Introduction to Machine Learning

Measures of Accuracy

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January 26, 2023

Outline

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What did we see until now?

The design of learning machines from two main points:

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

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

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 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...

Outline

How do we measure the difference

We have that

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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}
&= 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) + ... \\
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Outline

We have the Bias-Variance

Our Final Equation

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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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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.

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

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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

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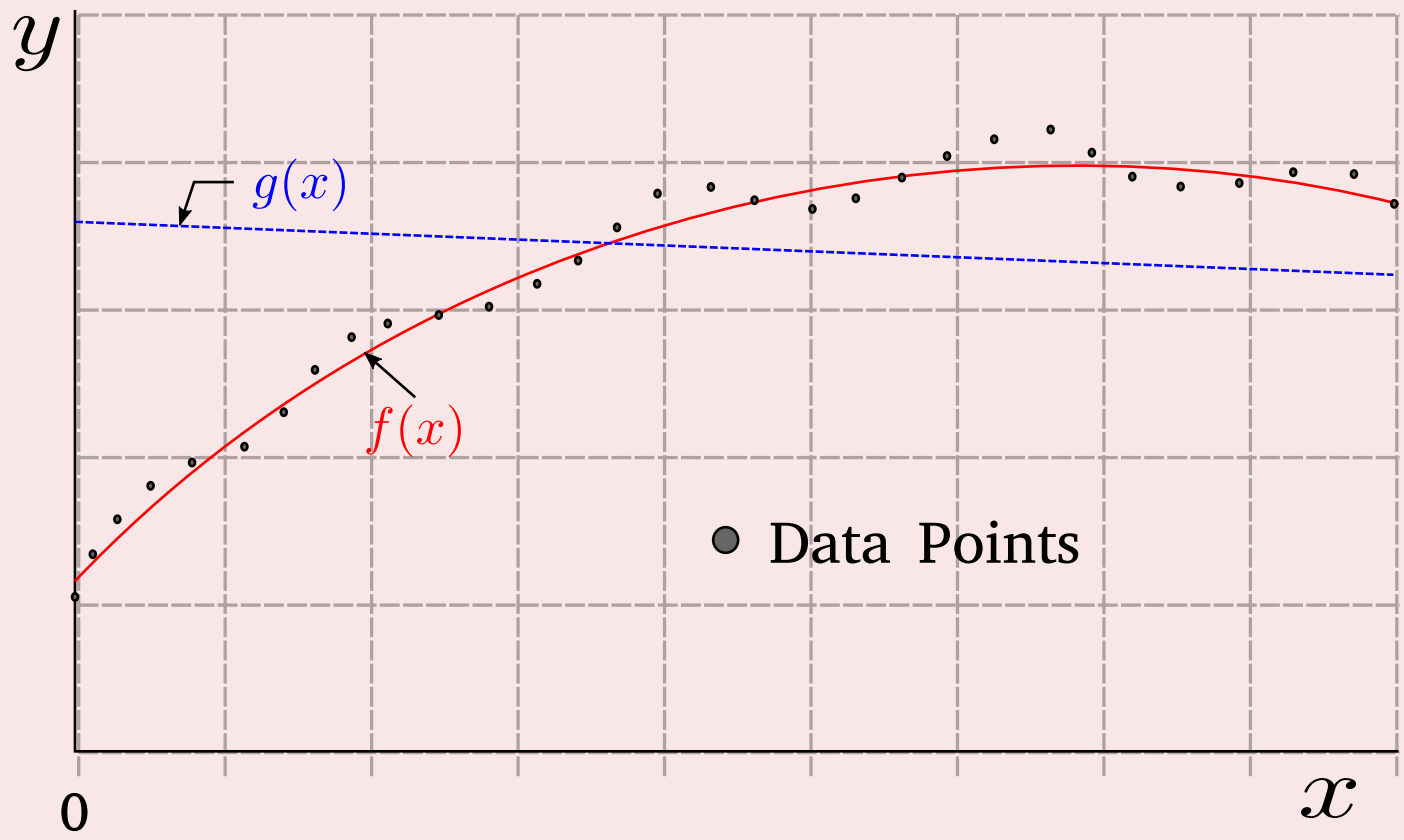
For example, the points are spread around $(x, f(x))$



