Deep Learning

A course about theory & practice

UNIVERSITÀ DI PAVIA

Predictions

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Feed-Forward Neural Network

Target function: $y = f^*(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d$

Dataset

$$D := \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$$

Representation

$$\tilde{y} = \boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b, \quad \boldsymbol{W} \in \mathbb{R}^{h \times d}, \ \boldsymbol{w}, \boldsymbol{b} \in \mathbb{R}^h, b \in \mathbb{R}$$

Evaluation *(Mean Squared Error)*

$$L(D) := \frac{1}{N} \sum_{i=1}^{N} (\tilde{y}(\boldsymbol{x}^{(i)}) - y^{(i)})^2$$

Optimization *(Gradient descent and its variants)*

$$\Delta \boldsymbol{W} = -\eta \frac{1}{N} \sum_{D} \frac{\partial}{\partial \boldsymbol{W}} L(\tilde{y}^{(i)}, y^{(i)}) \qquad \Delta \boldsymbol{b} = -\eta \frac{1}{N} \sum_{D} \frac{\partial}{\partial \boldsymbol{b}} L(\tilde{y}^{(i)}, y^{(i)})$$

$$\Delta \boldsymbol{w} = -\eta \frac{1}{N} \sum_{D} \frac{\partial}{\partial \boldsymbol{w}} L(\tilde{y}^{(i)}, y^{(i)}) \qquad \Delta b = -\eta \frac{1}{N} \sum_{D} \frac{\partial}{\partial b} L(\tilde{y}^{(i)}, y^{(i)})$$

Predictions?

Optimization:
The aim is finding the parameters that make the representation best approximating the target function over the dataset

Fundamental question:
How good is the approximator with data items that are *not* in the dataset?

Independent, Identically Distributed (iid)

Dataset

$$D = \left\{ (\boldsymbol{x}^{(i)}, y^{(i)}) \right\}_{i=1}^{N}$$

this what we use for optimization (a.k.a. learning)

Identically distributed

$$p^*(\boldsymbol{x}^{(i)}) = p^*(\boldsymbol{x}^{(j)}), \quad \forall i, j$$

where p^* is the (unknown) true probability that generated the sample

Independent

$$p^*\left(\{\boldsymbol{x}^{(i)}\}_{i=1}^{N}\right) = \prod_{i=1}^{N} p^*(\boldsymbol{x}^{(i)})$$

What we might look for

Evaluation *(Mean Squared Error)*

$$L(D) = \frac{1}{N} \sum_{i=1}^{N} \left(\tilde{y}(\boldsymbol{x}^{(i)}) - y^{(i)} \right)^2$$

this what we use for optimization (a.k.a. learning)

