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Class: Machine Learning

Machine Learning Evaluation

Instructor: Matteo Leonetti

- Define *overfitting*.
- Apply a strategy to avoid overfitting.
- List the main accuracy metrics to measure the performance of a classifier.
- Choose the appropriate metric for a given classification problem.
- Apply the metrics to real data sets and classifiers.

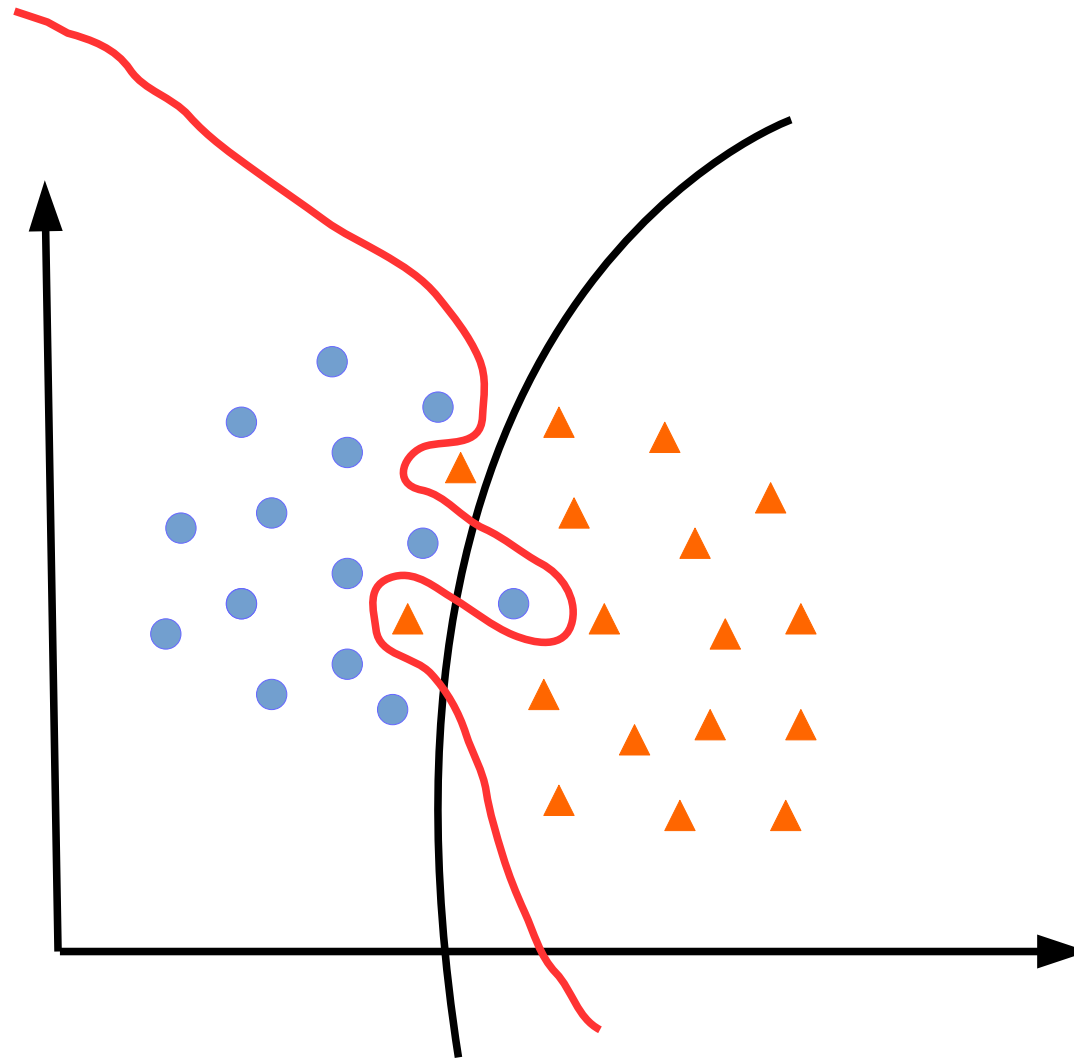
Feature Selection



The first step before any classification can take place is to decide what *features* we are considering when trying to discriminate two sets.

