Introduction to Machine Learning

Measures of Accuracy

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Outline

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What did we see until now?

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Under a data set

$$\mathcal{D} = \{(\boldsymbol{x}_i, y_i) \,|i = 1, 2, ..., N\} \tag{1}$$

Remark: Where the $\boldsymbol{x}_i \sim p(\boldsymbol{x}|\Theta)$!!!

Thus, we have that

Two main functions

- A function $g(\boldsymbol{x}|\mathcal{D})$ obtained using some algorithm!!!

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The approximation may be very good for a specific training data set but very bad for another.

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The key factor here is the dependence of the approximation on $\mathcal{D}$.

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The approximation may be very good for a specific training data set but very bad for another.

- This is the reason of studying fusion of information at decision level...

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How do we measure the difference?

We can use the variance

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Now, if we add and subtract

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Remark: The expected output of the machine $g\left(\boldsymbol{x}|\mathcal{D}\right)$

Thus, we have that

Or Original variance

$$
\begin{aligned}
Var_{\mathcal{D}}\left(g\left(\boldsymbol{x}|\mathcal{D}\right)\right) &= E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right) - E\left[y|\boldsymbol{x}\right]\right)^2\right) \\
&= E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] + E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right)^2\right) \\
&= E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)^2 + ... \right. \\
&...2\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)\right)\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right) + ... \\
&... \left.\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right)^2\right)
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Finally

$$E_D\left(\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)\right)\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right)\right) =? \quad (3)$$

Outline

We have the Bias-Variance

Our Final Equation

$$E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right)-E\left[y|\boldsymbol{x}\right]\right)^2\right)=\underbrace{E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right)-E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)^2\right)}_{VARIANCE}+\underbrace{\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]-E\left[y|\boldsymbol{x}\right]\right)^2}_{BIAS}$$

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Where the variance

It represents the measure of the error between our machine $g\left(\boldsymbol{x}|\mathcal{D}\right)$ and the expected output of the machine under $\boldsymbol{x}_i \sim p\left(\boldsymbol{x}|\Theta\right)$.

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Where the variance

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Where the bias

It represents the quadratic error between the expected output of the machine under $\boldsymbol{x}_i\sim p\left(\boldsymbol{x}|\Theta\right)$ and the expected output of the optimal regression.

Remarks

We have then

Even if the estimator is unbiased, it can still result in a large mean square error due to a large variance term.

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1. Increasing the bias decreases the variance and vice versa.

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Even if the estimator is unbiased, it can still result in a large mean square error due to a large variance term.

The situation is more dire in a finite set of data $\mathcal{D}$

We have then a trade-off:

1. Increasing the bias decreases the variance and vice versa.
2. This is known as the **bias–variance dilemma**.

Similar to...

Curve Fitting

If, for example, the adopted model is complex (many parameters involved) with respect to the number N, the model will fit the idiosyncrasies of the specific data set.

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Furthermore

If N grows we can have a more complex model to be fitted which reduces bias and ensures low variance.

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Furthermore

If N grows we can have a more complex model to be fitted which reduces bias and ensures low variance.

- However, N is always finite!!!

Thus

You always need to compromise

However, you always have some a priori knowledge about the data

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Allowing you to impose restrictions

Lowering the bias and the variance

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Nevertheless

We have the following example to grasp better the bothersome **bias–variance dilemma**.

For this

Assume

The data is generated by the following function

$$y = f(x) + \epsilon,$$
$$\epsilon \sim \mathcal{N}\left(0, \sigma_\epsilon^2\right)$$

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Furthermore

Assume that the randomness in the different training sets, $\mathcal{D}$, is due to the y_i's (Affected by noise), while the respective points, x_i, are fixed.

Outline

Sampling the Space

Imagine that $\mathcal{D} \subset [x_1, x_2]$ in which x lies

For example, you can choose $x_i = x_1 + \frac{x_2 - x_1}{N-1}(i-1)$ with $i = 1, 2, ..., N$

Case 1

Choose the estimate of $f(x)$, $g(x|\mathcal{D})$, to be independent of $\mathcal{D}$