Expected error *(over a population of interest)*

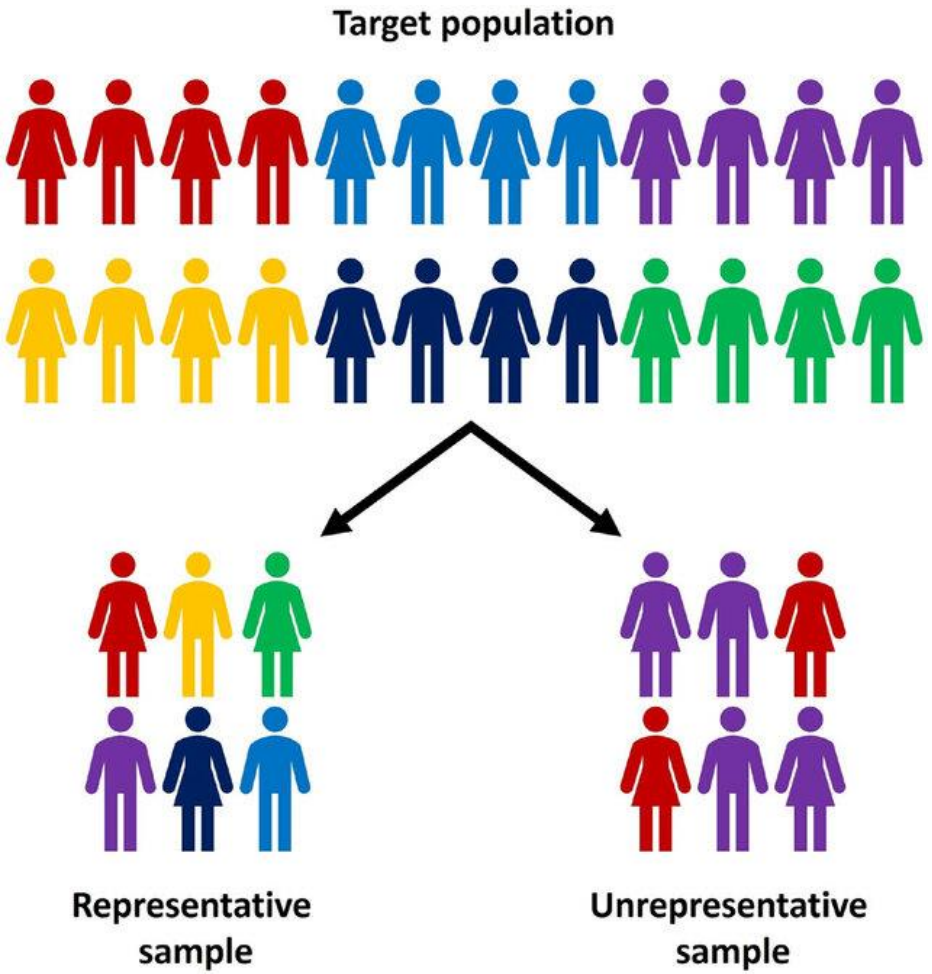
$$L_{p^*} := \mathbb{E}_{p^*} \left[\left(\tilde{y}(\boldsymbol{x}^{(i)}) - y^{(i)} \right)^2 \right]$$

this what we might want to minimize

where p^* is the (unknown) true probability of the population

Representativeness

Is the dataset representative of input features $p^*\left(\boldsymbol{x}^{(i)}\right)$ *?*



[Image from https://cms.galenos.com.tr/Uploads/Article_53618/Diagn%20Interv%20Radiol-28-450-En.pdf]

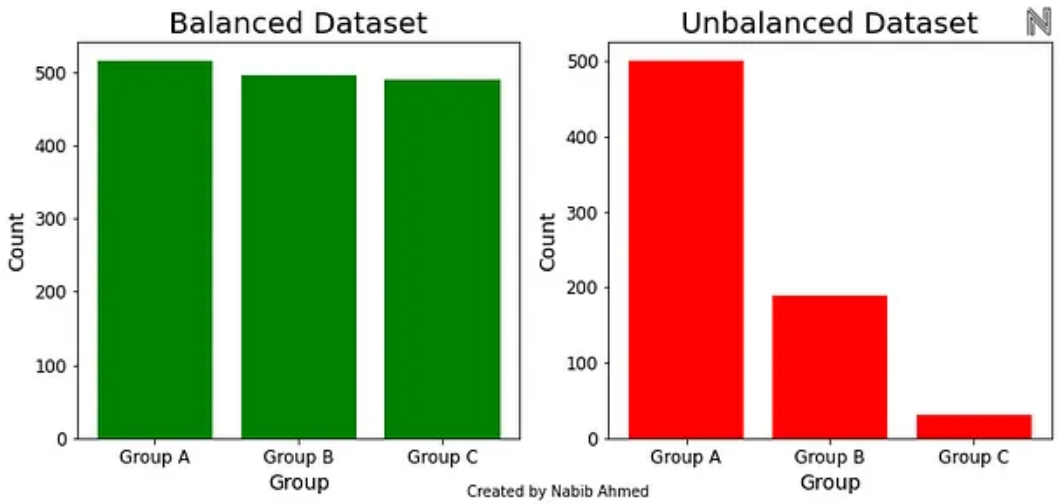
Balanced vs. Unbalanced

Sometimes, even the minimization of

$$L_{p^*} := \mathbb{E}_{p^*}\left[\left(\tilde{y}(\boldsymbol{x}^{(i)}) - y^{(i)}\right)^2\right]$$

might not be enough

When feature distributions are unbalanced a predictor minimizing the expected error will be biased towards over-represented classes



