# Ensembles of classifiers: Bagging and Boosting


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# The Misclassification Error

Let C(x, L ) be the classifier constructed by using the training sample L., and T another large sample from the same population as L was drawn from, then the misclassification error (ME) of the classifier C is the proportion of misclassified cases of T using C.

The ME can be descomposed as

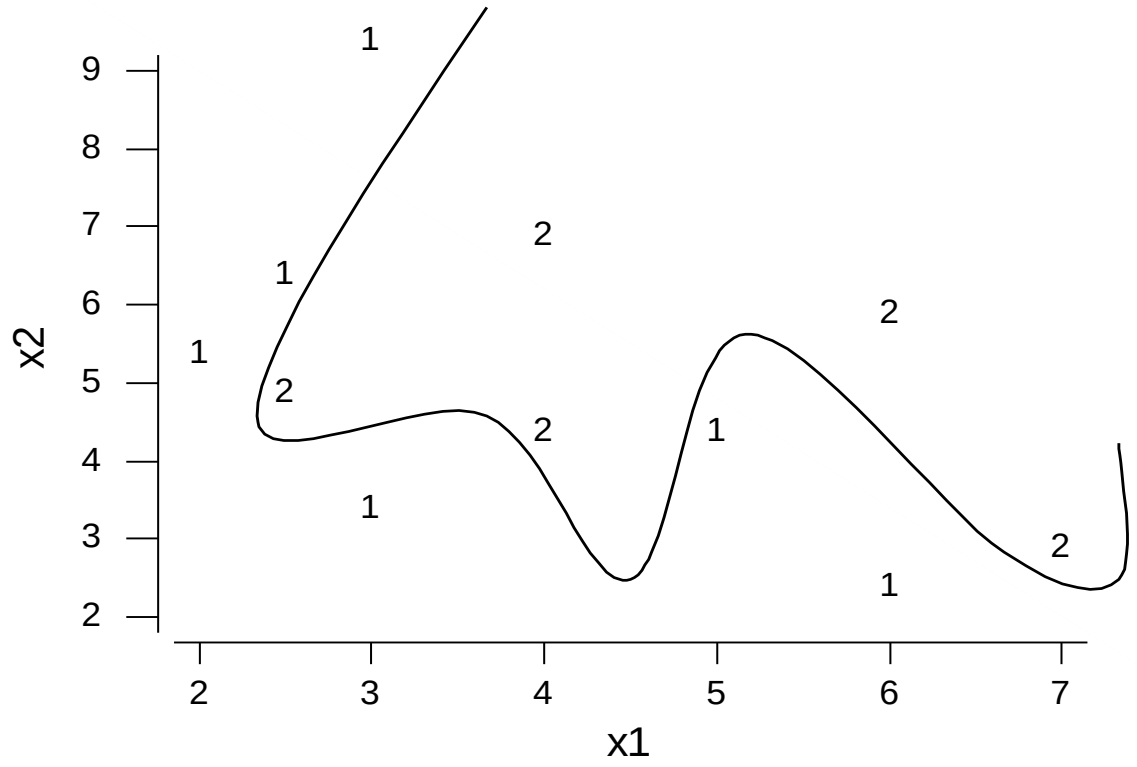
$$ME(C)=ME(C^*)+Bias^2(C)+Var(C)$$

where $C^*(x)=argmax_j P(Y=j/X=x)$ (Bayes Classifier)

Methods to estimate ME: Resubstitution, Crossvalidation, Bootstrapping

The classifier may either overfit the data (Low bias and large variance) or underfit the data ( Large bias and small variance).
Breiman (1996) heuristically defines a classifier as unstable if a small change in the data *L* can make large changes in the classification. Unstable classifiers have low bias but high variance.
CART and Neural networks are unstable classifiers.
Linear discriminant analysis and K-nearest neighbor classifiers are stable.

