# Metrics for Binary Classification

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14th December 2020

# Table of Contents

# What is classification?

- **Classification is the problem of dividing an observation in a certain category according to its properties.**
- Some examples: Is this a triangle, a rectangle or a circle? What kind of character we have?

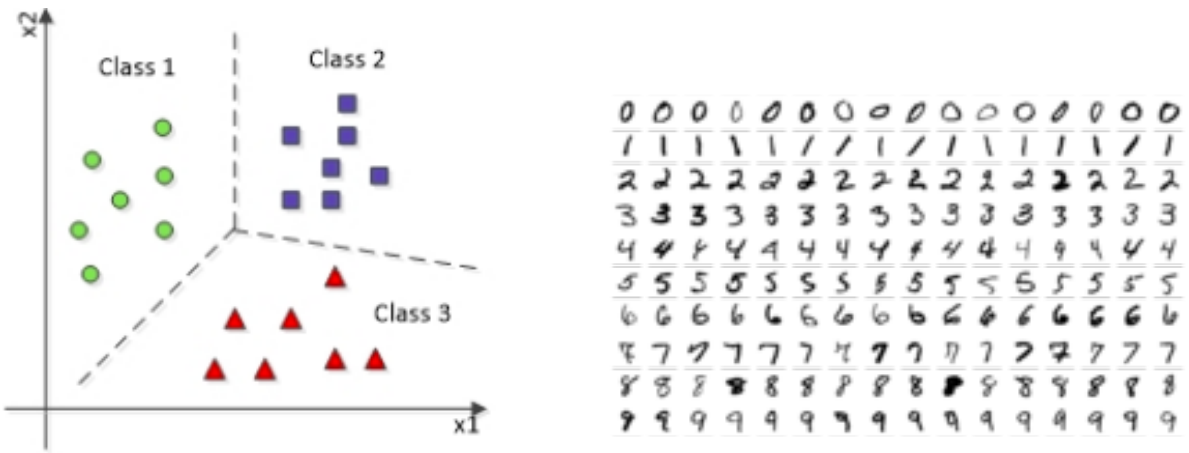



Figure: Two examples of classification

# Types of classification problems

- We can have two main types of classification: **binary** and **multiclass**.
- The classification can be **balanced** and **imbalanced**:
  - Balanced: in this case all the classes have similar frequencies.
  - Imbalanced: some classes are more frequent that other ones.
    Example: classification between rare and common events.

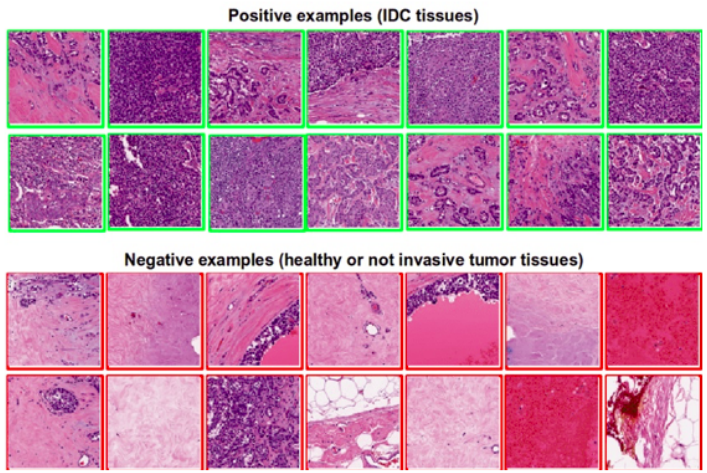



Figure: Disease vs not disease

# Mathematical model for classification

- A classifier (algorithm to classify) gives us a **probability** to belong to a class and with a **threshold** that we decide we obtain the **label** associated to a class.
- Classification is a **supervised machine learning problem**, where we have an input of features $X$, and an output $Y$, and we want to learn the relationship $f$ between them.
- The mathematical model is in the general form of:

$$p = f(X) + \varepsilon$$

where $p$ is the **estimated probability** to belong to a certain class $\in Y$, $X$ the **input**, $\varepsilon$ an **error term** related to the stochasticity, $f$ is the **relationship** between the input and the output and this is what the algorithm want to learn.