Case 1

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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$$Var_{\mathcal{D}}\left[g\left(x|\mathcal{D}\right)\right] = 0 \tag{5}$$

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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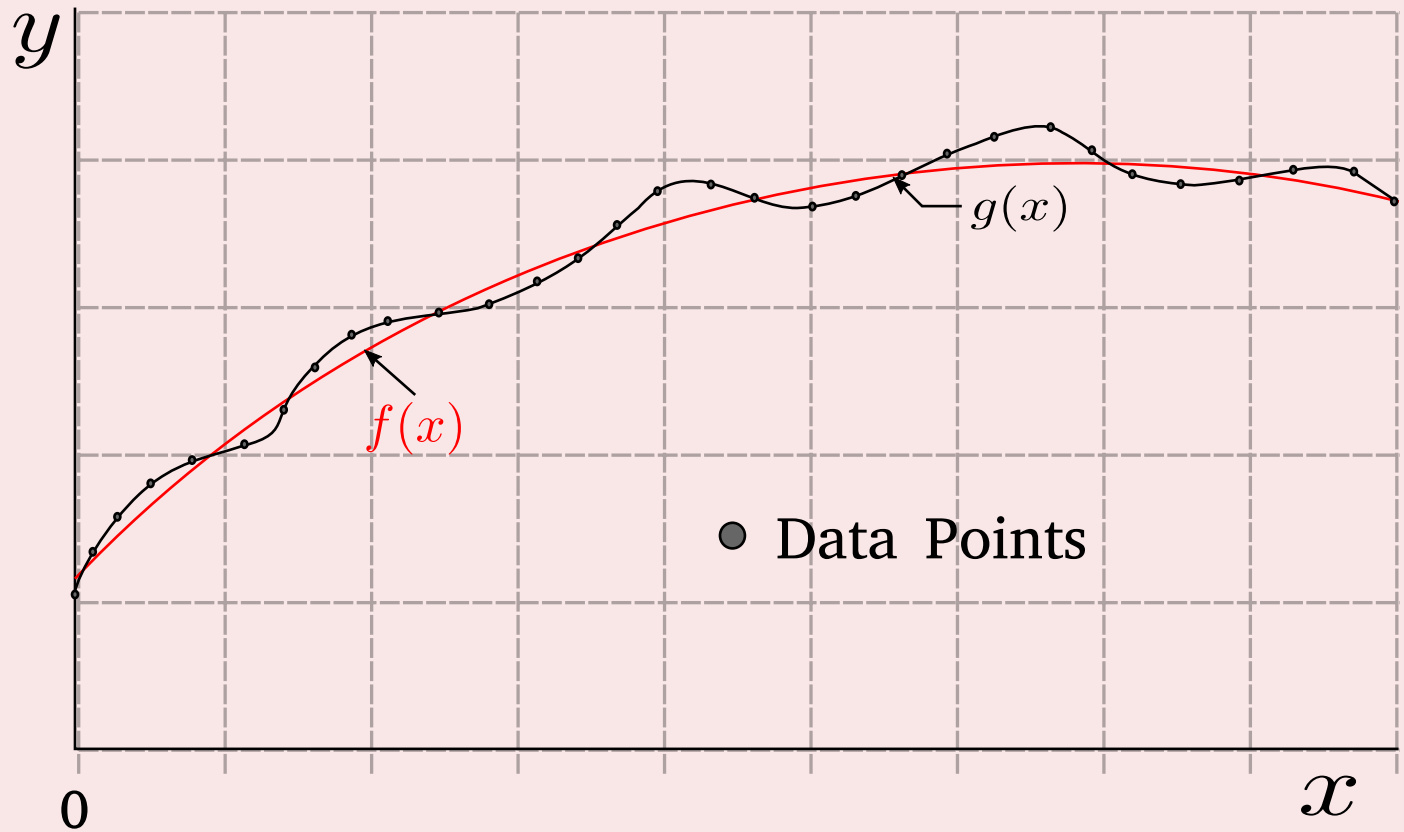
Example of $g_1(x)$