[Image from https://medium.com/@nahmed3536/data-bias-what-all-data-practitioners-should-be-aware-of-115eaeae48c]

Noisy observations

So far, we assumed that in a dataset D

$$y^{(i)} = f^*(\boldsymbol{x}^{(i)}), \quad \forall i$$

namely, that all annotations are noise-free

What if we have instead

$$y^{(i)} = f^*(\boldsymbol{x}^{(i)}) + \epsilon$$

where ϵ *is some random noise?*

If $\epsilon \sim \mathcal{N}(0, \sigma^2)$*, namely if noise is gaussian with zero mean (and any variance), we can still use the expected error as a target*

If this is not the case, our predictions will be biased

Training Set
Validation Set
Test Set

Overfitting

When the training process becomes too specific to the training set

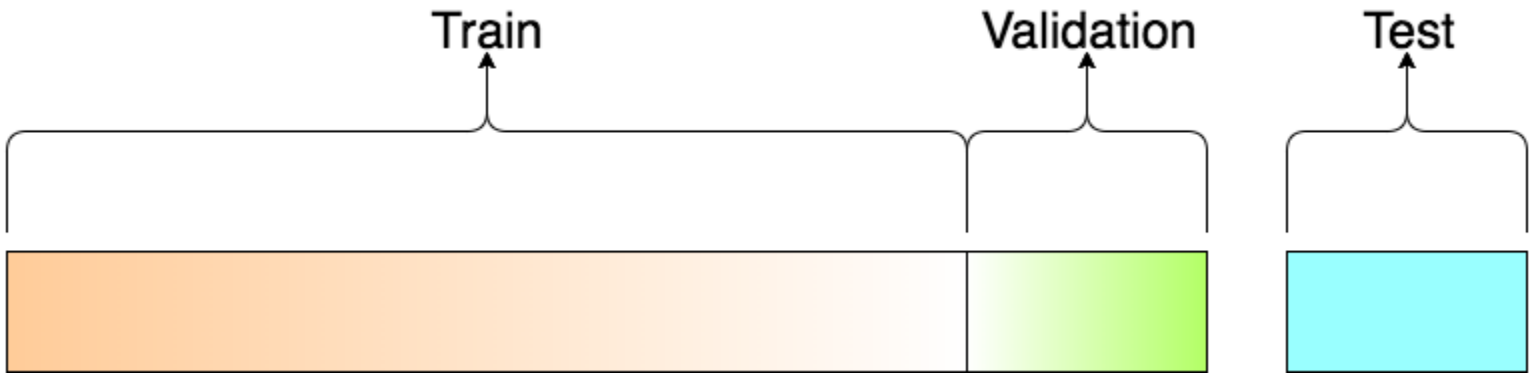
- ***Training set, validation set, test set***

  Splitting the dataset

$$D = D_{train} \cup D_{val} \cup D_{test}$$

$$\{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N} = \{(\boldsymbol{x}^{(j)}, y^{(j)})\}_{j=1}^{N_{train}} \cup \{(\boldsymbol{x}^{(k)}, y^{(k)})\}_{k=1}^{N_{val}} \cup \{(\boldsymbol{x}^{(l)}, y^{(l)})\}_{l=1}^{N_{test}}$$

$$N_{train} \gg N_{val}, N_{test}$$



Overfitting

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  $$N_{train} \gg N_{val}, N_{test}$$