# Binary classification

- In a binary problem we select one of the two class, that we call the "positive class" and $p$ is the probability to belong to this class, $1-p$ the probability for the other class, the "negative class".
- Example: the logistic regression is in the implicit form of:

$$\log(\frac{p}{1-p}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

and if we explicit $p$:

$$p = P(Y=1) = \frac{1}{1+e^{-(\beta_0+\beta_1 x_1+\beta_2 x_2)}}$$

# Calibration of the Probabilities

- We desire that the estimated class probabilities are reflective of the true underlying probability of the sample, that is, **well-calibrated**.
- Example: if we predict that a mail is spam with a 0.2 probability, we want that if we take 5 similar mails, only one of them is spam.
- To do it we use a **calibration plot**.
- The next definition is **only for balanced problems**.

# How to do a Calibration Plot

- First fix a set of bins like $[0, 10\%], (10\%, 20\%], ..., (90\%, 100\%]$.
- In each bin put all the observations you have according to the probability. Example: an observation with 0.15 probability will be assegnated to the bin $(10\%, 20\%]$.
- Compute the number of events with the class associated to the probability $p$, divide it by the number of observation in the bin: this is the **observed event rate**.
- If the probability reflects the true underlying probability of the sample, the observed event rate must stay on the diagonal. In this case we say that the probabilities are **well-calibrated**.

# An example of a Calibration Plot

- In the figure we have the results of two model predictions. We see both an example of well-calibrated and not-well calibrated plot.

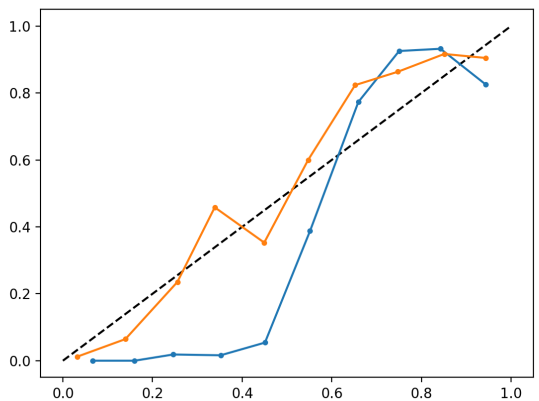
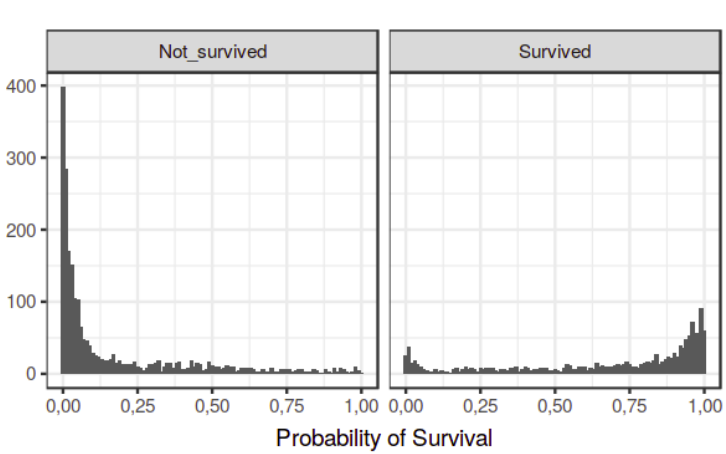



Figure: An example of well-calibrated in orange and not-well calibrated plot in blue

# Presenting Class Probabilities

- For a binary classification problem we have a good tool to understand the robustness of a model, i.e. if our model is very sure of its prediction.
- An easy tool is to plot an histogram of the probabilities for each class.
- We want the probabilities for the positive class distributed on the right and the probabilities for the negative one on the left.
- In this way we have a tool to understand how the model is sure of what is saying.