For example, we could use width and height, or colour, shape...

Two possible solutions



Which one would you say it's best?

A model *overfits* when it describes the randomness associated with the data, rather than the underlying relationship between the data points.

Occam's razor



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Attributed to William of Ockham (~1300 A.D.):

Entities should not be multiplied unnecessarily



Preventing Overfitting

Test set



Training data



Test data

Test on a portion of the data different from training.

Example: parametric classifier

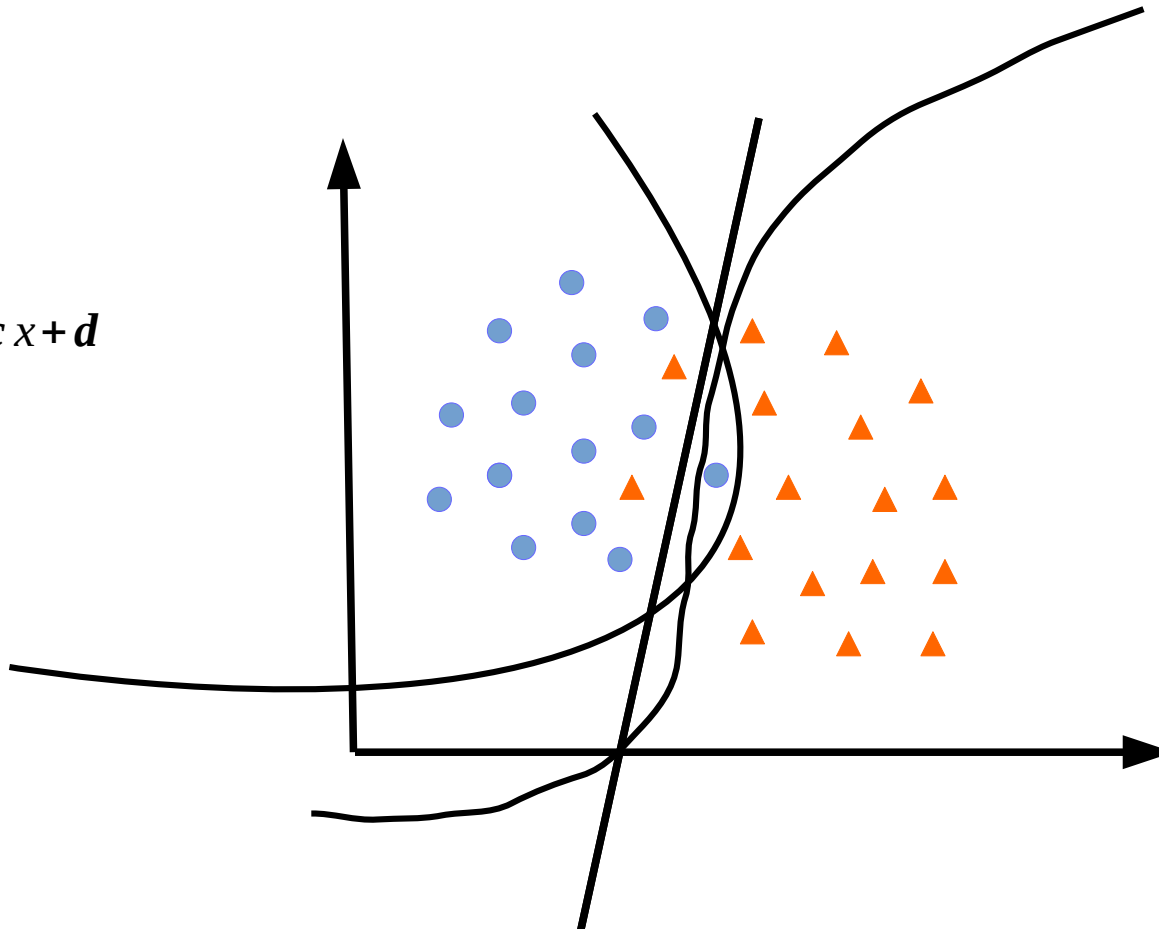
You may want to choose between different models, for instance:

Different orders of polynomials:

$$y = \mathbf{a}x + \mathbf{b}$$

$$y = \mathbf{a}x^2 + \mathbf{b}x + \mathbf{c}$$

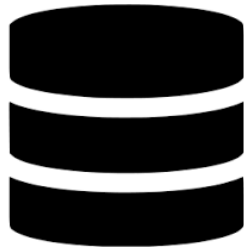
$$y = \mathbf{a}x^3 + \mathbf{b}x^2 + \mathbf{c}x + \mathbf{d}$$



Validation set



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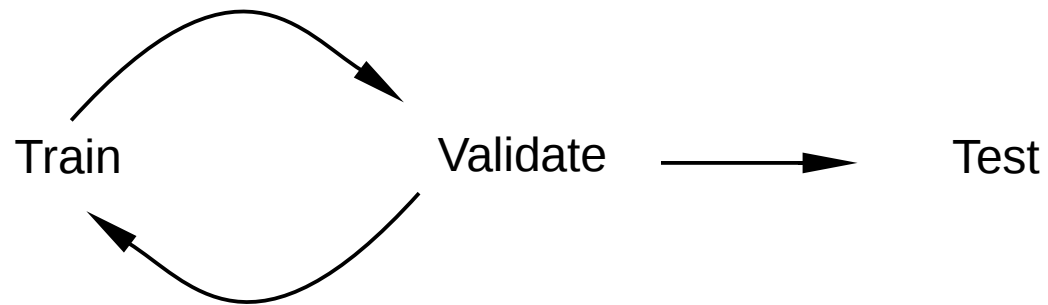
Training data