For example, $g(x) = w_1 x + w_0$

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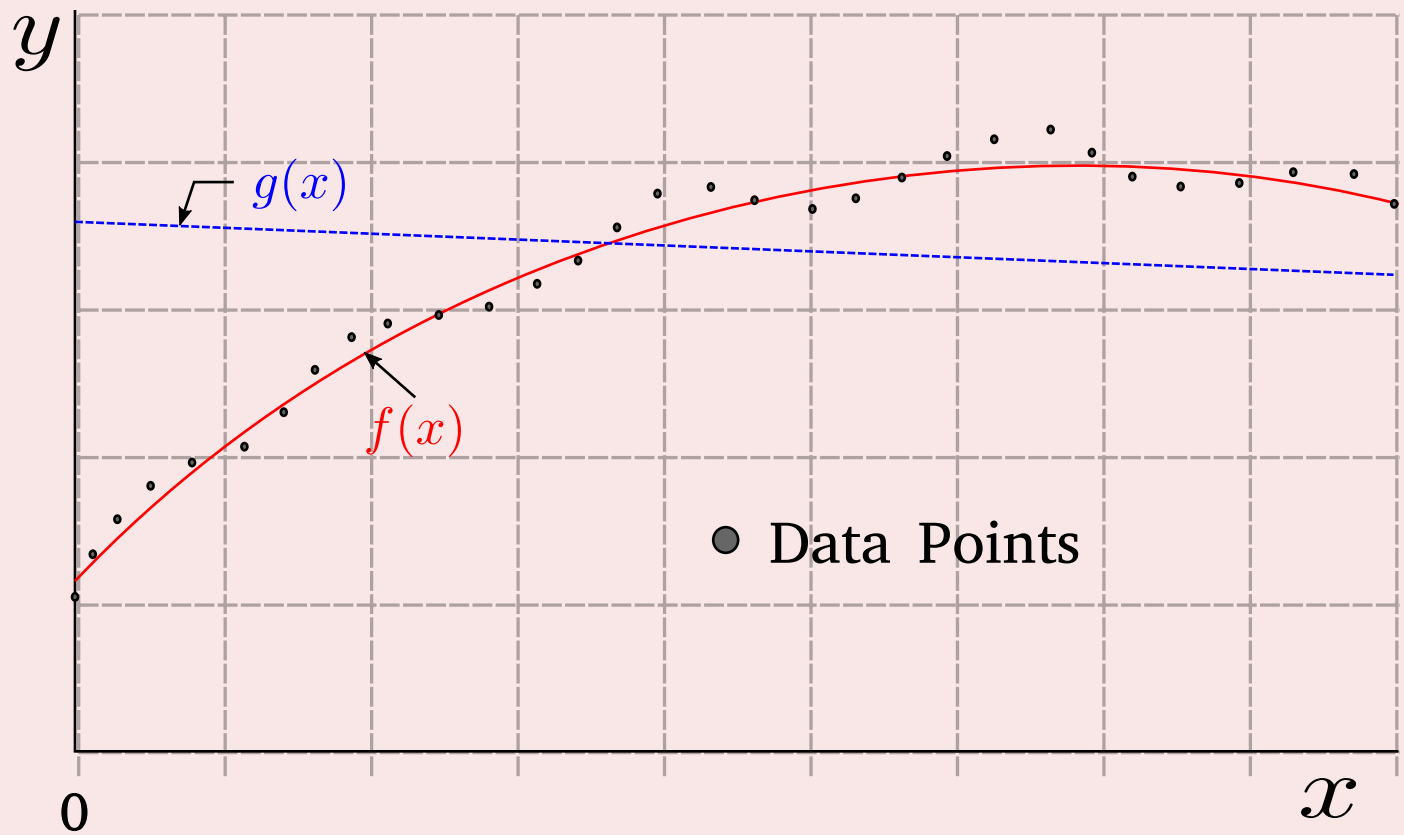
For example, the points are spread around $(x, f(x))$



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Since $g(x)$ is fixed

$$E_{\mathcal{D}}\left[g\left(x|\mathcal{D}\right)\right] = g\left(x|\mathcal{D}\right) \equiv g\left(x\right) \tag{4}$$

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On the other hand

Because $g(x)$ was chosen arbitrarily the expected bias must be large.

$$\underbrace{\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right)^2}_{BIAS} \tag{6}$$

Case 2

In the other hand

Now, $g_1(x)$ corresponds to a polynomial of high degree so it can pass through each training point in $\mathcal{D}$.

