ‘y’ (wine color) = white / red, two outcomes)
test_size=1000 (rows, before used percentage on train_test_split)
next() – built-in-function in python, 迭代
data.loc[train_idx, feature_cols]

GridSearchCV to prune tree

```
### BEGIN SOLUTION
from sklearn.model_selection import GridSearchCV

param_grid = {'max_depth':range(1, dt.tree_.max_depth+1, 2),
              'max_features': range(1, len(dt.feature_importances_)+1)}

GR = GridSearchCV(DecisionTreeClassifier(random_state=42),
                  param_grid=param_grid,
                  scoring='accuracy',
                  n_jobs=-1)

GR = GR.fit(X_train, y_train)
```

The number of nodes and the maximum depth of the tree.

```
GR.best_estimator_.tree_.node_count, GR.best_estimator_.tree_.max_depth
```

```
(99, 7)
```

remarks

param_grid (dict)
scoring='accuracy' (gridsearch need to maximize a value, here need to max 'accuracy')
n_jobs= -1 (paralyze across all of the power, all the functionality that's available on our computer)

DecisionTree Regressor

```
from sklearn.tree import DecisionTreeRegressor

dr = DecisionTreeRegressor().fit(X_train, y_train)

param_grid = {'max_depth':range(1, dr.tree_.max_depth+1, 2),
              'max_features': range(1, len(dr.feature_importances_)+1)}

GR_sugar = GridSearchCV(DecisionTreeRegressor(random_state=42),
                    param_grid=param_grid,
                    scoring='neg_mean_squared_error',
                     n_jobs=-1)

GR_sugar = GR_sugar.fit(X_train, y_train)
```

The number of nodes and the maximum depth of the tree. This tree has lots of nodes, which is not so surprising given the continuous data.

```
GR_sugar.best_estimator_.tree_.node_count, GR_sugar.best_estimator_.tree
```

```
(7475, 23)
```

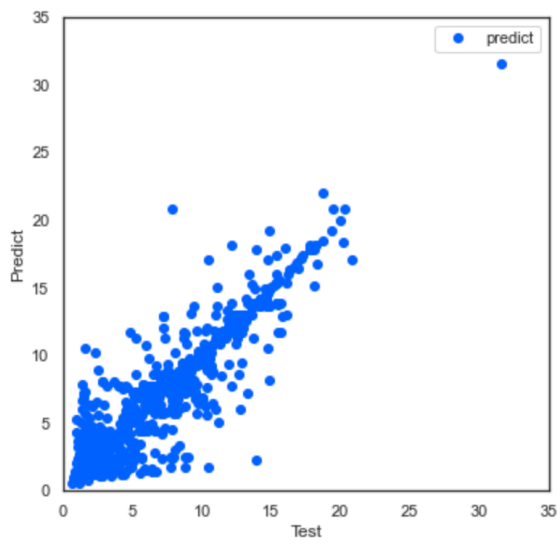
remarks

scoring='neg_mean_squared_error'
(gridsearch need to maximize a value, here need to

minimize the MSE, so equals to maximize neg_MSE)

Plot actual vs. predicted

```
sns.set_context('notebook')
sns.set_style('white')
fig = plt.figure(figsize=(6,6))
ax = plt.axes()

ph_test_predict = pd.DataFrame({'test':y_test.values,
                                'predict': y_test_pred_gr_sugar}).set_index('test').sort_index()

ph_test_predict.plot(marker='o', ls='', ax=ax)
ax.set(xlabel='Test', ylabel='Predict', xlim=(0,35), ylim=(0,35));
### END SOLUTION
```



If actual = predicted, 应该是一条对角线。

Plot the TREE (not prune vs. prune)

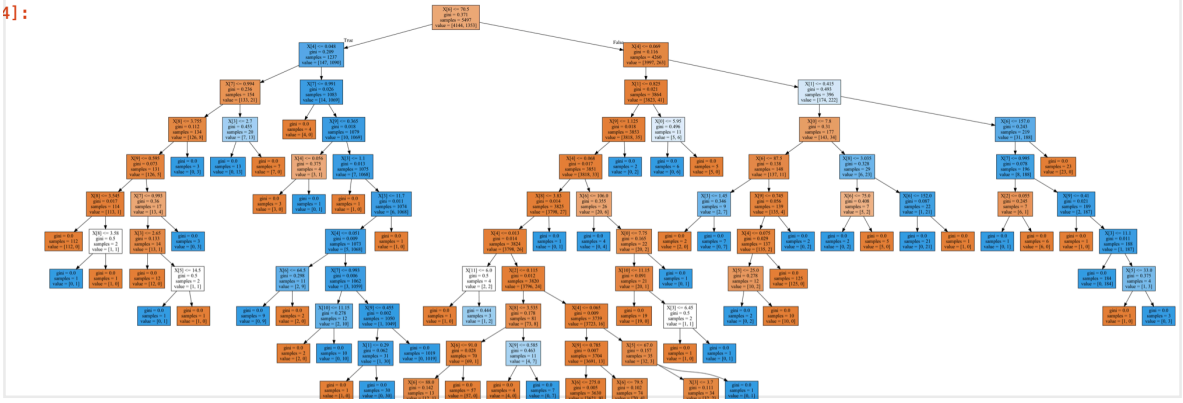
```
from io import StringIO
from IPython.display import Image
from sklearn.tree import export_graphviz
!pip install pydotplus
```

StingIO (we can dump out the file as a string)
Image (show image within Jupiter notebook)
sklearn.tree — export_graphviz (allow to take a graph which is our learned model and export into a file)
pydotplus (will take that file and allow us to render an actual image)

Not prune the tree: (original dt model)