  Training is made on D_{train} only

  At each *epoch* — *when the whole D_{train} has been processed*

  the loss function is evaluated on D_{val}

  After some epochs, the performance on D_{val} might get worse

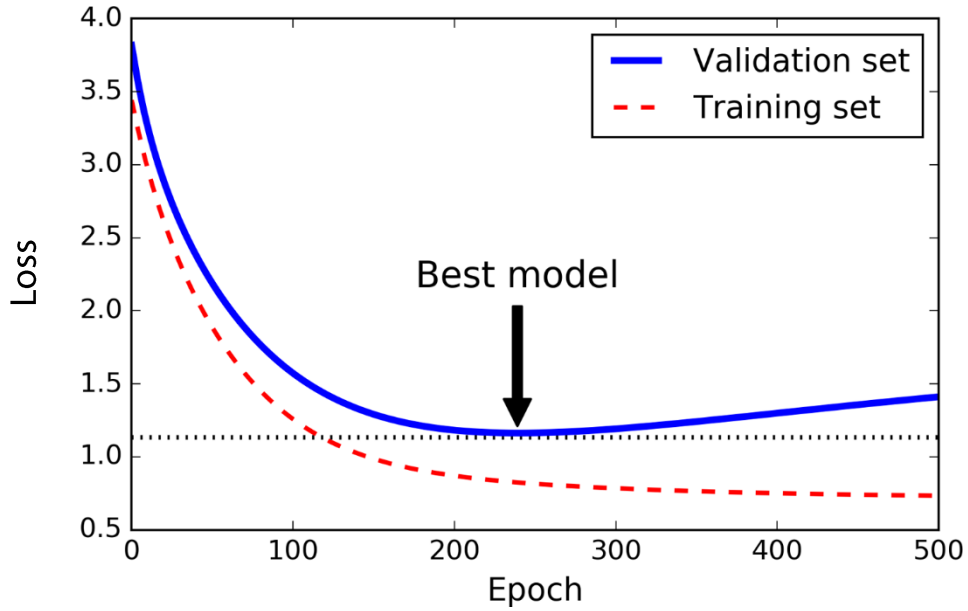


Image from https://www.safaribooksonline.com/library/view/hands-on-machine-learning/9781491962282/ch04.html

k-Fold Cross-Validation

- ***One dataset, multiple splits***
  1) Divide the dataset into k splits (i.e. *folds*)
  2) Use k - 1 folds for training and 1 fold for testing
  3) Unless all combinations have been considered, change combination and go back to 2)