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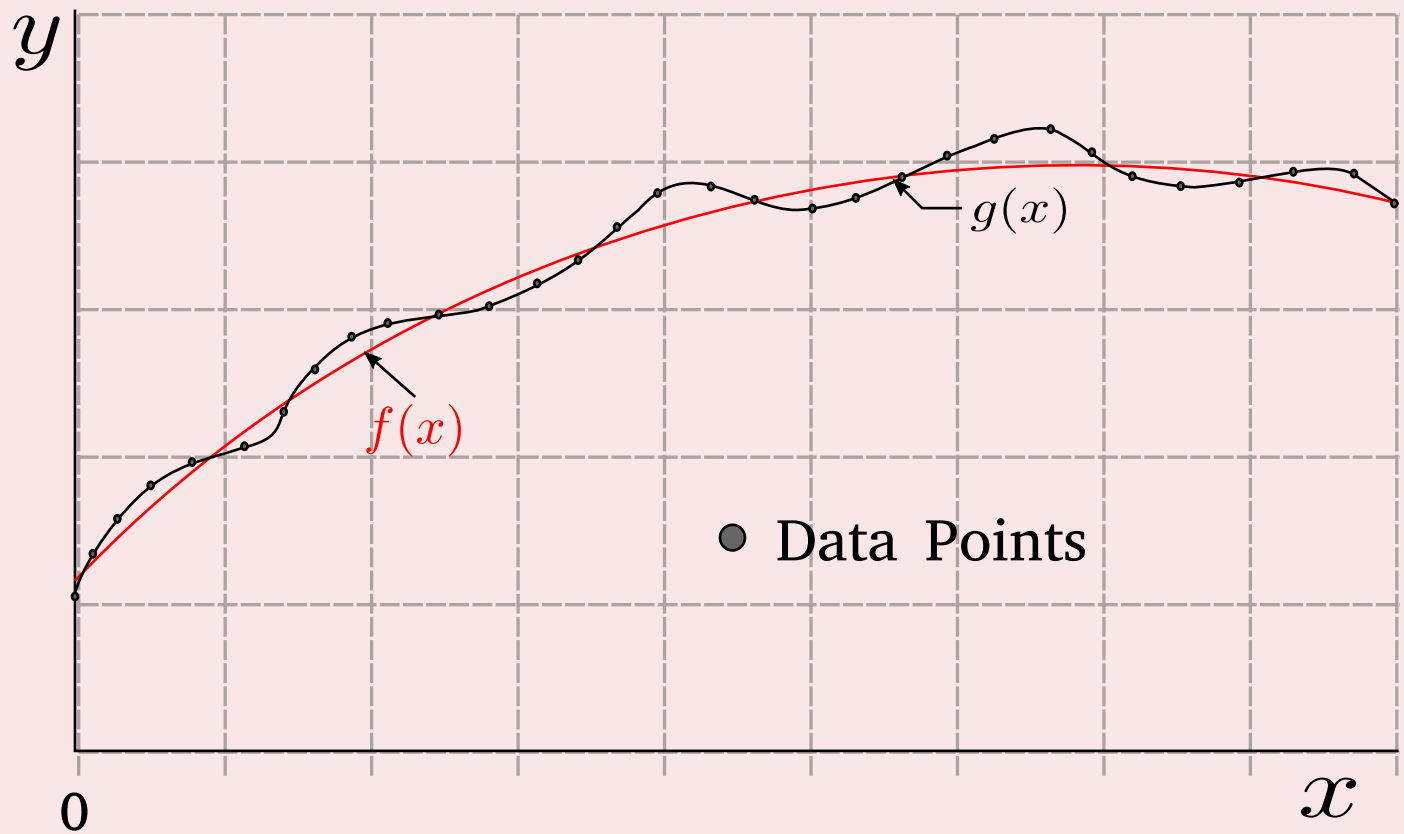
Example of $g_1(x)$



Case 2

Due to the zero mean of the noise source

$$E_D\left[g_1\left(\boldsymbol{x}|\mathcal{D}\right)\right] = f\left(x\right) = E\left[y|x\right] \text{ for any } x = x_i \tag{7}$$

Remark: At the training points the bias is zero.

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In other words

The bias becomes zero (or approximately zero) but the variance is now equal to the variance of the noise source.

Observations

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Everything that has been said so far applies to both the regression and the classification tasks.

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Think about

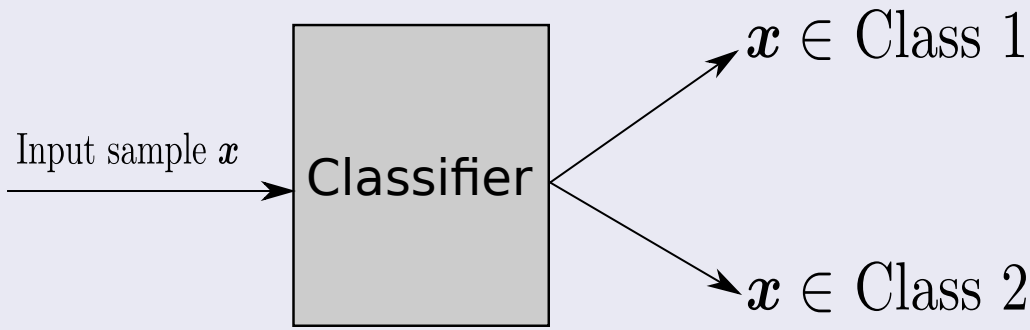
A classifier that sends everything far away of the hyperplane!!! Away from the values $+-1$!!!

Outline

Sooner of Latter you need to know how efficient is your algorithm

Thus, we need a measures of accuracy

Thus, we begin with the classic classifier for two classes



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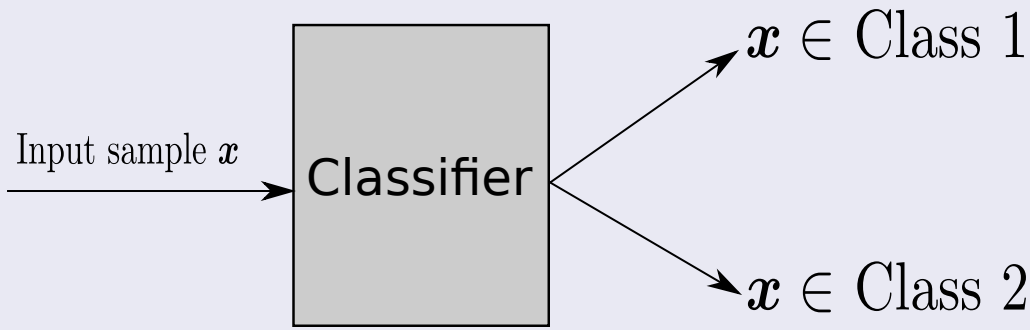

Here

A dataset used for performance evaluation is called a **test dataset.**

Therefore

It is a good idea to build a measure of performance

For this, we can use the idea of error in statistics.