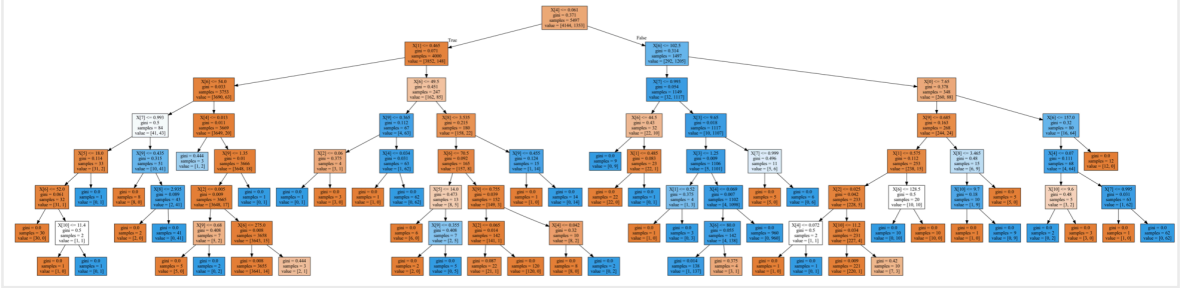
```
4]: ### BEGIN SOLUTION
    # Create an output destination for the file
    dot_data = StringIO()

    export_graphviz(dt, out_file=dot_data, filled=True)
    graph = pydotplus.graph_from_dot_data(dot_data.getvalue())

    # View the tree image
    filename = 'wine_tree_no_prune.png'
    graph.write_png(filename)
    Image(filename=filename)
```

4]:



Prune the tree (by grid search model)

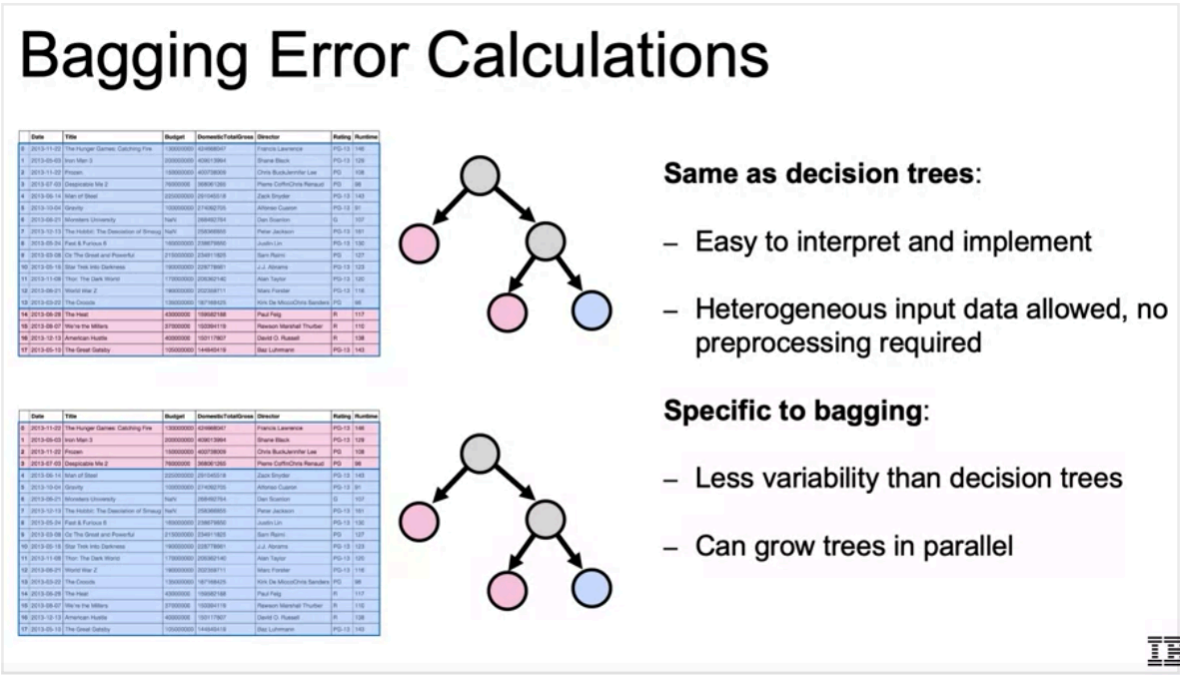
```
# Create an output destination for the file
dot_data = StringIO()

export_graphviz(GR.best_estimator_, out_file=dot_data, filled=True)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())

# View the tree image
filename = 'wine_tree_prune.png'
graph.write_png(filename)
Image(filename=filename)
### END SOLUTION
```



Wk3_Ensemble Based Methods and Bagging (2022.01.06)

Tree ensembles have been found to generalize well when scoring new data. Some useful and popular tree ensembles are bagging, boosting, and random forests.

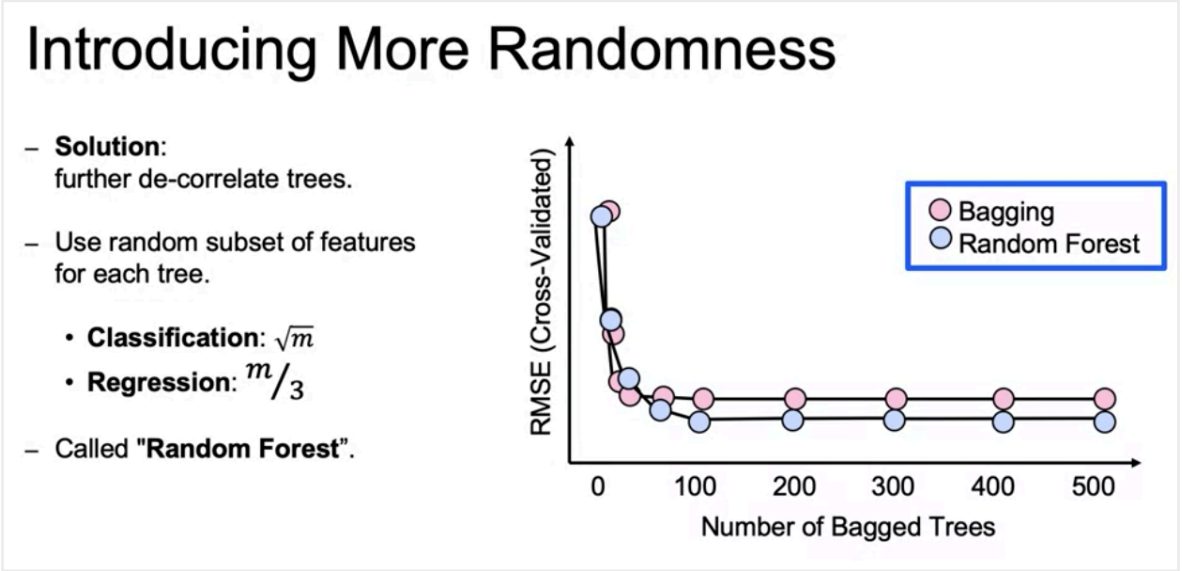
Bagging, which combines decision trees by using bootstrap aggregated samples.
An advantage specific to bagging is that this method can be multithreaded or computed in parallel. Most of these ensembles are assessed using out-of-bag error.