# Two examples of Class Probabilities



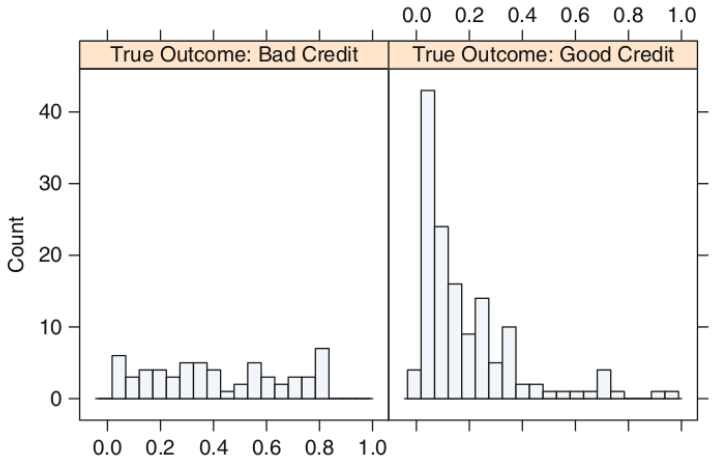




Figure: A robust classifier on the left and a not-robust one on the right

# Confusion matrix

- To understand the validity of a classifier we want to understand how many events we have right predicted, how many mistakes have been done, and which ones.
- A classical tool is the **confusion matrix**.

| Predicted | Observed | |
|---|---|---|
| | Event | Nonevent |
| Event | $TP$ | $FP$ |
| Nonevent | $FN$ | $TN$ |

Figure: A general confusion matrix

| Predicted | Observed | |
|---|---|---|
| | Bad | Good |
| Bad | 24 | 10 |
| Good | 36 | 130 |

Figure: An example of confusion matrix

- With this matrix we can create different metrics.

# Accuracy rate

- The accuracy rate is defined as:

$$\frac{\text{True predictions}}{\text{All the events}}$$

that we translate as:

$$\frac{TP + TN}{TP + TN + FP + FN}.$$

- This metric doesn't take into account:
  - **the errors that have been made**.
  - **the frequencies of each class**.

Ex: in an imbalanced problem the positive class could be 99%. In this case an algorithm that predict all the events as the most frequent class has an accuracy of 0.99 that seems good but it's not.

# An example of accuracy computation

Let's suppose we have a confusion matrix like that:

| Predicted — Reference | Positive | Negative |
|---|---|---|
| Positive + | 300 | 60 |
| Negative - | 200 | 855 |

In this case the accuracy is:

$$\frac{300 + 855}{300 + 855 + 200 + 60} \cdot 100 = 82\%$$

# Sensitivity (Recall) and Specificity

- **Sensitivity** $= \dfrac{\#\text{positive samples and predicted to be positives}}{\#\text{Positive samples}} = \dfrac{\text{TP}}{\text{TP} + \text{FN}}$.

  This is the ability to **detect positive samples**.

- **Specificity** $= \dfrac{\#\text{negative samples and predicted as negatives}}{\#\text{Negative samples}} = \dfrac{\text{TN}}{\text{TN+FP}}$.

  This is the ability to **detect negative samples**.

# An example of Sensitivy and Specificity computation

Let's suppose we have a confusion matrix like that:

| Predicted — Reference | Positive | Negative |
|---|---|---|
| Positive + | 300 | 60 |
| Negative - | 200 | 855 |

In this case the sensitivity is:

$$\frac{300}{300+200} \cdot 100 = 60\%$$

and the specificity:

$$\frac{855}{855+60} \cdot 100 = 93\%$$

# Probabilistic interpretation

- Sensitivity and specificity are two conditional probabilities.
- We use a medical explaination:
  - Sensitivity is defined as the probability of a positive test result given the presence of disease, written as:

$$P(\text{positive test}|\text{disease present}).$$

  - Specificity is defined as the probability of a negative test result given the absence of disease, written as:

$$P(\text{negative test}|\text{disease absent}).$$

- These quantities doesn't depend on prevalence, that is the frequence of the positive class definied as:

$$\text{Prevalence} = \frac{\#\text{Positive samples}}{\#\text{All samples}} = \frac{TP + FN}{TP + FN + FP + TN}$$

because these probabilities only depends on the test.

# Sensitivity-Specificity trade-off

- We know that changing the threshold we change the labels and so specificity and sensitivity.
- **Decreasing the threshold** we increase the number of true positives but the number of real positives is the same. So the **sensitivity increases**.
- **Decreasing the threshold** we also increase the number of false positives. So the **specificity decreases**.
- Increasing the threshold we have a similar discourse.
- We use the ROC curve to understand the Sensitivity-Specificity trade-off.