Consider the *average test loss* across all possible combinations

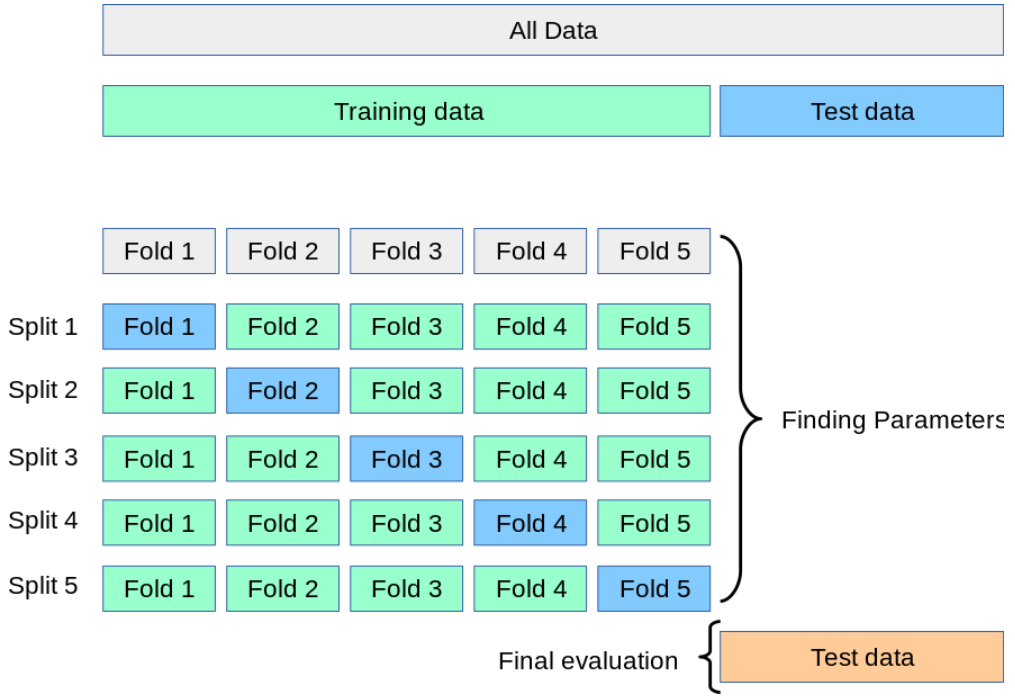


Image from https://www.kdnuggets.com/2020/01/data-validation-machine-learning.html