Random Forest

Random forest is a tree ensemble that has a similar approach to bagging. Their main characteristic is that they add randomness by only using a subset of features to train each split of the trees it trains.

Extra Random Trees is an implementation that adds randomness by creating splits at random, instead of using a greedy search to find split variables and split points.



Code

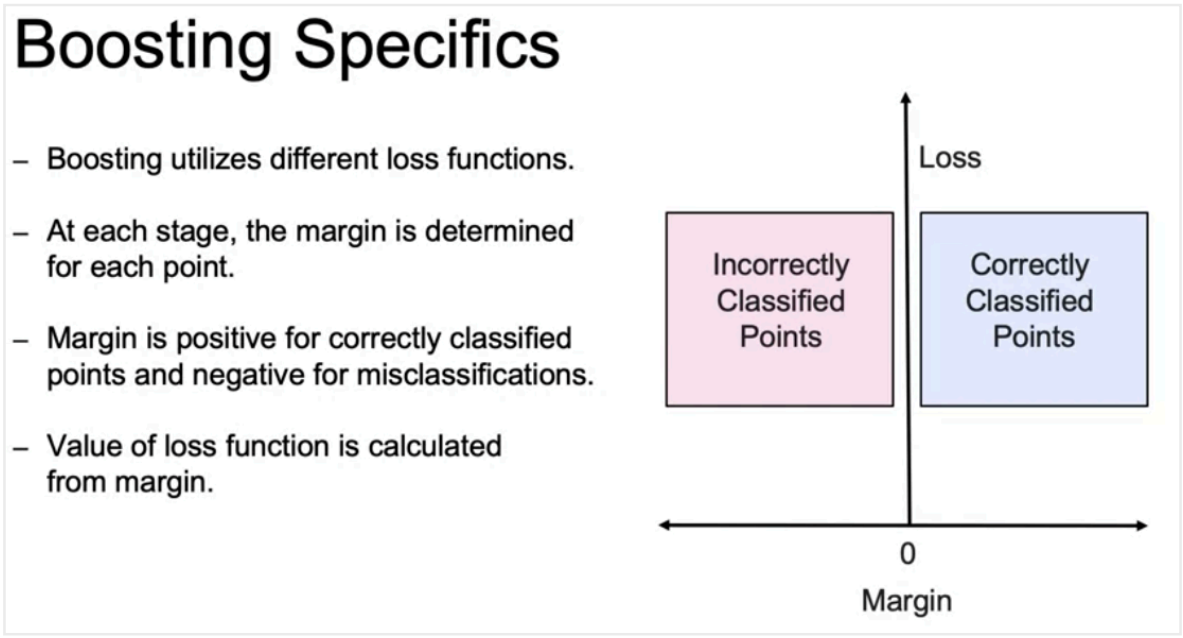
```
# Import the class containing the classification method
from sklearn.ensemble import RandomForestClassifier

# Create an instance of the class
RC = RandomForestClassifier(n_estimators=50)

# Fit the instance on the data and then predict the expected value
RC = RC.fit(X_train, y_train)
y_predict = RC.predict(X_test)

Tune parameters with cross-validation. Use RandomForestRegressor for regression.
```

Code

```
# Import the class containing the classification method
from sklearn.ensemble import ExtraTreesClassifier

# Create an instance of the class
EC = ExtraTreesClassifier (n_estimators=50)

# Fit the instance on the data and then predict the expected value
EC = EC.fit(X_train, y_train)
y_predict = EC.predict(X_test)

Tune parameters with cross-validation. Use ExtraTreesRegressor for regression.
```

Boosting

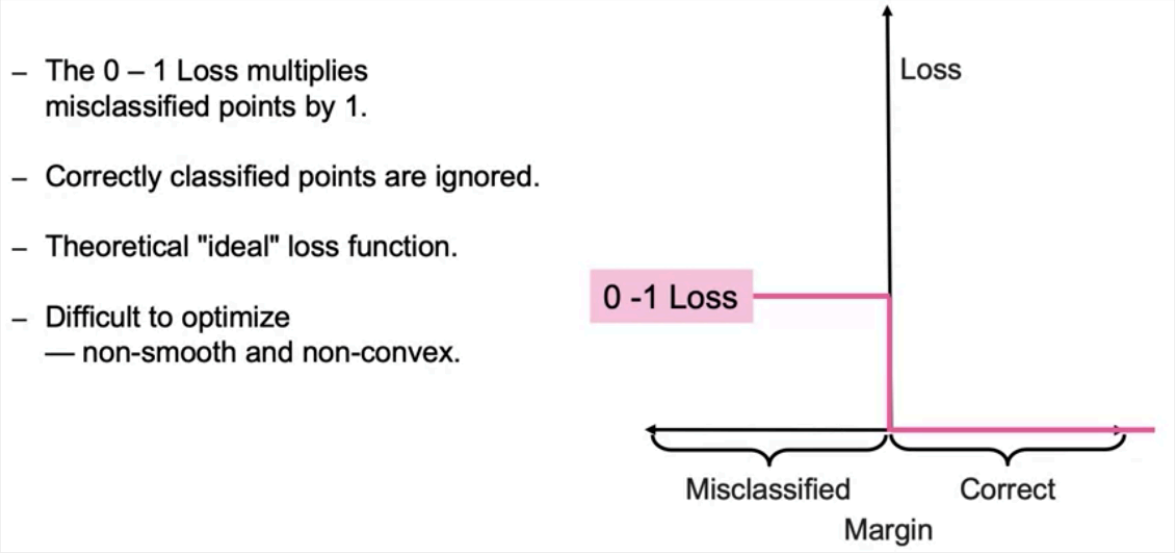
Boosting methods are additive in the sense that they sequentially retrain decision trees using the observations with the highest residuals on the previous tree.
To do so, observations with a high residual are assigned a higher weight.