# Overfitting



# Combination of clasiffiers (Ensembles)

It is possible to reduce the bias and variance of the misclassification error by combining the prediction of several classifiers. This combination is called an **Ensemble** and in general is more precise than the individual classifiers. Among the methods used to build ensembles are the following:

**Bagging** (Bootstrap aggregating by Breiman, 1996)

**AdaBoosting** (Adaptive Boosting by Freund and Schapire, 1996)

**Arcing** (Adaptively resampling and combining, by Breiman (1998).

**Gradient Boosting** ( Friedman,1999)

**XGboosting (Chen, 2014)**

# Bootstrap Sample

A bootstrap sample of a training sample L is a sample with replacement taken from L and of the same size than L

```
x=[5,3,12,13,21,31,8,9,15,17,24,32]  # This is the original sample
boot1=np.random.choice(x,12)  #Extracting one bootstrap sample
print boot1
[31 8 5 31 24 13 21 3 32 9 9 17]
np.unique(boot1)
array([ 3, 5, 8, 9, 13, 17, 21, 24, 31, 32])
boot2=np.random.choice(x,12) #Second bootstrap sample
print boot2
[ 5 12 12 13 13 15 9 13 24 15 21 12]
np.unique(boot2)
array([ 5, 9, 12, 13, 15, 21, 24])
```

Note: Approximately, 37% of the instances of the training sample L DO NOT appear in any bootstrap sample. In the above examples 16.67% and 41.67% of instances do not appear in each of the bootstrap samples.

# The Bagging Algorithm: Breiman (1996)

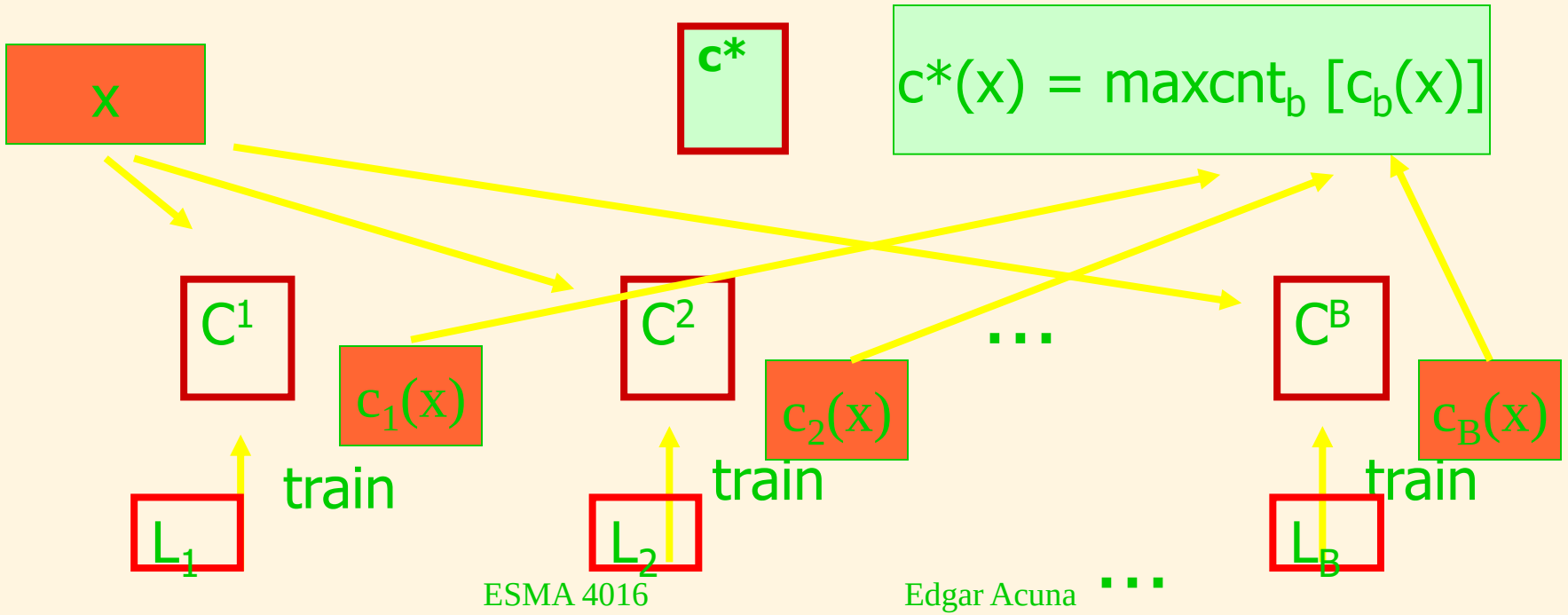
**Input:** learning set $\iota$ , classifier C, integer T (number of bootstrap samples), J classes.