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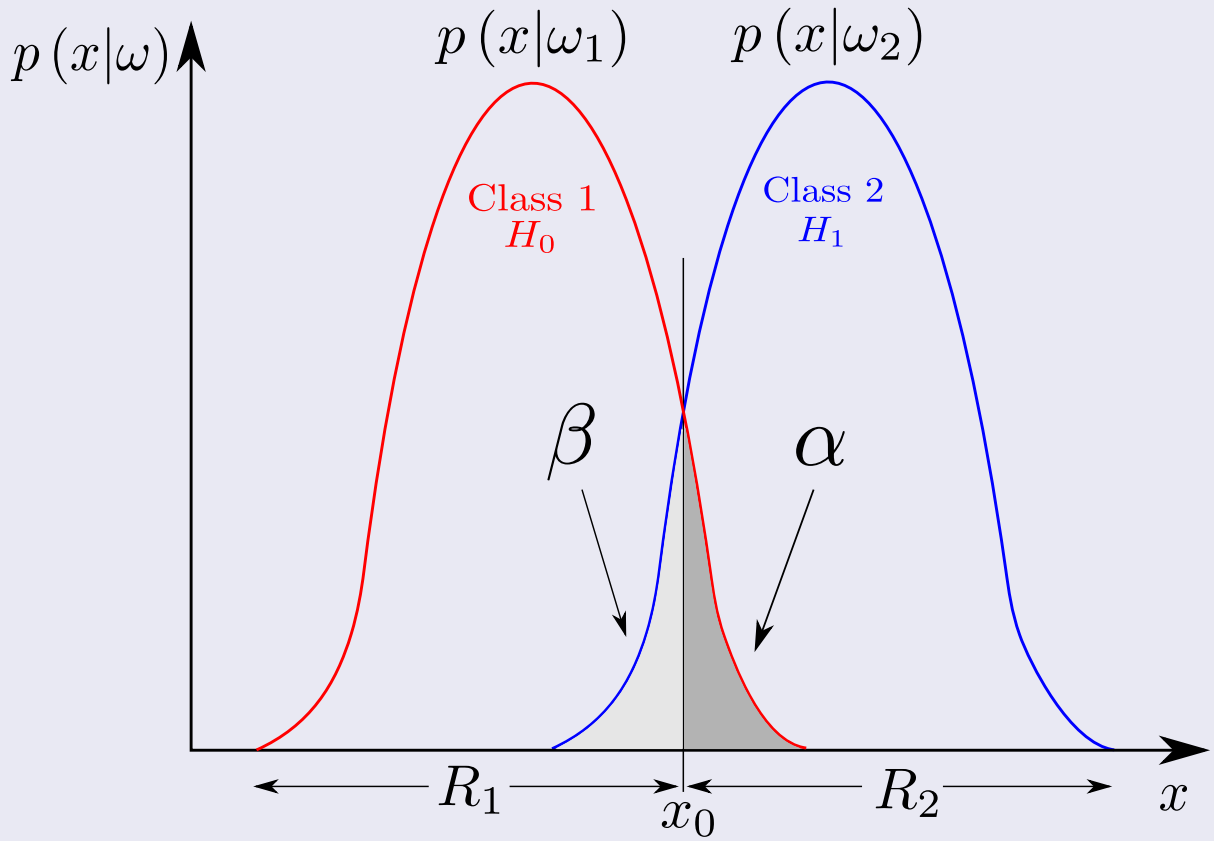
We have two distribution for each class



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α error

Definition (Type I Error - False Positive)

α is the probability that the test will lead to the rejection of the hypothesis H_0 when that hypothesis is true.