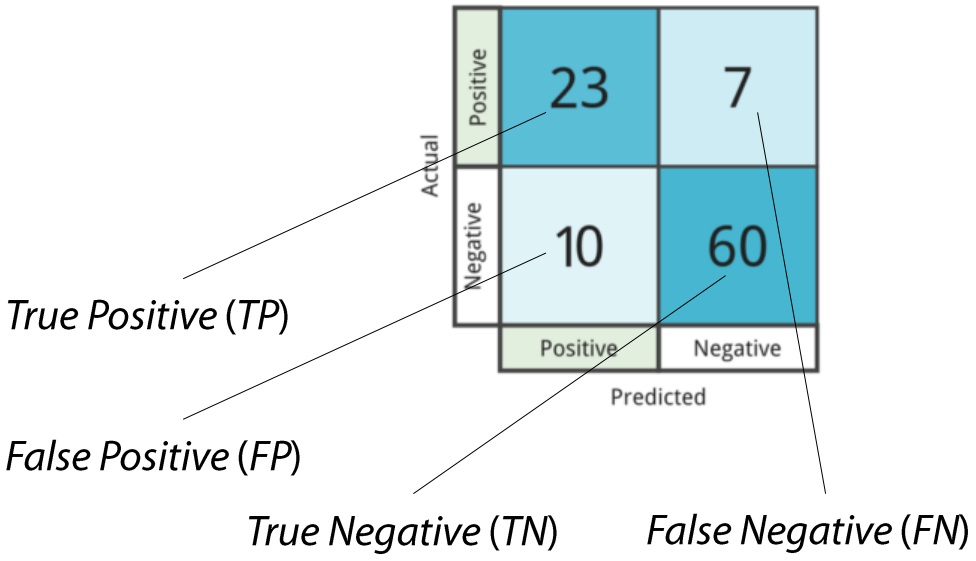
Evaluating a Classifier

Classifier: Confusion Matrix

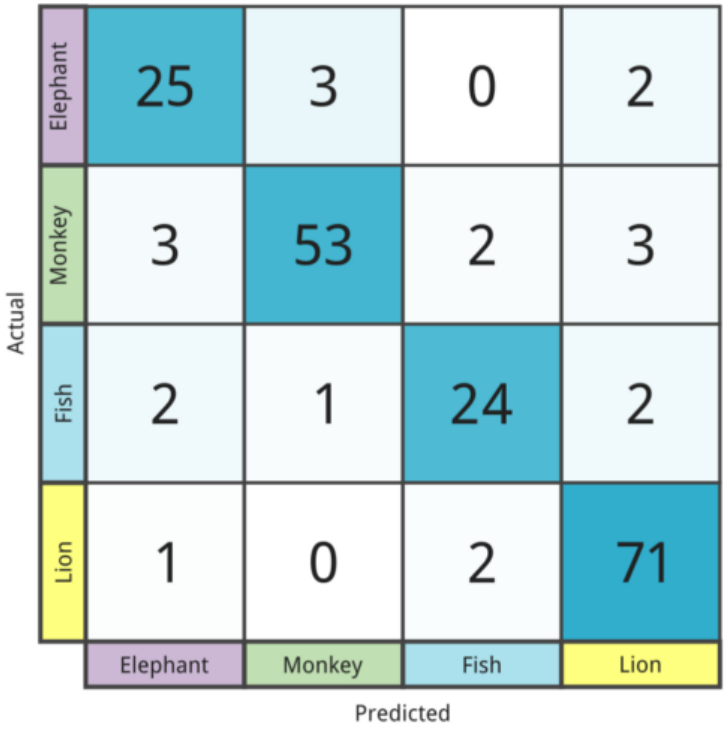
- Actual VS. Predicted Classes

  Predicted:
  the class with the highest probability

Binary

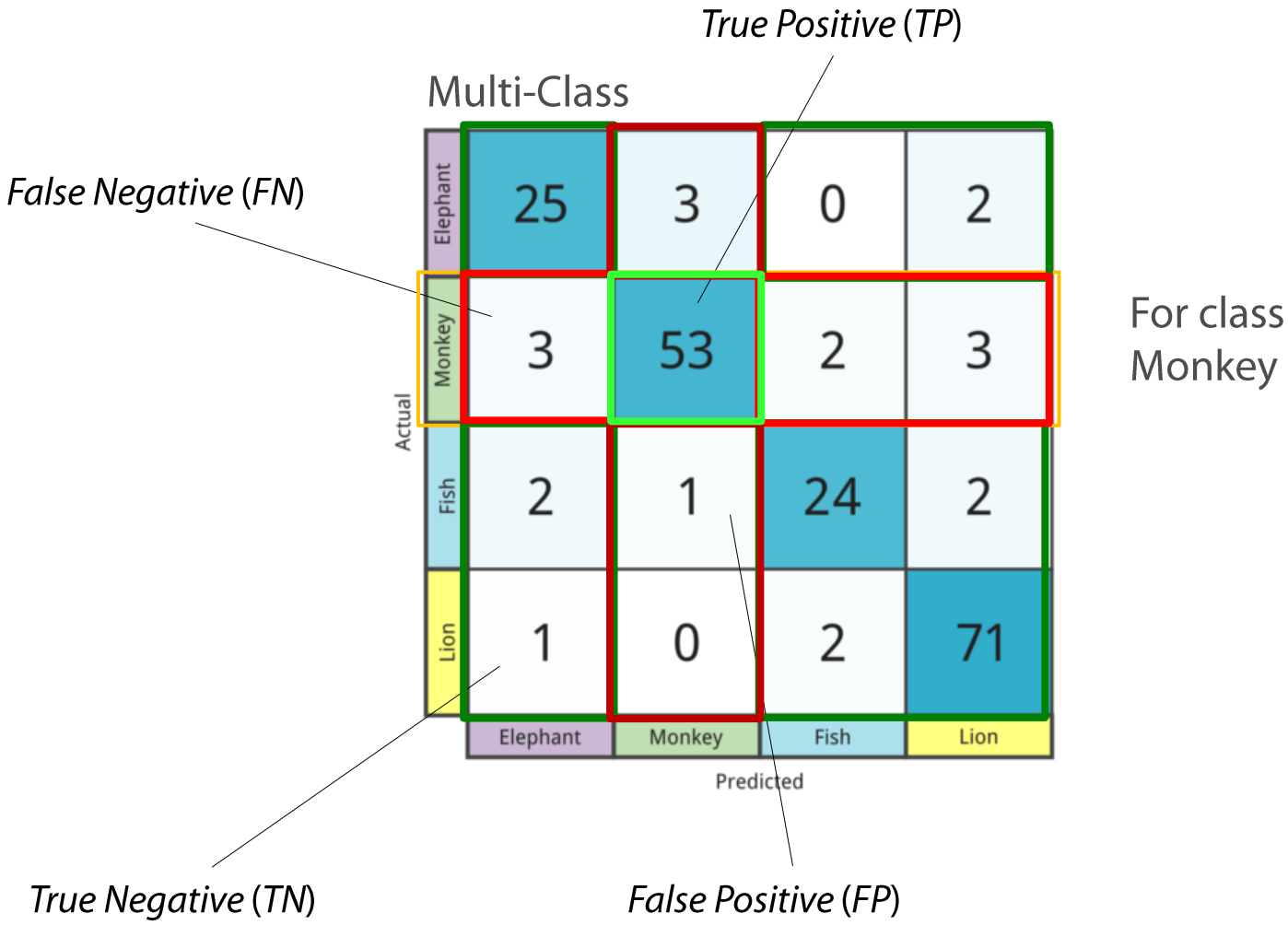


Multi-Class



Classifier: Confusion Matrix

- Actual VS. Predicted Classes



Classifier: Metrics

- **Accuracy**

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

- **Recall**

$$\text{recall} := \frac{TP}{TP + FN}$$

also called 'sensitivity'

- **Precision**

$$\text{precision} := \frac{TP}{TP + FP}$$

- **F_1**

$$F_1 := 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}}$$

typically preferred when
when positive and negative cases are highly unbalanced