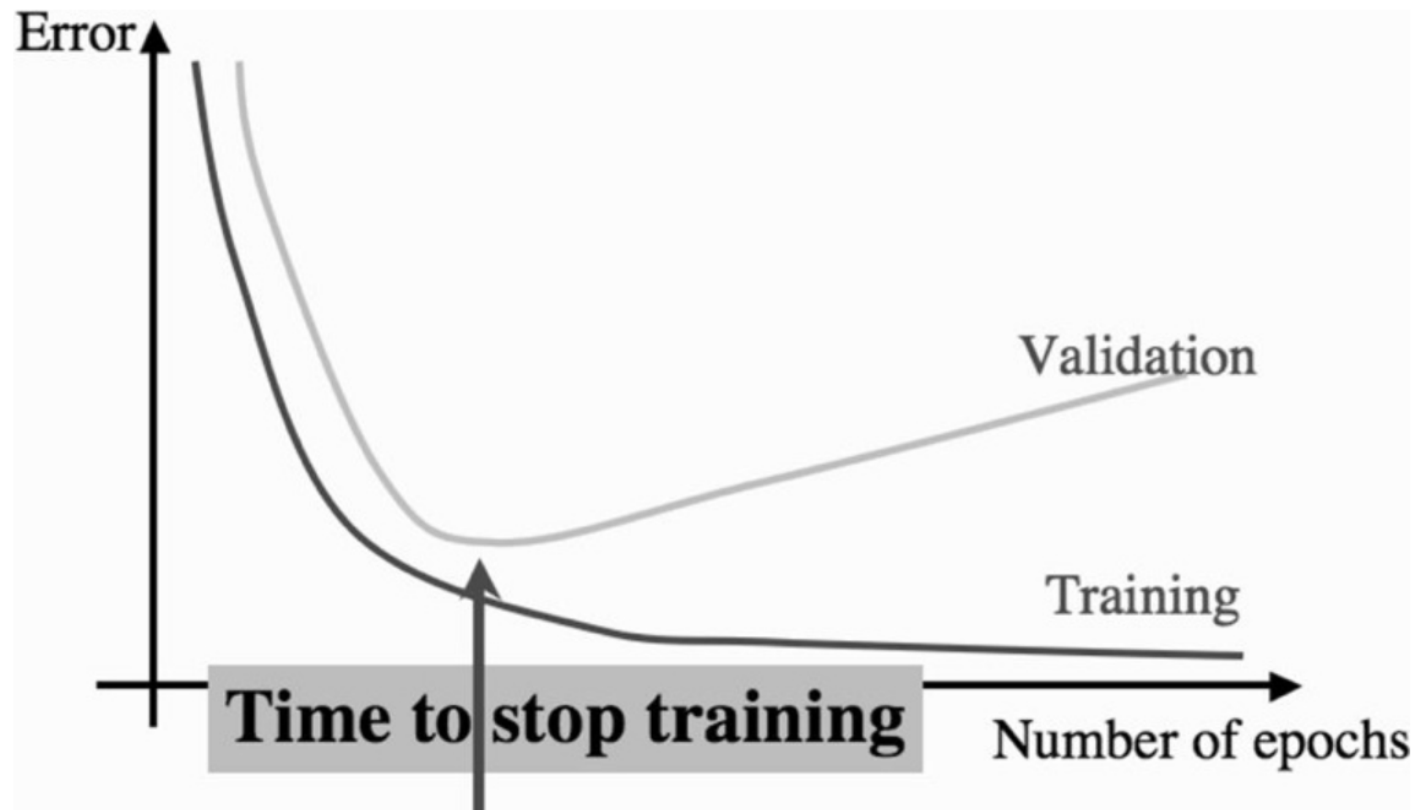
Validation data



Test data



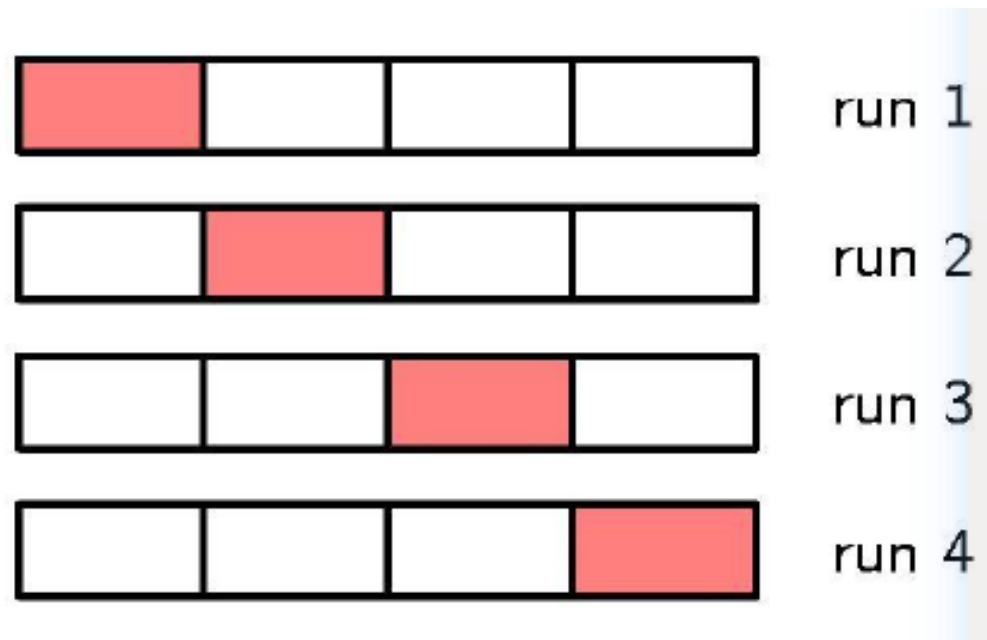
When to stop learning