1. For i=1 to T {
2. $B_i$= Bootstrap sample from $\iota$ ( sample with replacement)
3. $C_i=C(B_i)$
4. }
5. $C_A(x)= \underset{j\in\{1,\ldots..J\}}{\operatorname{argmax}} \sum_{i:C_i(x)=j} 1$ (The class most voted)

**Output:** Ensemble $C_A$

# Bagging with cross validation

- From the training sample **L** select B random samples with replacement (bootstrap samples) obtaining **B** different training samples $L_1,...,L_B$ of size N.
- For each sample $L_b$ a classifier $C^b$ is built .
- Using 10-fold cross validation , each case x of L is assigned to the class c*(x)=j by voting.



# Bagging using scikit-learn

```
url= "http://academic.uprm.edu/eacuna/diabetes.dat"
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
data = pd.read_table(url, names=names,header=None)
#The response varaiable must be binary  (0,1)
y=data['class']-1
X=data.iloc[:,0:8]
modeltree = tree.DecisionTreeClassifier()
bagging = BaggingClassifier(modeltree,n_estimators=100)
# Accuracy rate
bagging.fit(X, y)
predictions = bagging.predict(X)
print(classification_report(y, predictions))
#Estimating the accuracy by cross validation
kfold = model_selection.KFold(n_splits=10, random_state=99)
results = model_selection.cross_val_score(bagging, X, y, cv=kfold)
print(results.mean())
```

0.756459330144

# Out-of-Bag (OOB) error estimation

Assuming that K=100 bootstrap sample are drawn from the original sample L, then an instance of L will not be chosen in approximately 37 percent of these samples, therefore they can be considered as a test sample T.

Hence any instance would have something like 37 predictions. Using voting we can have a final prediction.

The missclassfication error rate estimated Out-of-bag is the average of the number of errors using those final predictions.

# Out-of-bag error estimation using sckit-learn

```
bagging1 = BaggingClassifier(modeltree,n_estimators=100, oob_score=True)
bagging1.fit(X, y)
bagging1.score(X,y)
1.0
```

# Boosting

In  this method, also bootstrap samples are chosen but given a selection weight to each instance. In the first bootstrap sample, all the instances have the same weight 1/N to be chosen, where N is the number of instances.

In the following steps this weight changes in such way the instances classified incorrectly in the previous sample have more weight to be selected in the next step. The instances correctly classified have less weight to be chosen in a later step.

The goal is to force the classifier to learn to classify correctly an instance, which is not easy to classify.

There are plenty versions of boosting, the first one is known as AdaBoosting. But the ones that are being used at the present are Gradient Boosting and XGBoost

**Adaboosting Algorithm:Freund & Schapire[1996]**

**Input:** Learning set $L$ , classifier C, integers N, T

1. B= $L$ with weights $w_1(x_j)=1/N$. For j=1,…..N

2. For i=1 to T { $C_i=C(B)$

3. Set $e_i = \sum_{x_j \in B: C_i(x_j) \neq y_j} w_i(\mathbf{x}_j)$ . If either $e_i>1/2$ or $e_i=0$ then restart assigning equal weights.

4. Set $\beta_i=e_i/(1-e_i)$

5. Udpate the weights: for each $x_j \in B$, if $C_i(x_j)\neq y_j$ then $w_{i+1}(x_j)=w_i(x_j)/2e_i$ , else $w_{i+1}(x_j)=w_i(x_j)/2(1-e_i)$}

6.$C^*(x)=\arg\max_{j\in\{1,\ldots..J\}} \sum_{i:C_i(x)=j} \log \frac{1}{\beta_i}$

**Output:** Ensemble C*

# Boosting

Below are the steps for performing the AdaBoost algorithm:
1.Initially, all observations are given equal weights.
2.A model is built on a subset of data.
3.Using this model, predictions are made on the whole dataset.
4.Errors are calculated by comparing the predictions and actual values.
5.While creating the next model, higher weights are given to the data points which were predicted incorrectly.
6.Weights can be determined using the error value. For instance,the higher the error the more is the weight assigned to the observation.
7.This process is repeated until the error function does not change, or the maximum limit of the number of estimators is reached.