Receiver operating characteristic (ROC)

Typically, a classifier produces a probability distribution
Where do we put the threshold γ *?*

$$\tilde{y}(\boldsymbol{x}^{(i)}) = y_1 \quad \text{if} \quad \boldsymbol{x} > \gamma$$

Consider the probability distribution

$$p^*(y^{(i)} \mid \tilde{y}(\boldsymbol{x}^{(i)}))$$

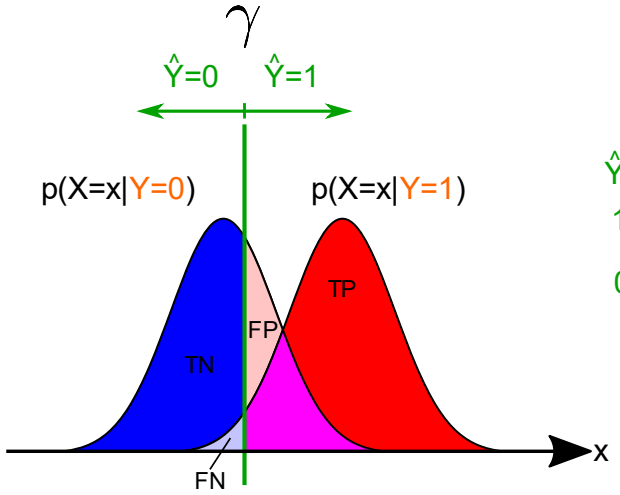
which could be estimated as

same as 'recall'

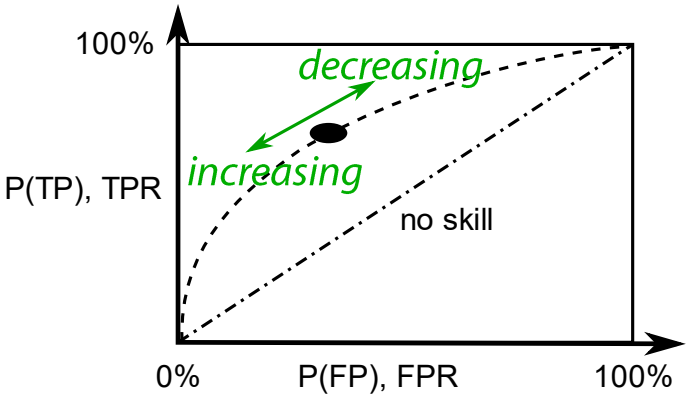
$$\text{true positive rate (TPR)} := \frac{TP}{TP + FN}$$

$$\text{false positive rate (FPR)} := \frac{FP}{FP + TN}$$

these values depend on the threshold γ *we choose*



Ŷ \ Y	1	0
1	TP	FP
0	FN	TN



[Images from https://en.wikipedia.org/wiki/Receiver_operating_characteristic]