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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$$\begin{aligned} E_D\left[\left(g_1\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g_1\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)^2\right] &= E_D\left[\left(f\left(x\right) + \epsilon - f\left(x\right)\right)^2\right] \\ &= \sigma_\epsilon^2, \text{ for } x = x_i, i = 1, 2, ..., N \end{aligned}$$

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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

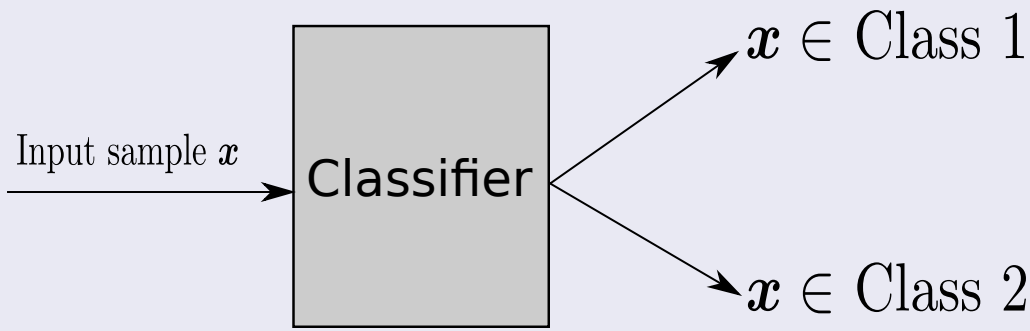
A classifier that sends everything far away of the hyperplane!!! Away from the values $+-1$!!!

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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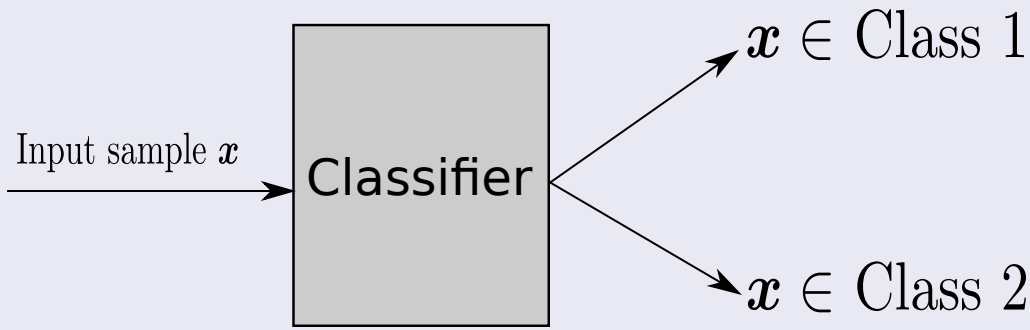