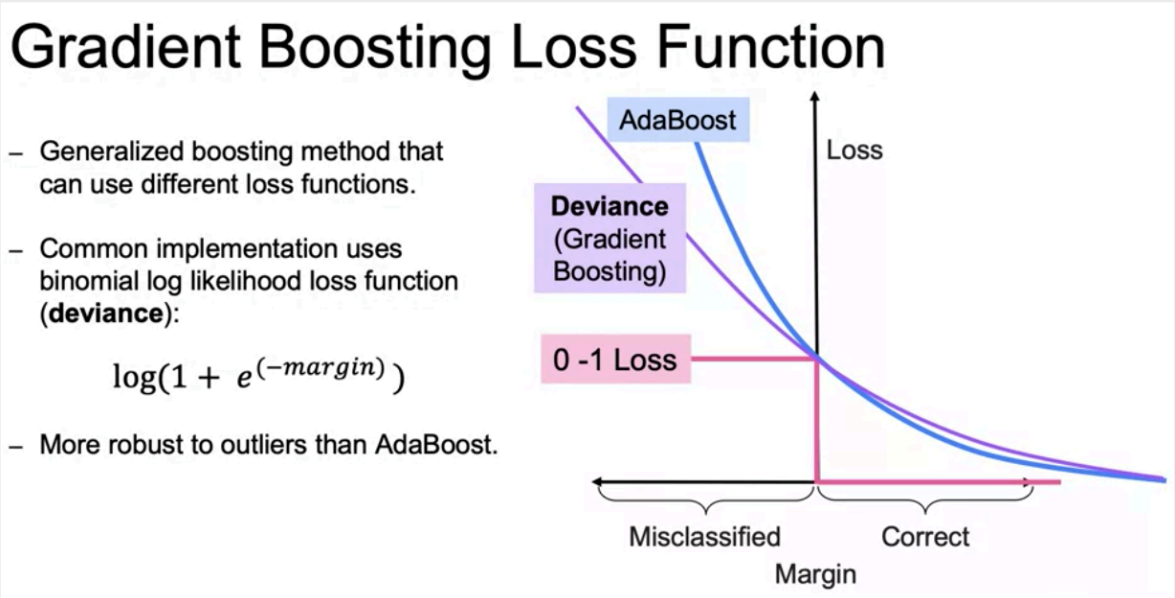
Gradient Boosting

The main loss functions for boosting algorithms are:

- *0-1 loss function*, which ignores observations that were correctly classified. The shape of this loss function makes it difficult to optimize.



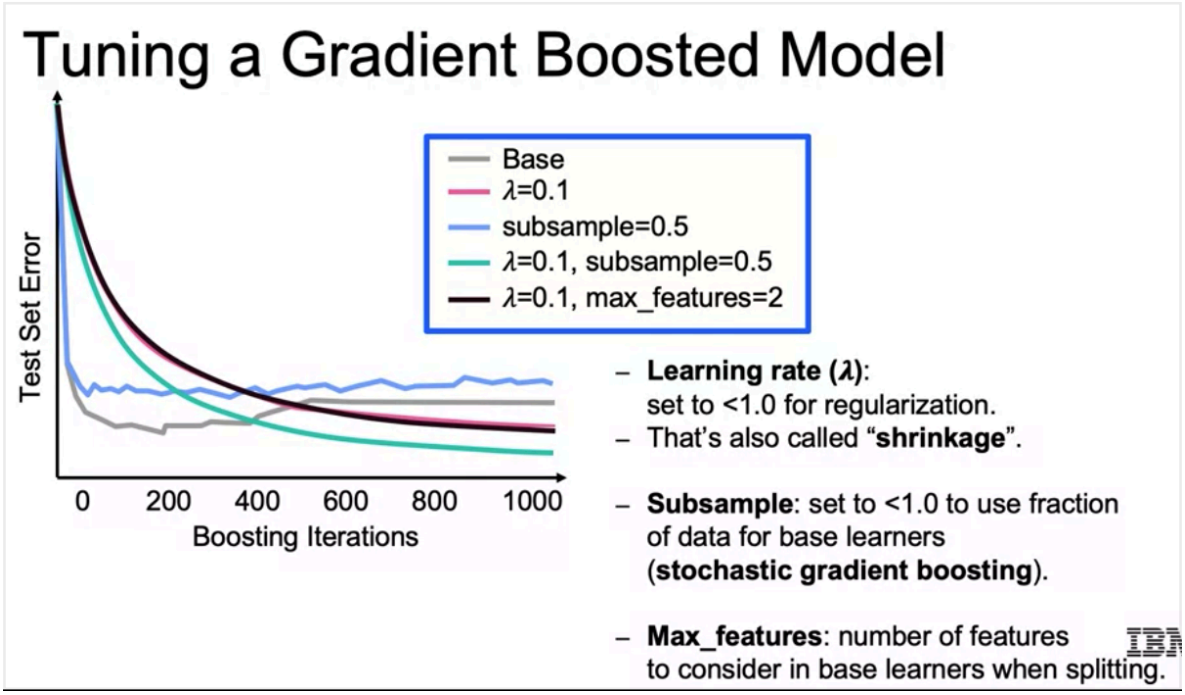
- *Adaptive boosting loss function*, which has an exponential nature. The shape of this function is more sensitive to outliers.



- *Gradient boosting loss function*. The most common gradient boosting implementation uses a binomial log-likelihood loss function called deviance. It tends to be more robust to outliers than AdaBoost.

The additive nature of gradient boosting makes it prone to overfitting.
This can be addressed using cross validation or fine tuning the number of boosting iterations.
Other hyperparameters to fine tune are:

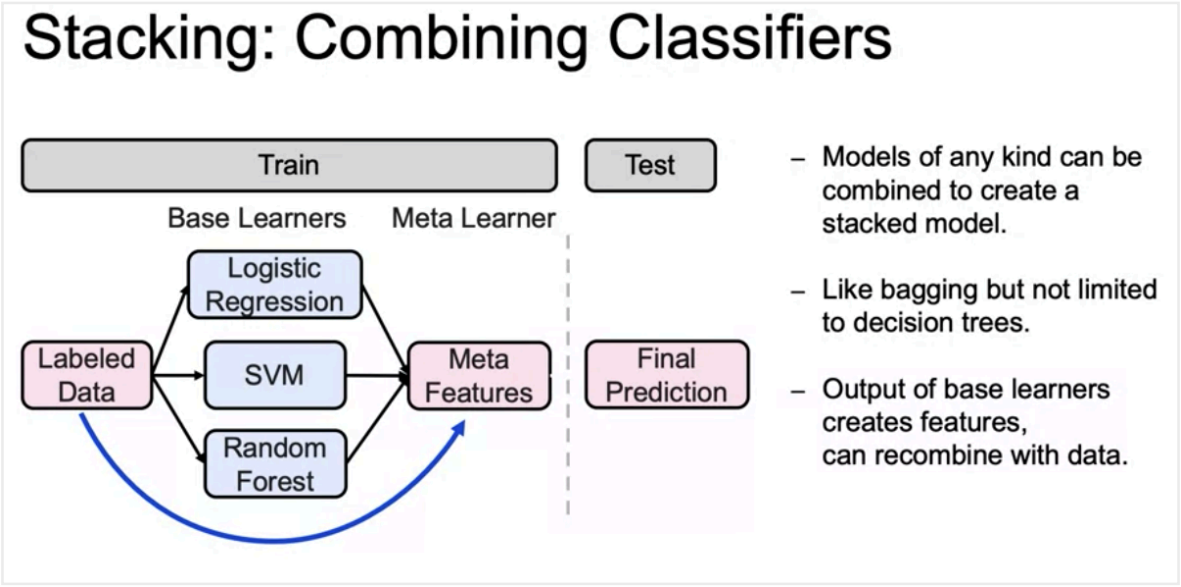
- learning rate (shrinkage). <1
- subsample. 0.5
- number of features. max_features