# ROC curve

- We have $1 -$ Specificity on the $x-$ axis and Sensitivity on the $y$-axis.

$$1 - \text{Specificity} = 1 - \frac{\text{TN}}{\text{TN+FP}} = \frac{\text{FP}}{\text{TN+FP}}.$$

- The ROC curve is created changing the threshold for the model and predicting the associated label. After that we measure for each threshold/prediction step the Sensitivity and $1 -$ Specificity.

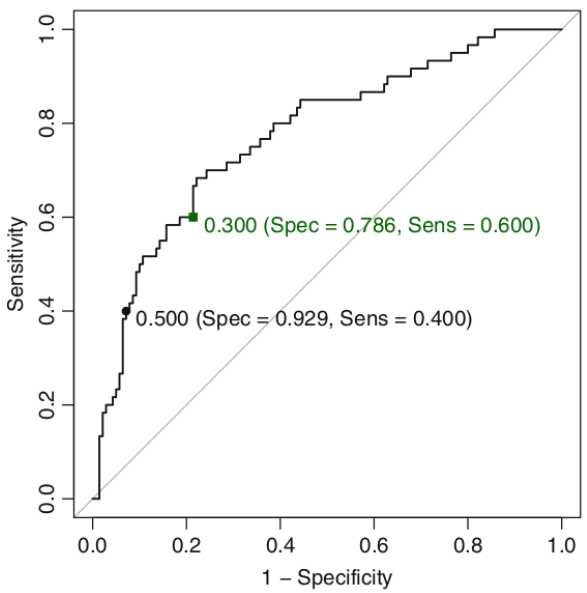



Figure: ROC curve of a classifier against random guess

# Some observations on the ROC curve

- The bisector is the ROC curve for the random guessing.
- A perfect classifier has a ROC curve of the type $y = 1$.
- We can use the AUC of the ROC curve to select a model. This method is threshold-insensitive and insensitive to disparity in the class proportions (it's a function of sensitivity and specificity).
- Problems:
  - different curves could cross
  - maybe the threshold is an important discriminating factor.
  - when we will deal with very imbalanced dataset is not reliable.

# Select a threshold using ROC curve

- When we are interested in the threshold selection we have to find a trade-off between specificity and sensitivity.
- We can use the ***Youden's J index***:

$$J = Sensitivity + Specificity - 1$$

  and finding the threshold that maximizes this function.
- Sometimes we can also use this indicator:

$$I = Sensitivity \cdot Specificity$$

# PPV and NPV

We introduce two other important metrics:

- Positive Predicted Value (or precision) definied as:

$$\text{PPV} = \frac{\#\text{positive samples and predicted to be positives}}{\#\text{Samples predicted as positive}} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

- Negative Predicted Value definied as:

$$\text{NPV} = \frac{\#\text{negative samples and predicted to be negative}}{\#\text{Samples predicted as negative}} = \frac{\text{TN}}{\text{TN} + \text{FN}}$$

- With the PPV and NPV we are seeing how a prediction is reliable.

# An example of PPV and NPV computation

Let's suppose we have a confusion matrix like that:

| Predicted — Reference | Positive | Negative |
|---|---|---|
| Positive + | 300 | 60 |
| Negative - | 200 | 855 |

In this case the PPV is:

$$\frac{300}{300+60} \cdot 100 = 83\%$$

and the NPV is:

$$\frac{855}{855+200} \cdot 100 = 83\%$$

# Probabilist interpretation

- PPV and NPV are two conditional probabilities too.
- We use a medical explaination:
  - PPV is defined as the probability of the presence of disease given a positive test result, i.e.,

$$P(\text{disease present}|\text{positive test}).$$

  - NPV is defined as the probability of the absence of disease given a negative test result, i.e.,

$$P(\text{disease absent}|\text{negative test}).$$

- We can find a relationship with Sensitivity and Specificity using the Prevalence.

# Understanding the role of prevalence in PPV and NPV

- We have seen that Sensitivity and Specificity depends only on the test/algorithm.
- The PPV and NPV cannot be independent from it.
- We first see some examples to better understand the idea and we see the mathematical proof of the fact.

# Prevalence effect example

We take two medical examples where we use the same test with :

- Sensitivity = 90%
- Specificity = 90%
- 1000 people

and we change the prevalence from 0.5% to 20%.