Here

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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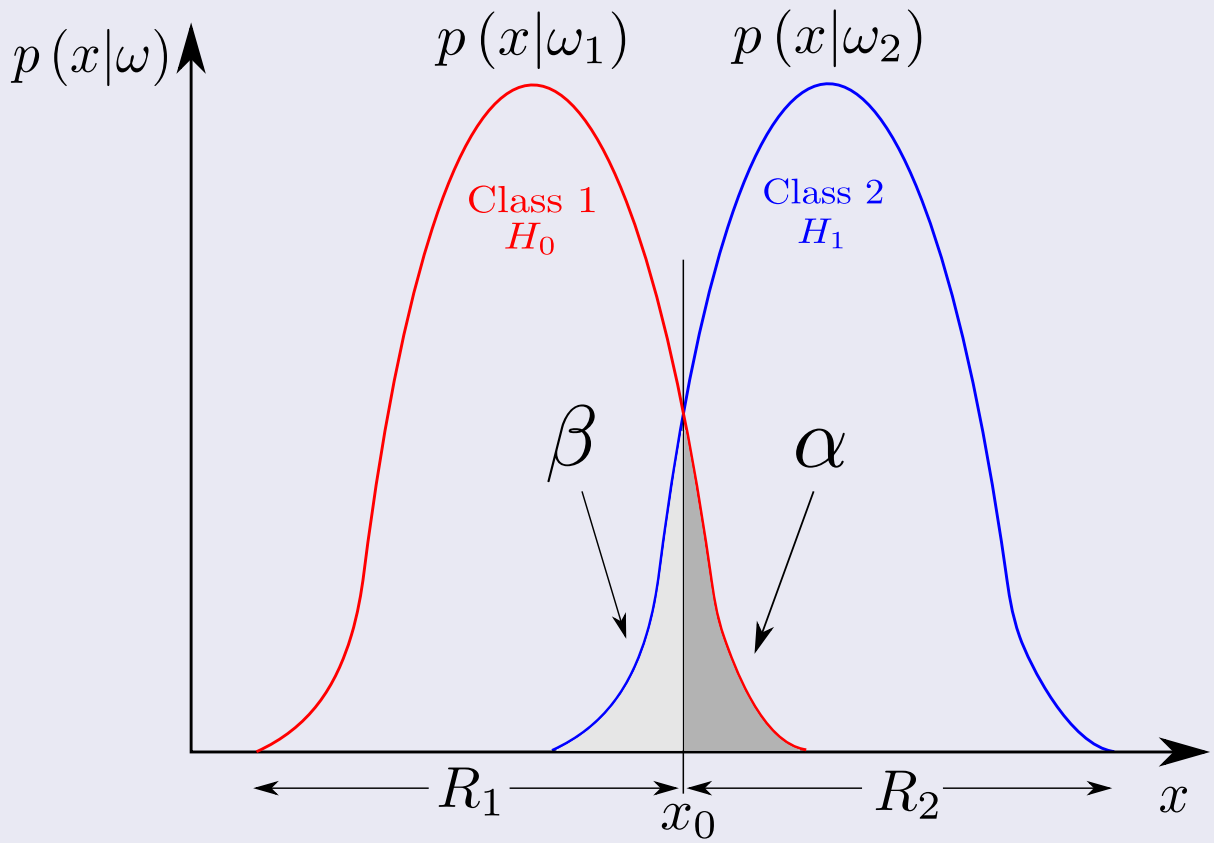
Do you remember?



Outline

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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2. You have a device that fails $\alpha = 0.05$ meaning that it fails 5 of the time.