Cross validation



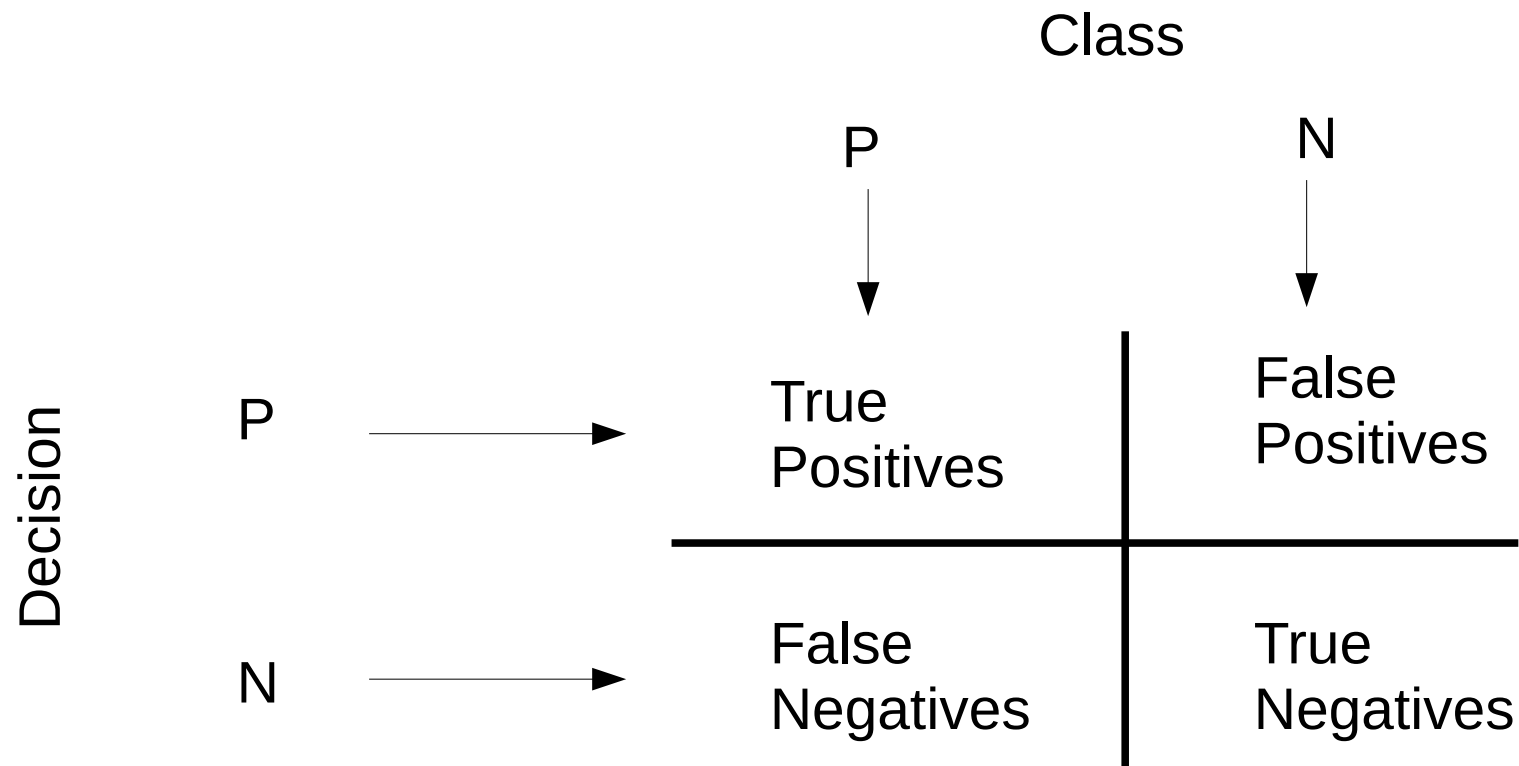
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Measuring Accuracy