# Prevalence = 5%

- First case: Prevalence = 5% so we have 50 positive people and 950 negative ones. So the confusion matrix is:

| Predicted — Reference | Disease | No Disease |
|---|---|---|
| Test + | 45 | 95 |
| Test - | 5 | 855 |

Table: Prevalence = 5%

The PPV is:

$$PPV = \frac{45}{140} \cdot 100 = 32\%$$

that is very low.

# Prevalence = 20%

- Second case: Prevalence = 20% so we have 200 positive people and 800 negative ones. So the confusion matrix is:

| Predicted — Reference | Disease | No Disease |
|---|---|---|
| Test + | 180 | 80 |
| Test - | 20 | 720 |

Table: Prevalence = 5%

The PPV is:

$$PPV = \frac{180}{260} \cdot 100 = 69\%$$

that is quite good.

# Observation on the examples

- The PPV is dependent on the prevalence.
- The PPV can change from one population to another and the same test can be useful or not.

# How PPV, specificity, sensitivity and prevalence are related?

We know that:

$$P(\text{disease}|\text{positive test}) = \frac{P(\text{positive test}|\text{disease}) \cdot P(\text{disease})}{P(\text{positive test})}$$

from Bayes theorem and:

$$P(\text{disease}) = \text{prevalence}$$

and

$$P(\text{positive test}) = P(\text{positive test}|\text{disease}) \cdot P(\text{disease}) \quad (1)$$
$$+ P(\text{positive test}|\text{not disease}) \cdot P(\text{not disease}) \quad (2)$$

and so we obtain:

$$\text{PPV} = \frac{\text{Sensitivity} \times \text{Prevalence}}{(\text{Sensitivity} \times \text{Prevalence}) + ((1 - \text{Specificity}) \times (1 - \text{Prevalence}))}$$

# Some observations on the PPV

- The PPV is strongly dependent on the prevalence.
- This dependence is a problem. It's not easy to have an idea of the prevalence.
  In a spam classifier we can have troubles because there are more schemes to invent spam.
  In medecine the prevalence can also change according to the geografical position.

# Precision-Recall Curve

- If the prevalence is known and fixed the PPV/precision can be useful.
- There is a trade-off between precision and recall related to the threshold chosen. If we increase the threshold we increase the precision but decrease the recall.

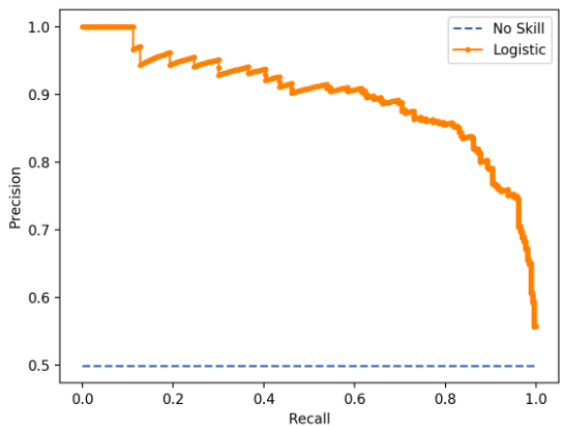



Figure: Precision-Recall curve

# Select a threshold using precision-recall curve

- When we are interested in the threshold selection we have to find a trade-off between precision and recall.
- We can use the ***F1 score***:

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{recall}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \tag{3}$$

  and finding the threshold that maximizes this function.
- Sometimes we can also be more interested on precision or more on recall and we don't want to maximize the trade-off. It depends on the situation.

# What curve is better?

- It can be difficoult to chose between the ROC and precision-recall curve to select the best threshold.
- In a very imbalanced dataset (1:100), if the prevalence is known and constant, it's better to use the precision-recall curve because the ROC is optimistic.
- This is related to the fact that the false positive rate is:

$$FPR = 1 - \text{Specificity} = \frac{FP}{TN + FP}$$

and $FP$ can be very different in order of magnitude with respect to $TN$. So we can have a $FP$ number high w.r.t. $TP$ but low w.r.t. $TN$. Therefore we can have a very good recall and sensitivity and low precision.

# Example of ROC problem

Let's see an example of the previous problem.

| Predicted — Reference | Negative | Positive |
|---|---|---|
| Negative | 9.4e+04 | 10 |
| Positive | 4.4e+03 | 1.6e+02 |

In this case we have:

- Sensitivity: 0.94
- Specificity: 0.95
- Precision: 0.035

*Thank you for your attention!!*