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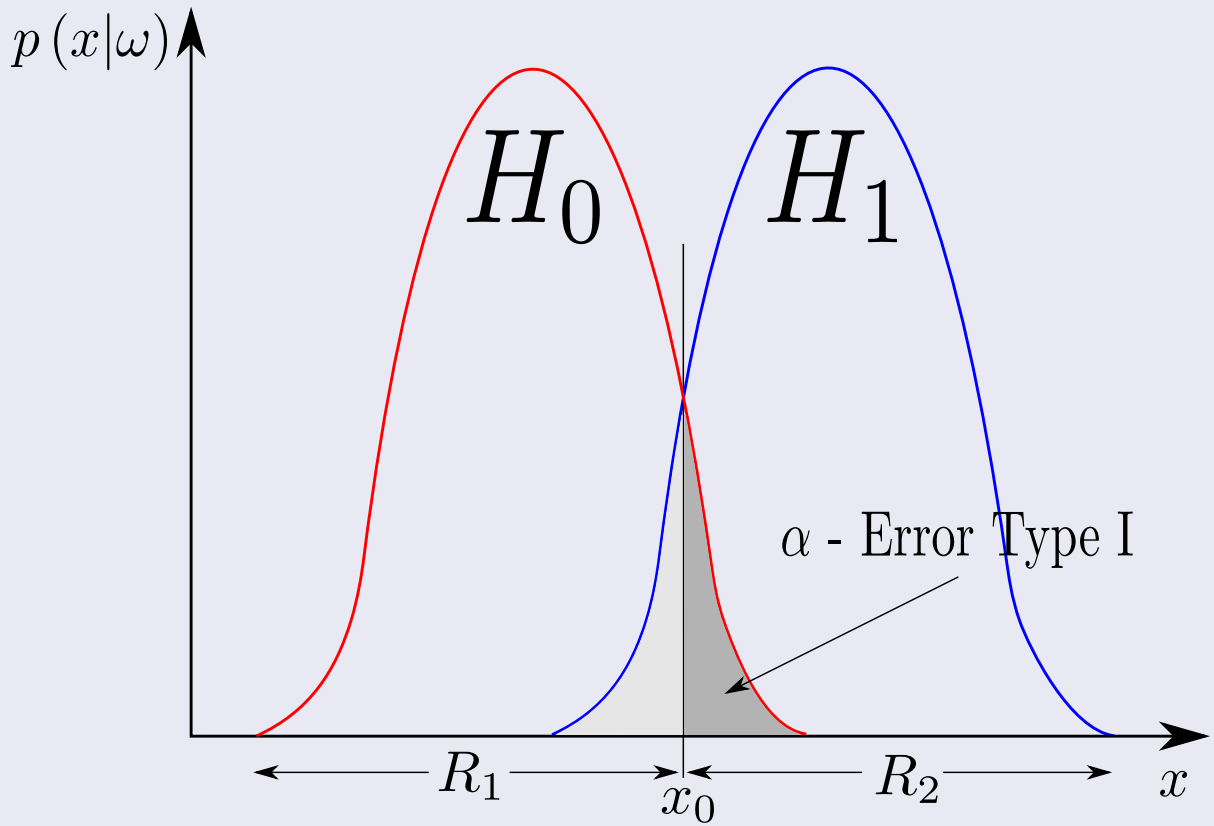
3. This says that you ha low chance of a wrong circuit.

Basically

We have



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2. Then $\beta = 0.05$ meaning that you have a chance of 5 of the time.
3. This says that you ha 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		Null Hypothesis AKA H_0	
		True	False
Decision about H_0	Reject	Type I Error - α **False Positive**	Correct Inference **True Positive**
	Fail to reject	Correct Inference **True Negative**	Type II Error - β **False Negative**

In the case of two classes, we have

We have the following

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

Outline

Accuracy

Definition

The proportion of getting correct classification of the Positive and Negative classes.

Accuracy

Definition

The proportion of getting correct classification of the Positive and Negative classes.

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.

True Positive Rate

Also called

Sensitivity or Recall Rate

True Positive Rate

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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.