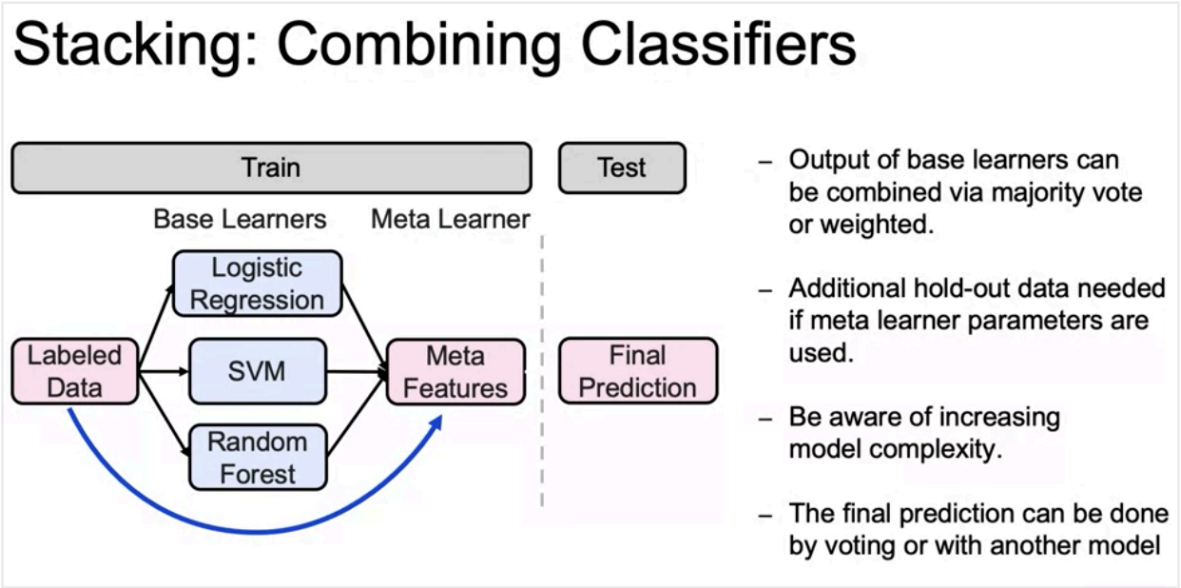


Stacking

Stacking is an ensemble method that combines any type of model by combining the predicted probabilities of classes.
In that sense, it is a generalized case of bagging.
The two most common ways to combine the predicted probabilities in stacking

are: using a majority vote or using weights for each predicted probability.





Code

```
# Import the class containing the classification method
from sklearn.ensemble import VotingClassifier

# Create an instance of the class
VC = VotingClassifier(estimator_list)

# Fit the instance on the data and then predict the expected value
VC = VC.fit(X_train, y_train)
y_predict = VC.predict(X_test)

Use VotingRegressor for regression.

The StackingClassifier (or StackingRegressor) works similarly:
SC = StackingClassifier(estimator_list, final_estimator=LogisticRegression())
```

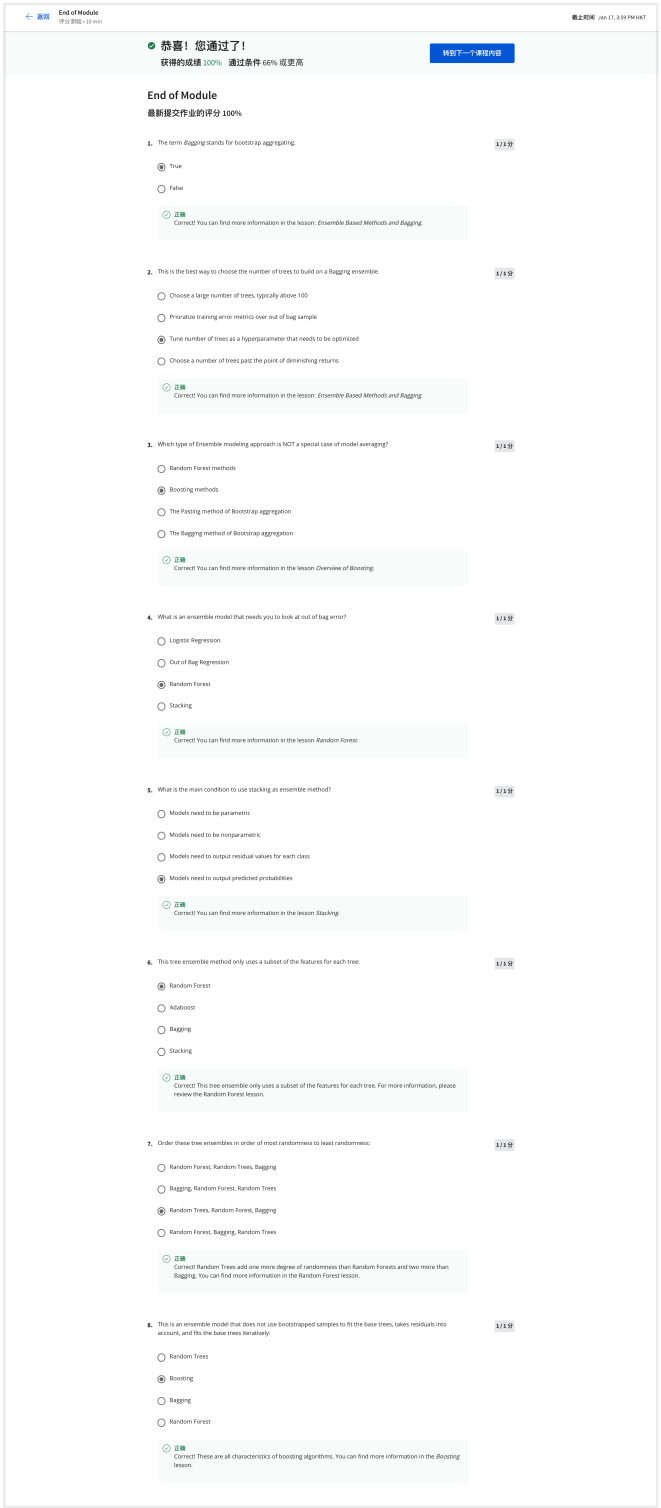
In this section, we discussed:

- The Boosting approach to combining models
- Types of Boosting models: Gradient Boosting, AdaBoost
- Boosting loss functions
- Combining heterogeneous classifiers

Further reading:

- XGBoost is another popular boosting algorithm (not in Scikit-Learn).

Exam (Check every question!!)



Wk4_Unbalanced Classes (2022.01.07)

Modeling Unbalanced Classes

Classification algorithms are built to optimize accuracy, which makes it challenging to create a model when there is not a balance across the number of observations of different classes.

Common methods to approach balancing the classes are:

- Downsampling or removing observations from the most common class

Downsampling adds tremendous importance to the minor class, typically shooting up recall and bringing down precision.

Values like 0.8 recall and 0.15 precision isn't uncommon.

- Upsampling or duplicating observations from the rarest class or classes

Upsampling mitigates some of the excessive weight on the minor class. Recall is still typically higher than precision, but the gap is lesser.

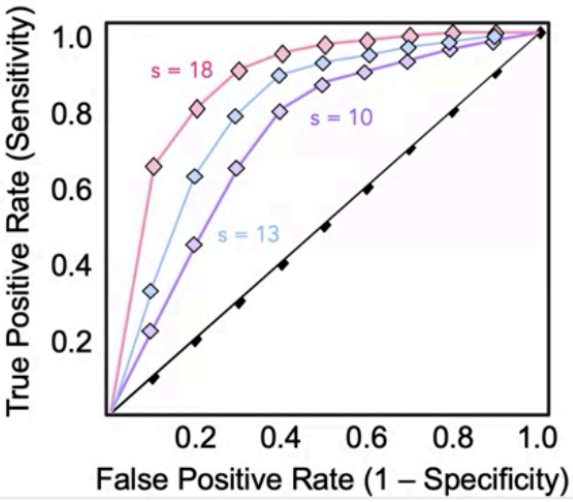
Values like 0.7 recall and 0.4 precision isn't uncommon. And are often considered good results for an unbalanced dataset.

- A mix of downsampling and upsampling

Steps for unbalanced datasets:

- Do a stratified test-train split
- Up or down sample the full dataset
- Build models

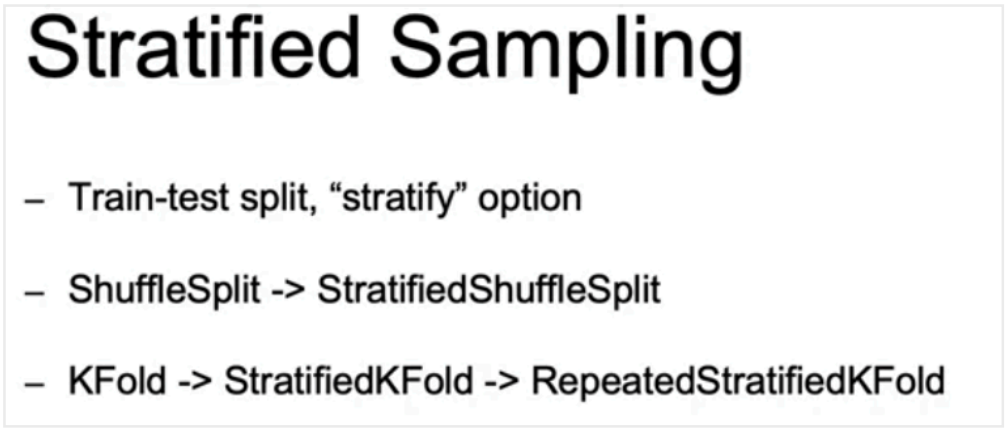
Cross-validation works for any global model-making choice, including sampling.



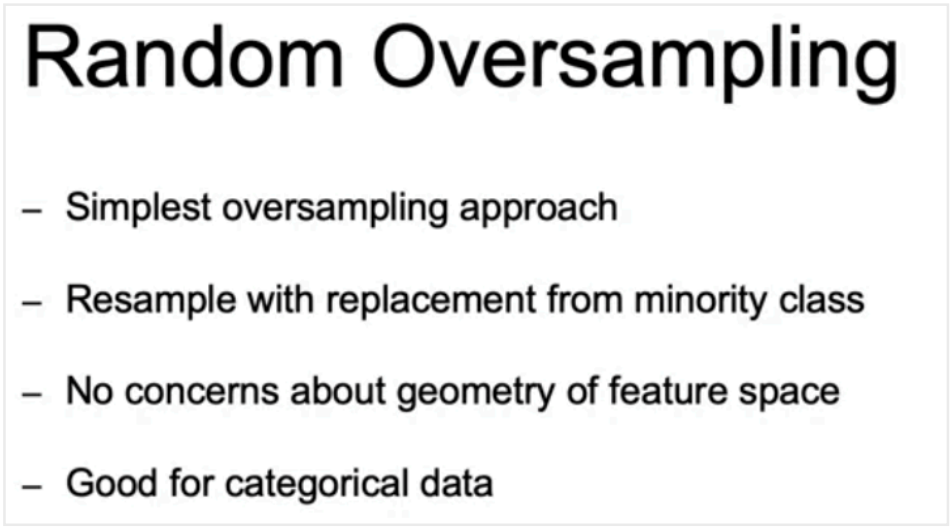
Modeling Approaches for Unbalanced Classes

Specific algorithms to upsample and downsample are:

- Stratified sampling



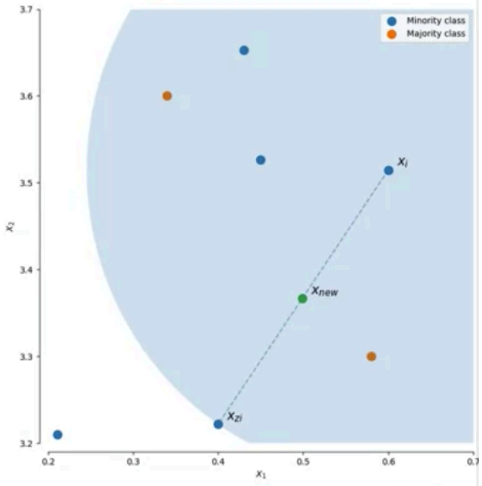
- Random oversampling



- Synthetic oversampling,
    - the main two approaches being :
        - Synthetic Minority Oversampling Technique **(SMOTE)** and;
        - Adaptive Synthetic sampling **(ADASYN)**

Synthetic Oversampling

- Start with a point in the minority class
- Choose one of K nearest neighbors
- Add a new point between them
- Two main approaches:
  - SMOTE
  - ADASYN



http://contrib.scikit-learn.org/imbalanced-learn/stable/over_sampling.html#a-practical-guide

SMOTE:
Synthetic Minority Oversampling Technique

- **Regular**: Connect minority class points to any neighbor (even other classes)
- **Borderline**: Classify points as outlier, safe, or in-danger
  - **1**: Connect minority in-danger points only to minority points
  - **2**: Connect minority in-danger points to whatever is nearby
- **SVM**: Use minority support vectors to generate new points

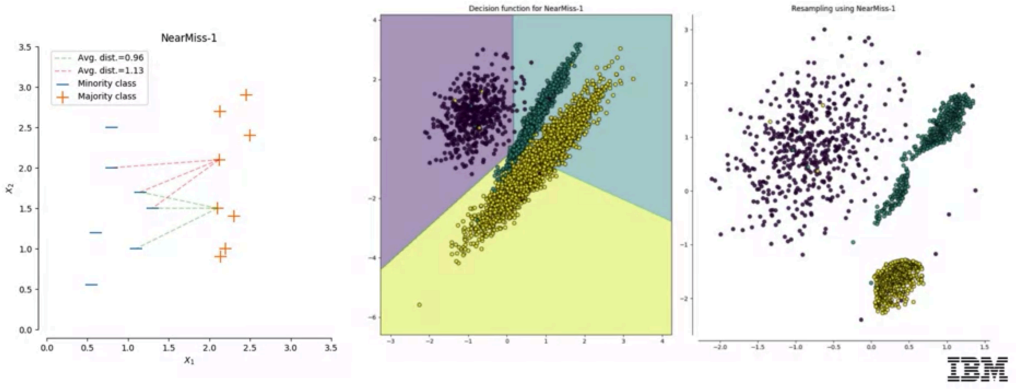
ADASYN:
ADAptive SYNthetic sampling

- For each minority point:
  - Look at classes in neighborhood
  - Generate new samples proportional to competing classes
- Motivated by KNN, but helps other classifiers as well

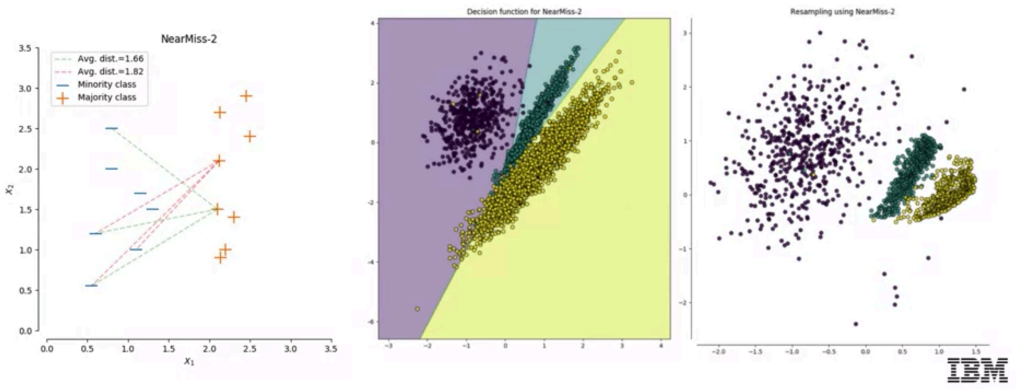
- Cluster Centroids implementations like:
  - NearMiss 1,2,3
  - Tomek Links, and;
  - Nearest Neighbors

imbalanced-learn documentation:
https://imbalanced-learn.org/stable/index.html

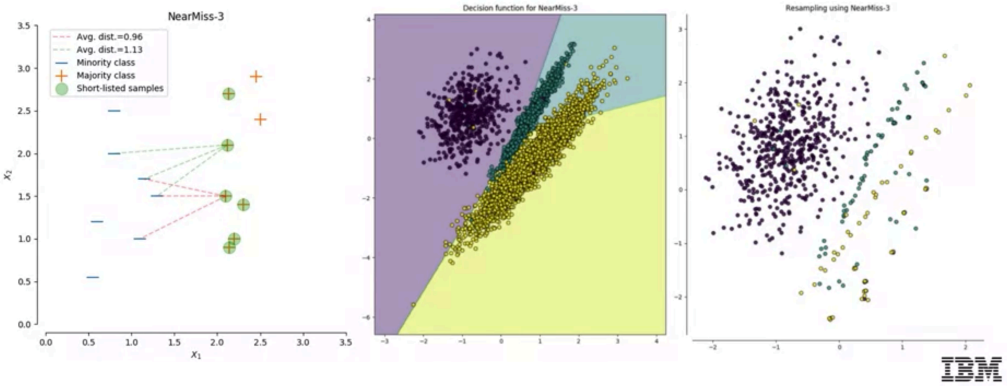
NearMiss-1: Which Points to Keep? Those Closest to Nearby Minority Points