# AdaBoosting using scikit-learn

```
adaboost = AdaBoostClassifier(modeltree,n_estimators=100,learning_rate=1)
adaboost.fit(X, y)
predictions = adaboost.predict(X)
print(classification_report(y, predictions))
      precision recall f1-score support
0      1.00     1.00      1.00      500
1      1.00     1.00      1.00      268
 avg / total 1.00 1.00 1.00     768
kfold = model_selection.KFold(n_splits=10, random_state=999)
results = model_selection.cross_val_score(adaboost, X, y, cv=kfold)
print(results.mean())
```

0.7252734108

# Gradient Boosting

Below are the steps for performing the Gradien Boosting algorithm:
1.A model is built on a subset of data.
2.Using this model, predictions are made on the whole dataset.
3.Errors are calculated by comparing the predictions and actual values.
4.A new model is created using the errors calculated as target variable. Our objective is to find the best split to minimise the error.
5.The predictions made by this new model are combined with the predictions of the previous.
6.New errors are calculated using this predicted value and actual value.
7.This process is repeated until the error function does not change, or the maximum limit of the number of estimators is reached.

# Gradient Boosting using scikit-learn

```
gboost = GradientBoostingClassifier(n_estimators=100)
gboost.fit(X, y)
predictions = gboost.predict(X)
print(classification_report(y, predictions))
             precision recall f1-score support
0             0.90      0.96   0.93      500
1             0.91      0.81   0.86      268
avg / total 0.91 0.91   0.90      768
kfold = model_selection.KFold(n_splits=10, random_state=999)
results = model_selection.cross_val_score(gboost, X, y, cv=kfold)
print(results.mean())
```

0.766900205058

# Gradient Boosting using h2o

```
diabetes = h2o.import_file("https://academic.uprm.edu/eacuna/diabetes.dat")
myx=['C1','C2','C3','C4','C5','C6','C7','C8']
diabetes['C9']=diabetes['C9'].asfactor()
myy="C9"
gbm1 = H2OGradientBoostingEstimator(model_id="gbm_covType_v1",ntrees = 100,
max_depth=3,nfolds=10, sample_rate = 1,col_sample_rate = 1,seed=2000000
)
gbm1.train(myx, myy, training_frame=diabetes)
y_pred=gbm1.predict(diabetes)
print (y_pred['predict']==diabetes['C9']).mean()
[0.9010416666666666]
```

# Previous results on combining classifiers

| Reference | Classifier | Relative Improv. (%) | |
|---|---|---|---|
| | | Bagging | Boosting |
| Breiman (1996) | CART | 29.0 | ------ |
| Freund & Schapire (1996) | C4.5 | 20.0 | 24.8 |
| Quinlan (1996) | C4.5 | 10.0 | 15.01 |
| Maclin & Opitz (1997) | C4.5 | 18.5 | 22.0 |
| Maclin & Opitz (1997) | Neural Net | 13.3 | 17.1 |
| Breiman (1998) | CART | 36.0 | 48.4 |
| Bauer & Kohavi (1999) | MC4 | 14.5 | 27.0 |
| Dietterich(2000) | C4.5 | 16.9 | 22.4 |
| Daza (2002) | G.M. | 10.1 | 0.8 |
| Acuna & Rojas (2002) | Kernel | 4.9 | 1.9 |

- Bagging reduces variance. AdaBoosting reduces both bias and variance
- Bagging can be parallelized easily, but Boosting is essentially sequential and only some part of the algoruthm can be parallelized.
- Boosting is only useful for large sample datasets and for classifiers that perform poorly.

# XGBoosting (Extreme Gradient Boosting)

- Extreme Gradient Boosting is an advanced implementation of the Gradient Boosting. This algorithm has high predictive power and is ten times faster than any other gradient boosting techniques. Moreover, includes a variety of regularisation which reduces overfitting and improves overall performance.
- Execution Speed: Generally, XGBoost is fast. Really fast when compared to other implementations of gradient boosting.
- Model Performance: XGBoost dominates structured or tabular datasets on classification and regression predictive modeling problems. The evidence is that it is the go-to algorithm for competition winners on the Kaggle competitive data science platform.

# XGBoosting (Extreme Gradient Boosting)

- **What is the difference between the gradient boosting machine) and xgboost (extreme gradient boosting)?**
- Both xgboost and gbm follows the principle of gradient boosting. There are however, the difference in modeling details. Specifically, xgboost used a more regularized model formalization to control over-fitting, which gives it better performance.
- Objective Function : Training Loss + Regularization
- The regularization term controls the complexity of the model, which helps us to avoid overfitting.