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

True Negative Rate

Also known as

Specificity

True Negative Rate

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Specificity

Defined as

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

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

Precision

Also known as

Positive Predictive Value

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Positive Predictive Value

Defined as

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

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

Significance Level

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Defined as

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Outline

We can do better than these simple measures of accuracy

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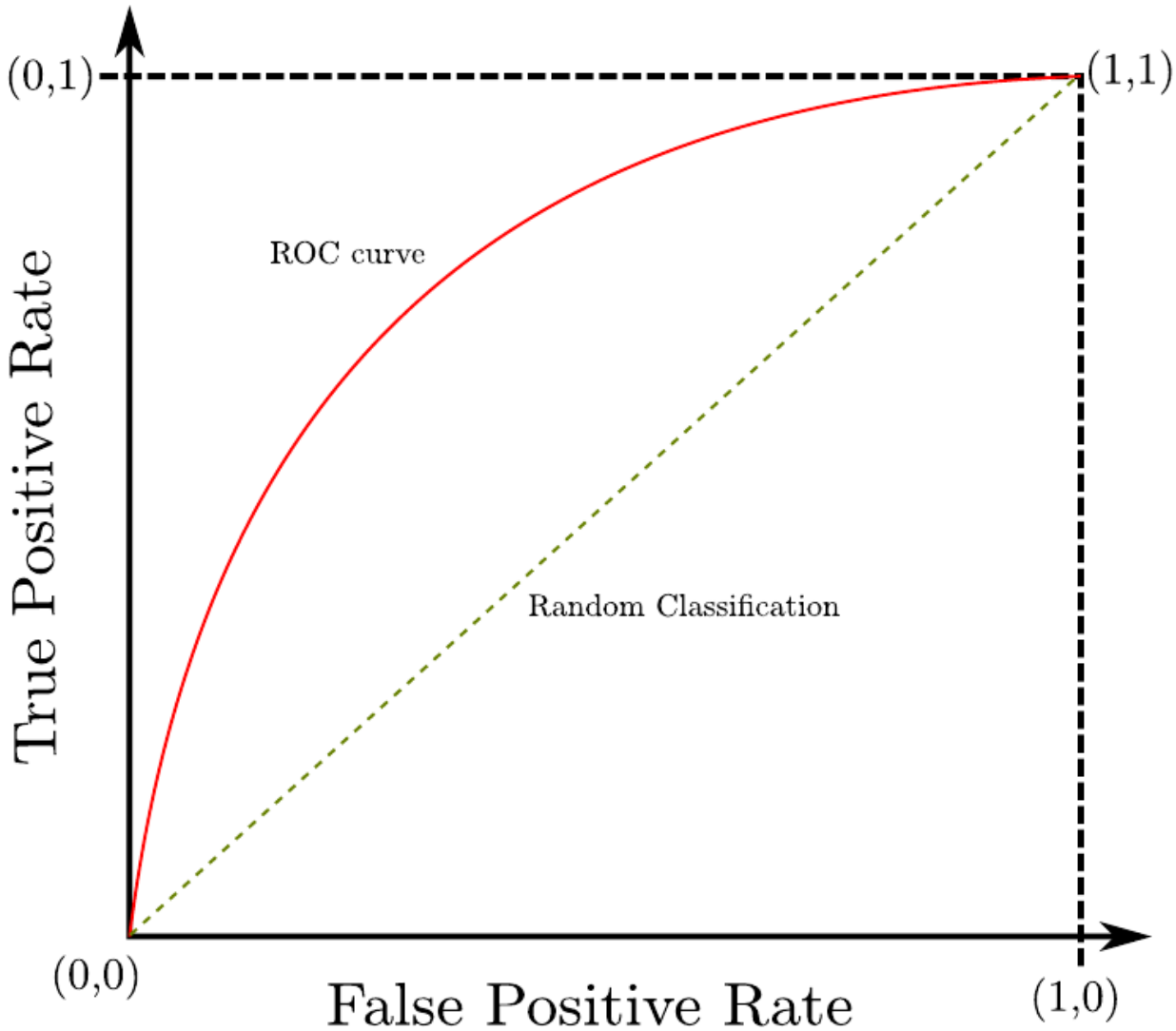
1. A ROC curve is created by connecting all ROC points of a classier in the ROC space.
2. Two adjacent ROC points can be connected by a straight line.
3. The curve starts at (0.0, 0.0) and ends at (1.0, 1.0).