NearMiss-2: Which Points to Keep? Those Closest to Distant Minority Points



NearMiss-3: Those Closest to Majority Neighbors of Minority Points



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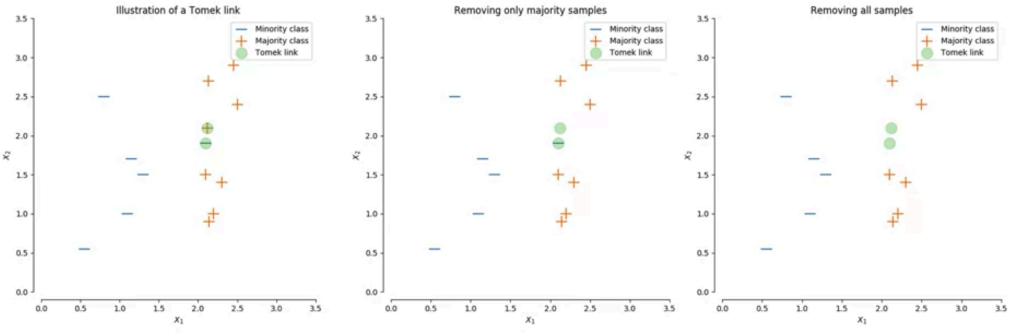
Tomek Links: Mixed Mutual Nearest Neighbors



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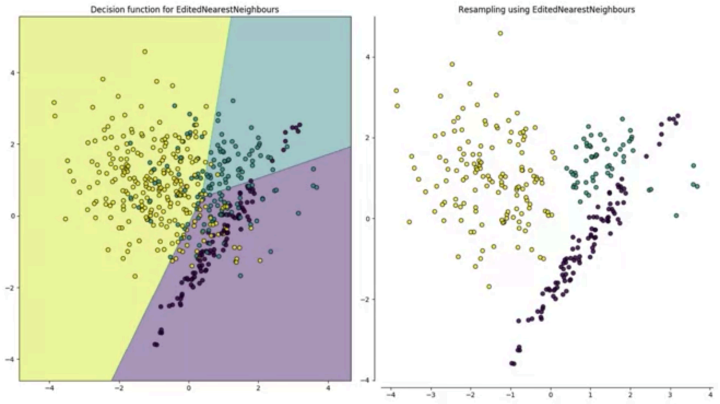
Edited Nearest Neighbors

- Remove points that don't agree with neighbors



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Combination Over/Under

- SMOTE + Tomek's link
- SMOTE + Edited Nearest Neighbors

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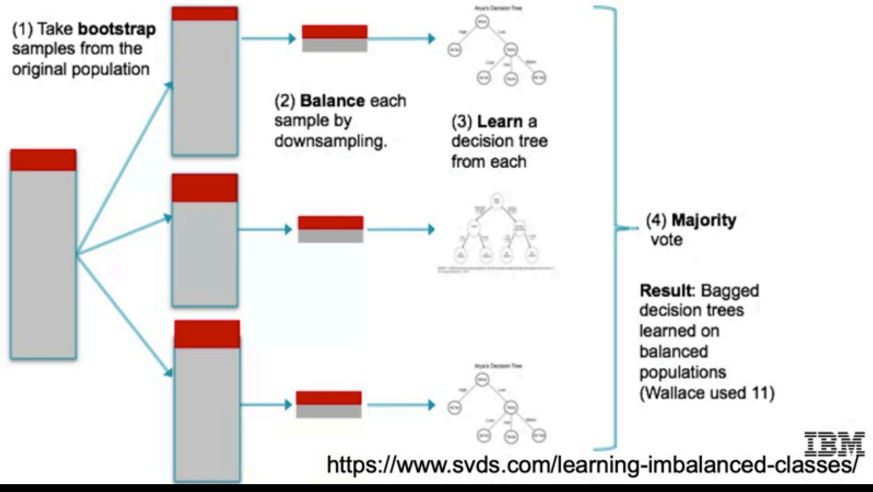
Blagging (Balanced Bagging)



https://www.svds.com/learning-imbalanced-classes/

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Unbalanced Classes: Summary

- All of this happens after the test set has been split.
- Use sensible metrics
  - AUC
  - F1
  - Cohen's Kappa
  - Not accuracy - too easy to fool in this case

Now that first step is going to ensure that you first do your train test split before doing any of this over or undersampling. Recall that if we do this oversampling first, we can end up with values being both represented in the train and test set, which means we can very easily overfit, have that data leakage and even if we're synthetically creating those new samples, those values will be very close to those train set samples and we can still have that overfitting. So always do your train test split first.

Then we have here Cohen's Kappa. This is a new one that we haven't discussed, but we felt it was worth at least letting you all know that it's available. This is best if you're working with a team and it's actually a measure of agreement between two different raters or two different models, where each rater will be classifying n items into mutually exclusive categories so just performing classification, and the goal here is to come up with a ratio of observed agreement between these two models as compared to the probability of there being agreement just by chance. So with unbalanced classes, we want to make sure that we have strong agreement and that agreement between those two different models are better than just agreement by chance. So the higher this value is for Cohen's Kappa, the more you can trust the agreed upon predictions of those two models.

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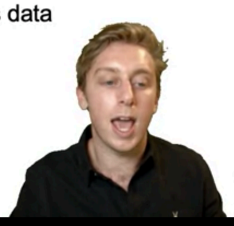
Learning Recap

In this section, we discussed:

- Additional approaches to dealing with unbalanced outcomes
- Random and Synthetic Over Sampling
- Techniques for Under Sampling
- Using Balanced Bagging (Blagging) to address unbalanced class data

Note: I want you to note here that for both of them, they each have their advantages and practices for each one of them, for the specific techniques for each of them. But it'll often be difficult to tell for oversampling or undersampling which technique to use without cross-validation since we can almost never visualize as clearly as we did in each one of these examples. But when deciding between under or oversampling in general, remember what we discussed earlier. Undersampling will probably lead to a bit of a higher recall for that minority class at the cost of precision whereas oversampling will keep all the values from our majority class and thus will have a bit of a lower recall than undersampling, but better precision on those predictions.



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← 返回 Modeling Unbalanced Classes
练习测验 • 4 min

⚠ 准备好后再次尝试
获得的成绩 50% 通过条件 66% 或更高

再试

Modeling Unbalanced Classes

总分 2

1. These are all methods of dealing with unbalanced classes EXCEPT: 1 / 1 分

- ○ Downsampling.
- ◉ Mix of in-sample and out-of-sample.
- ○ Mix of downsampling and upsampling.
- ○ Upsampling.

✓ 正确
Correct! You can find more information in the lesson *Upsampling and Downsampling.*

2. (True/False) A best practice to build a model using unbalanced classes is to split the data first, then apply an upsample or undersample technique. 0 / 1 分

- ○ True
- ◉ False

✗ 错误
Incorrect. A best practice is to do a stratified train/test split before, then use an upsample or downsample technique, and last build a predictive model. You can find more information in the lesson *Upsampling and Downsampling.*