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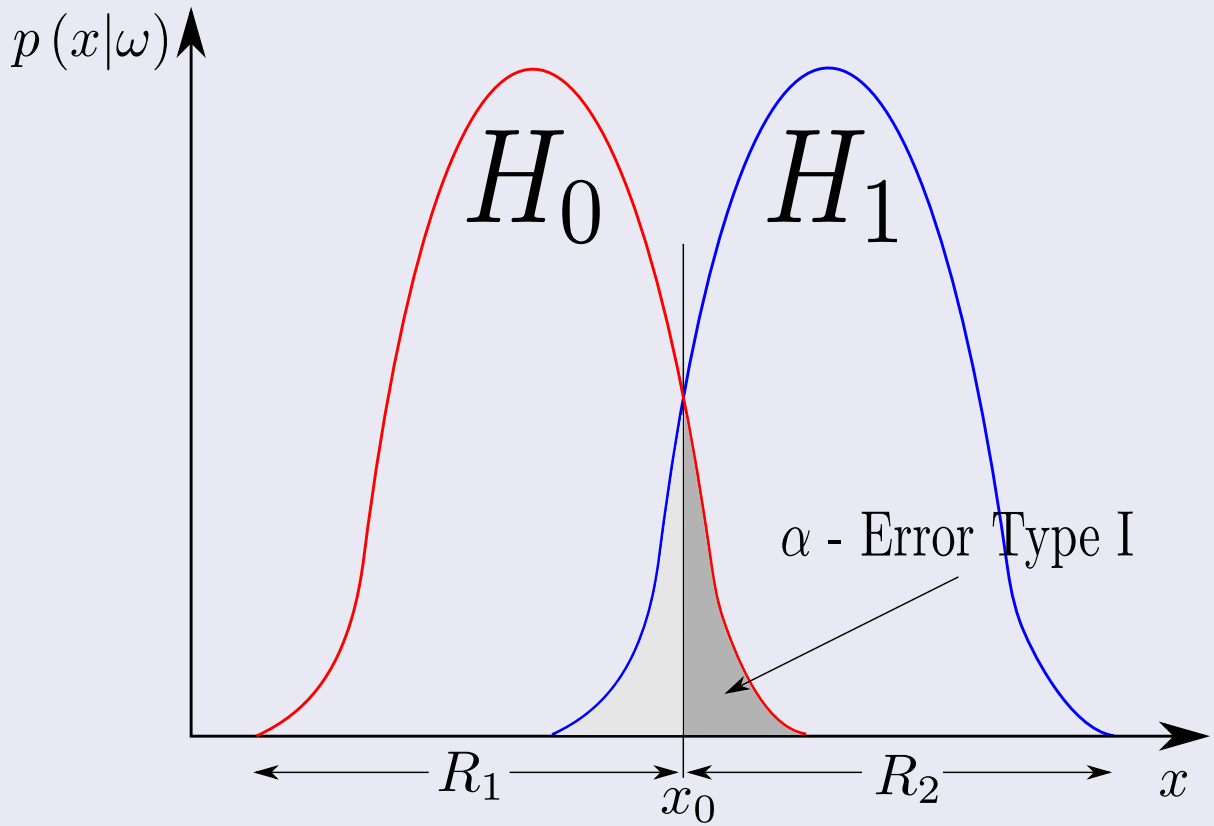
Basically

We have



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1. H_1: “Adding fluoride to toothpaste protects against cavities."
2. Then $\beta = 0.05$ meaning that you have a chance of 5 of the time.
3. This says that you have a low chance of having a cavity using fluoride in the water.

Outline

This can be seen as a table

Confusion Matrix

Table of error types		True H_0, False H_1	False H_0, True H_1
Decisions	Reject H_1	Correct Inference **True Positive**	Type I Error - α **False Positive**
	Reject H_0	Type II Error - β **False Negative**	Correct Inference **True Negative**

In the case of two classes, we have

We have finally the Confusion Matrix

		Actual Class	
		Positive	Negative
Predicted Classes	Positive	**True Positive (TP)**	**False Positives (FP)**
	Negative	**False Negatives (FN)**	**True Negatives (TN)**

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Definition

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Thus

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

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Problem - accuracy assumes equal cost for both kinds of errors

Is 99% accuracy good, bad or terrible? It depends on the problem.

Another Problem

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The True Positive or

- The Recall Rate...

True Positive Rate

Also called

- Sensitivity or **Recall Rate**

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True Positive Rate

Also called

- Sensitivity or **Recall Rate**

Defined as

- True Positive Rate is the proportion of getting a correct classification of the Positive Class vs the True Positive and False Negatives.

$$\text{True Positive Rate} = \frac{TP}{TP + FN}$$

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We also need to measure the Class 2

For this, we have

- Specificity

True Negative Rate

Also known as

- Specificity

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Predicted Classes	Positive	True Positive (TP)	**False Positives (FP)**
	Negative	False Negatives (FN)	**True Negatives (TN)**

True Negative Rate

Also known as

- Specificity

Defined as

- It is the proportion of True Negative vs the elements classified as True negatives.

$$\text{True Negative Rate} = \frac{TN}{FP + TN}$$

		Actual Class	
		Positive	Negative
Predicted Classes	Positive	True Positive (TP)	**False Positives (FP)**
	Negative	False Negatives (FN)	**True Negatives (TN)**

We also need to measure the rate of TP

We have for this

- The Precision

Precision

Also known as

- **Positive Predictive Value**

Precision

Also known as

- **Positive Predictive Value**

Defined as

- The proportion of the elements classified as true positive vs the total of all the real true positives.

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

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Predicted Classes	Positive	**True Positive (TP)**	**False Positives (FP)**
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Significance Level

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Defined as

False Positive Rate is the probability of getting an incorrect classification of the Positive Class vs the True Negative and the False Positive.

$$\text{False positive rate} = \frac{FP}{TN + FP}$$

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Given these initial measures of validity

it is possible to obtain a more precise model evaluation, the ROC curves.