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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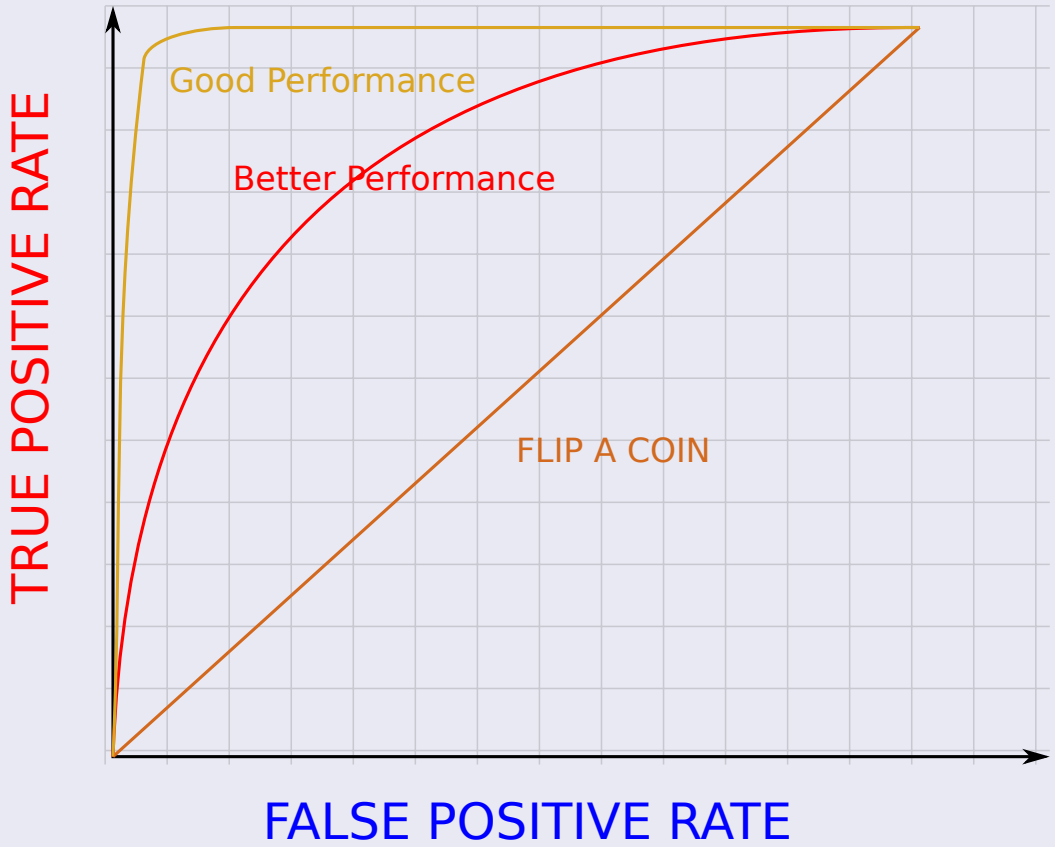
10. $R.append\left(\frac{FP}{N}, \frac{TP}{P}\right)$**, this is** $(1, 1)$

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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This equation has the following meaning

- 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

Outline

Also known as F_1 score

It is a measure of a test's accuracy

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An interesting fact

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

Remember

Precision

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Comparison of Measures

Something Notable

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

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

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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

General Form

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

What we want

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

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3. Compute the Cross Validation (CV) estimate:

$$\hat{R}_{CV}\left(f\left(x|\gamma\right)\right) = \frac{1}{N_v}\sum_{k=1}^{N_v} L\left(y_i, f_k\left(\boldsymbol{x}_{k(i)}|\gamma\right)\right) \tag{10}$$

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

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

Outline

How to choose K

Extremal cases

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

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2. Important concept: By removing substantial parts of the sample in turn and at random, we can simulate this variance.
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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Definition

- It involves using p-observation as validation data, and remaining data is used to train the model.

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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

Pros and Cons

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- Simple, easy to understand, and implement.

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Cons

- 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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- Not suitable for an imbalanced dataset.
- 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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Pros

- The model has low bias and Low time complexity
- The entire dataset is utilized for both training and validation.

Finally

We take the mean accuracy of the k-folds

$$acc_{cv} = \frac{1}{K}\sum_{i=1}^{K} acc_i$$

Pros

- The model has low bias and Low time complexity
- The entire dataset is utilized for both training and validation.

Cons

- Not suitable for an imbalanced dataset.

Outline

Empty

Definition

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

Empty

Definition

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

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.

Finally

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.

Therefore

Final Score

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

Pros

- Works well for an imbalanced dataset.

Therefore

Final Score

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

Pros

- Works well for an imbalanced dataset.

Cons

- Now suitable for time series dataset.

Outline

A Combination

An Image Better than 100 words