Area under curve (AUC)

A random classifier is right / wrong an equal number of times, regardless of γ

$$\mathrm{TPR} = \mathrm{FPR}, \quad \forall\gamma$$

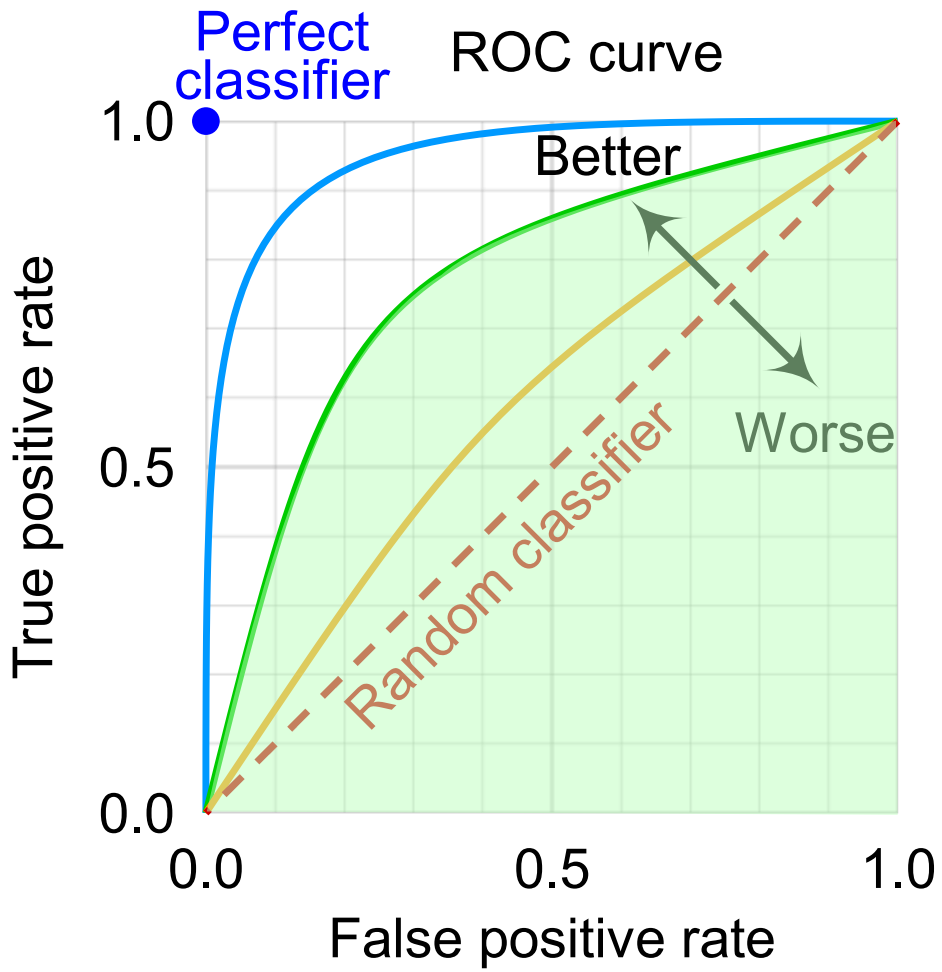
whereas a good classifier should have

$$\mathrm{TPR} \geq \mathrm{FPR}, \quad \forall\gamma$$

The Area Under Curve of the ROC measures the overall efficiency of a classifier

For a random classifier: $\mathrm{AUC} = 0.5$

For a perfect classifier: $\mathrm{AUC} = 1.0$



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