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The ROC Curves plot

It is a model-wide evaluation measure that is based on two basic evaluation measures:

1. **Specificity** is a performance measure of the whole negative part of a dataset.
2. **Sensitivity** is a performance measure of the whole positive part.

What the ROC Curves uses

We have a plot where

The ROC plot uses specificity on the x-axis and sensitivity on the y-axis.

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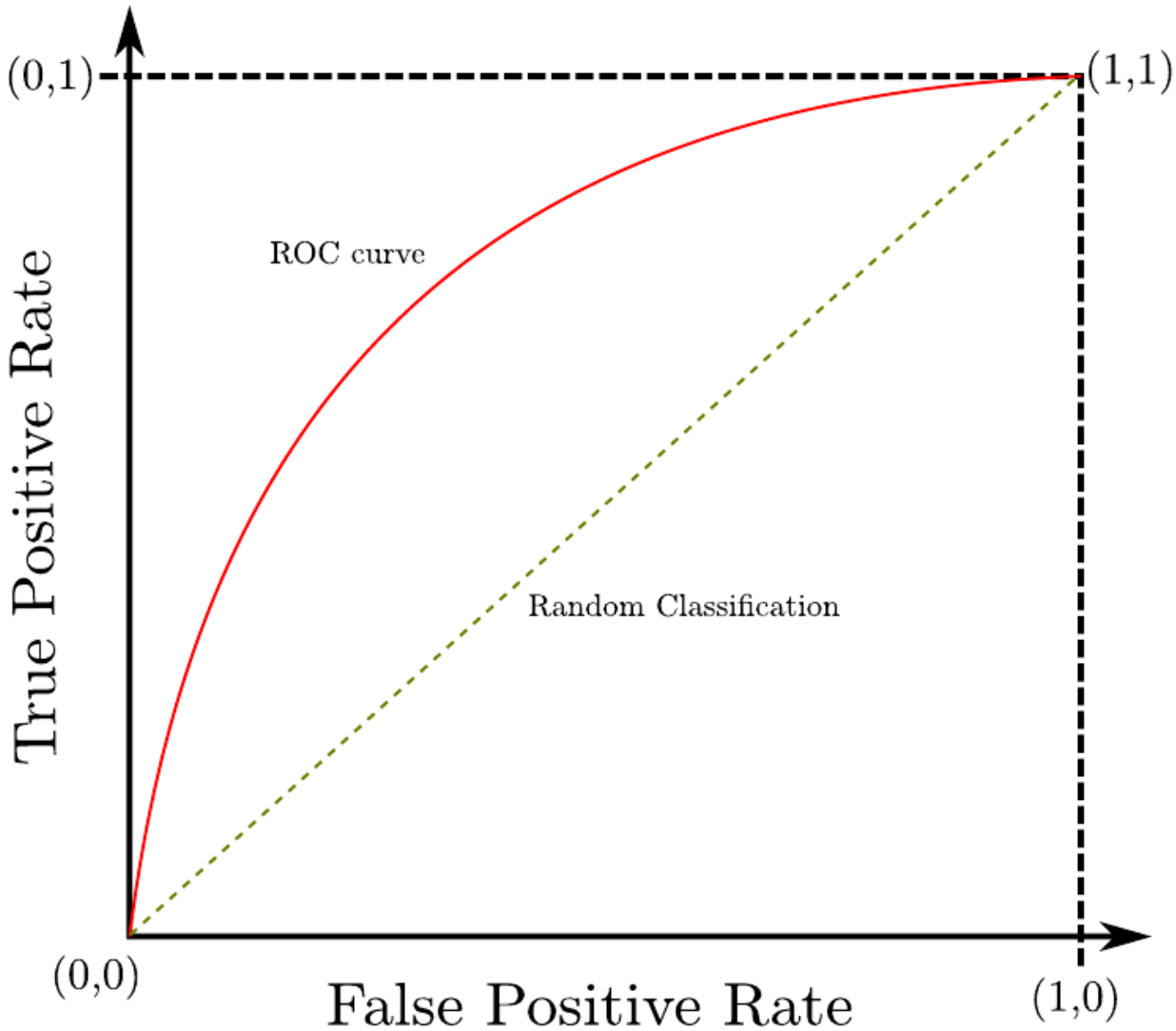
Then

1. A ROC curve is created by connecting all ROC points of a classier in the ROC space.
2. Two adjacent ROC points can be connected by a straight line.
3. The curve starts at (0.0, 0.0) and ends at (1.0, 1.0).

Outline

For Example


(0,1)
(1,1)
ROC curve
Random Classification
True Positive Rate
(0,0)
False Positive Rate
(1,0)

Outline

We have

Algorithm ROC point generation

Input: L, the set of test examples; $f(i)$, the probabilistic classifier estimate that example i is positive; P and N, the number of positive and negative examples.

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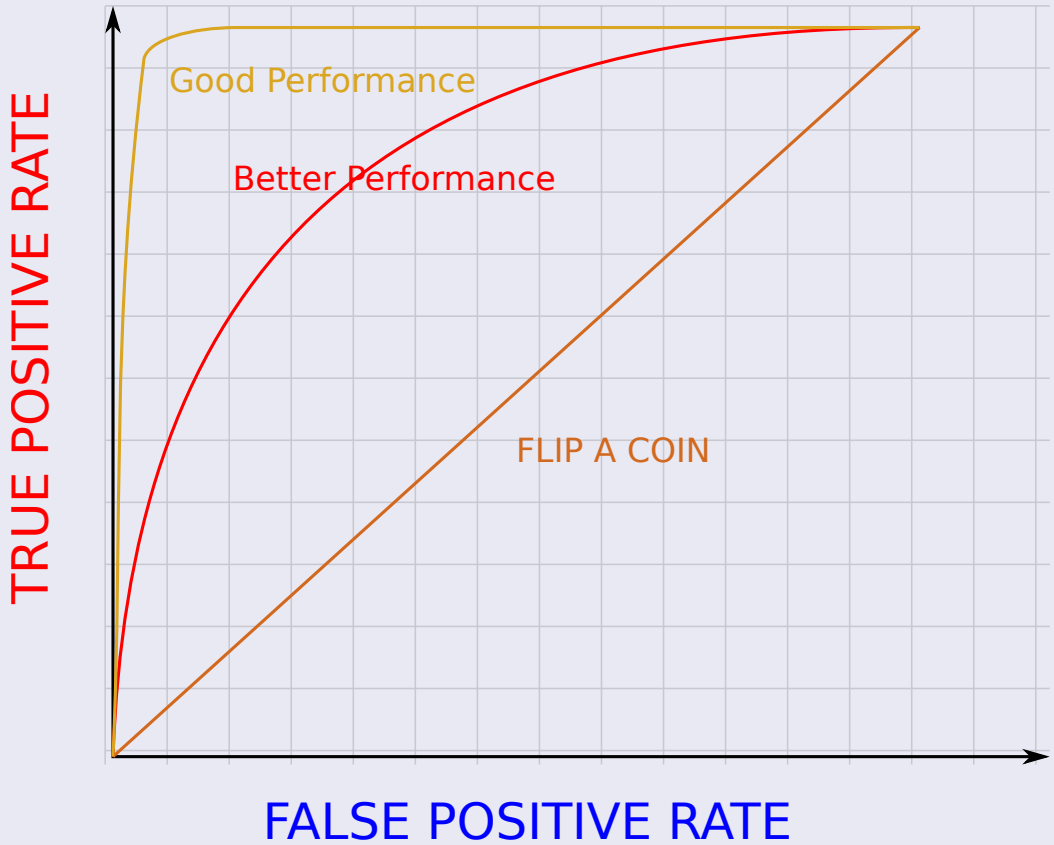
For Example

We could have multiple methods



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A Partial List is

1. Area Under the Curve (AUC)
2. Equal Error Rate (EER)
3. Likelihood Ratio

Outline

A Simple Defintion

We have

$$AUC = \int ROC\left(p\right) dp = \sum_{i=1}^{N} ROC\left(f\left(\frac{1}{i}\right)\right)\left[\frac{i}{N} - \frac{i-1}{N}\right]$$

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- The probability that a randomly selected observation X from the **positive class** would have a higher score than a randomly selected observation Y from the **negative class.**

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The AUC gives the mean **true positive** rate averaged uniformly across the **false positive** rate.

Therefore

AUC curves are a good measure of how good are our results

- However, we need to combine this results with something more powerful
  - Cross Validation - to understand the variation in the machine estimation

Outline

Also known as F_1 score

It is a measure of a test's accuracy

- It considers both the precision P and the recall R of the test to compute the score.

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An interesting fact

- It computes some average of the information retrieval precision and recall.

Remember

Precision

- The proportion of the elements classified as true positive vs the total of all the real true positives.

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

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Recall

- True Positive Rate is the proportion of getting a correct classification of the Positive Class vs the True Positive and False Negatives.

$$\text{True Positive Rate} = \frac{TP}{TP + FN}$$

Building the F_1 score

Something Notable

$$Average = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$Harmonic = \frac{N}{\sum_{i=1}^{N} \frac{1}{x_i}}$$

Building the F_1 score

Something Notable

$$Average = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$Harmonic = \frac{N}{\sum_{i=1}^{N} \frac{1}{x_i}}$$

When $x_1 = Precision$ and $x_2 = Recall$

$$Average = \frac{1}{2}(P + R)$$

$$Harmonic = \frac{2}{\frac{1}{P} + \frac{1}{R}} = \frac{2PR}{P + R}$$

Thus

Important

- The harmonic mean is more intuitive than the arithmetic mean when computing a mean of ratios.

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Example

- Suppose that you have a finger print recognition system and its precision and recall be 1.0 and 0.2

Therefore, we have

The Average will report

$$\frac{1}{2}(P+R) = \frac{1.0+0.2}{2} = 0.6$$

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At the F_2 score

$$\frac{2PR}{P+R} = \frac{0.4}{1.2} = 0.33$$

General Form F_β

Then for Precision and Recall, we have a general function

$$F_\beta = \frac{(\beta^2 + 1)\, Precision \times Recall}{\beta^2 Precision + Recall} \quad (0 \leq \beta \leq +\infty)$$

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Thus, for the basic case F_1

$$F_1 = 2\frac{Precision \times Recall}{Precision + Recall}$$

Outline

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We want to measure

A quality measure to measure different classifiers (for different parameter values).

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$$R(f) = E_{\mathcal{D}}\left[L\left(y, f\left(\boldsymbol{x}\right)\right)\right]. \tag{8}$$

Example: $L\left(y, f\left(x\right)\right) = \left\|y - f\left(\boldsymbol{x}\right)\right\|_2^2$

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Example: $L\left(y, f\left(x\right)\right) = \left\|y - f\left(\boldsymbol{x}\right)\right\|_2^2$

More precisely

For different values γ_j of the parameter, we train a classifier $f\left(\boldsymbol{x}|\gamma_j\right)$ on the training set.

Then, calculate the empirical Risk

Do you have any ideas?

Give me your best shot!!!

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Empirical Risk

We use the validation set to estimate

$$\hat{R}\left(f\left(x|\gamma\right)\right) = \frac{1}{N_v}\sum_{i=1}^{N_v} L\left(y_i, f\left(\boldsymbol{x}_i|\gamma\right)\right) \tag{9}$$

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3. Report error estimate $\hat{R}\left(f\left(x|\gamma_i\right)\right)$ computed on the test set.

Idea

Something Notable

- Each of the **error estimates computed on validation set** is computed from a single example of a trained classifier.
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$$\hat{R}_{CV}\left(f\left(x|\gamma\right)\right) = \frac{1}{N}\sum_{i=1}^{N} L\left(y_i, f_k\left(\boldsymbol{x}_{k(i)}|\gamma\right)\right) \tag{10}$$

where $k\left(i\right)$ is the fold containing $\boldsymbol{x}_i$.

Example

$K = 5, k = 3$

Train	Train	Testing	Train	Train
1	2	3	4	5

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Actually, we have

- A more general setup

$\overbrace{\text{SPLIT All Train Set}}^{\text{Train Data + Validation Data}}$	Test

Outline

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Extremal cases

- $K = N$, called leave one out cross validation (loocv)

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3. By removing a single point (loocv), we cannot make this variance visible.

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2. This should not weaken the classifier considerably, but should be large enough to make measure variance effects.

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Notes

- A variant of LpOCV with $p = 2$ known as leave-pair-out cross-validation has been recommended as a nearly unbiased method for estimating the area under ROC curve of a binary classifier.

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Definition

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Train	Train	Train	Test $= 1$	Train	Train

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- Simple, easy to understand, and implement.

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- The model may lead to a low bias.
- The computation time required is high.

Outline

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- The holdout technique is an exhaustive cross-validation method.
- It randomly splits the dataset into train and test data.
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- Requieres large amount of data

Outline

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- In k-fold cross-validation, the original dataset is equally partitioned into k subparts or folds.

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Thus

- Out of the k-folds or groups, for each iteration, one group is selected as validation data,
- The remaining $(k-1)$ groups are selected as training data.

Finally

We take the mean accuracy of the k-folds

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- Repeated random subsampling validation also referred to as Monte Carlo cross-validation splits the dataset randomly into training and validation.

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Something Notable

- Unlikely k-fold cross-validation split of the dataset into not in groups or folds but splits in this case in random.
- Using multiple Iterations to performa an average accuracy

Finally

Pros

- The proportion of train and validation splits is not dependent on the number of iterations or partitions.

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Pros

- The proportion of train and validation splits is not dependent on the number of iterations or partitions.

Cons

- Some samples may not be selected for either training or validation.
- Not suitable for an imbalanced dataset.

Outline

Stratisfied K-fold Cross-Validation

Something Notable

- For all the cross-validation techniques discussed above, they may not work well with an imbalanced dataset.
  - Stratified k-fold cross-validation solved the problem of an imbalanced dataset.

Stratisfied K-fold Cross-Validation

Something Notable

- For all the cross-validation techniques discussed above, they may not work well with an imbalanced dataset.
  - Stratified k-fold cross-validation solved the problem of an imbalanced dataset.

Definition

- In Stratified k-fold cross-validation, the dataset is partitioned into k groups or folds
  - The validation data has an equal number of instances of target class label.

Therefore

Final Score

- The final score is computed by taking the mean of scores of each fold.

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Pros

- Works well for an imbalanced dataset.

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Pros

- Works well for an imbalanced dataset.

Cons

- Now suitable for time series dataset.

Outline

A Combination

An Image Better than 100 words