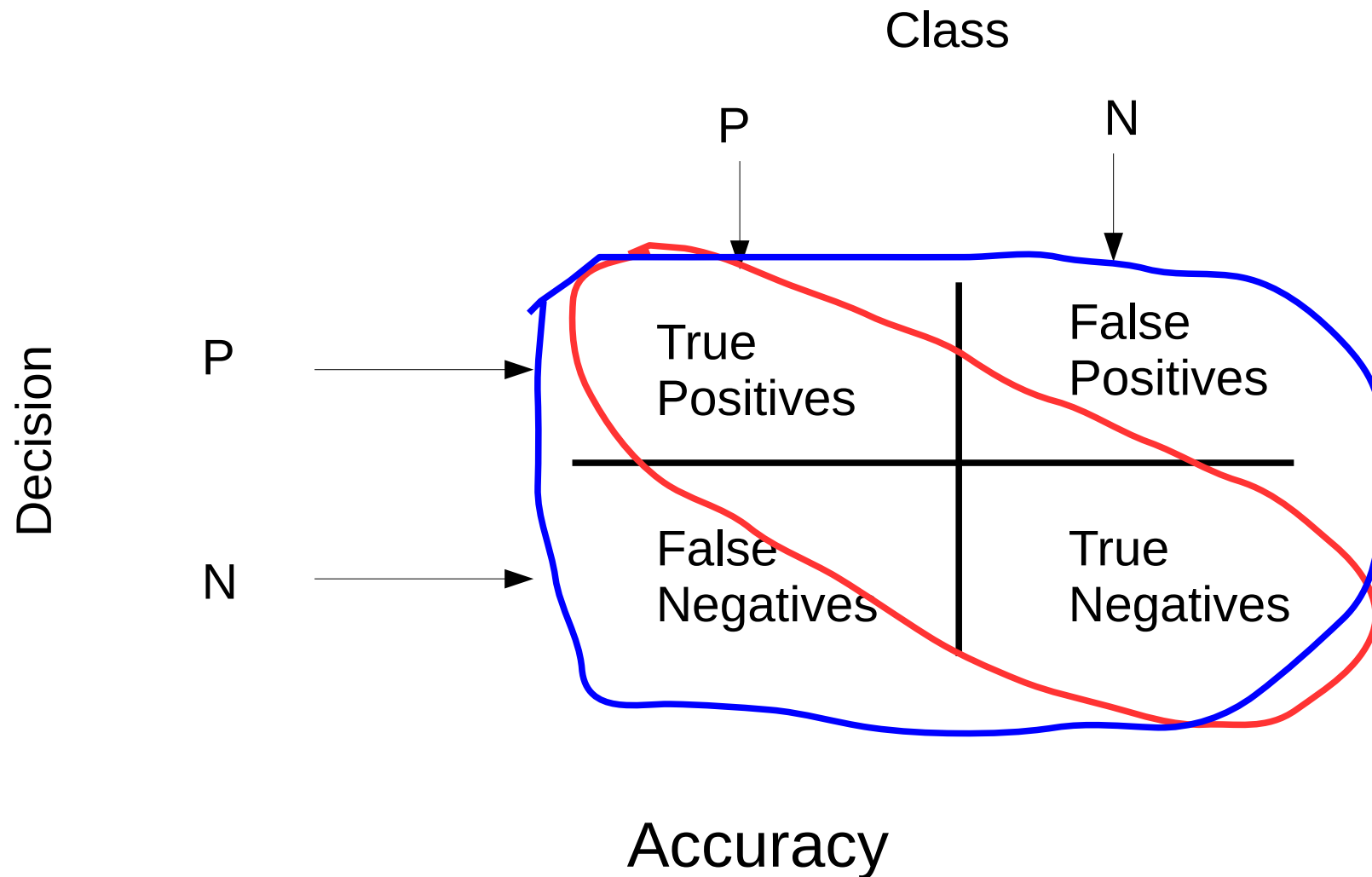
Accuracy on a binary classifier



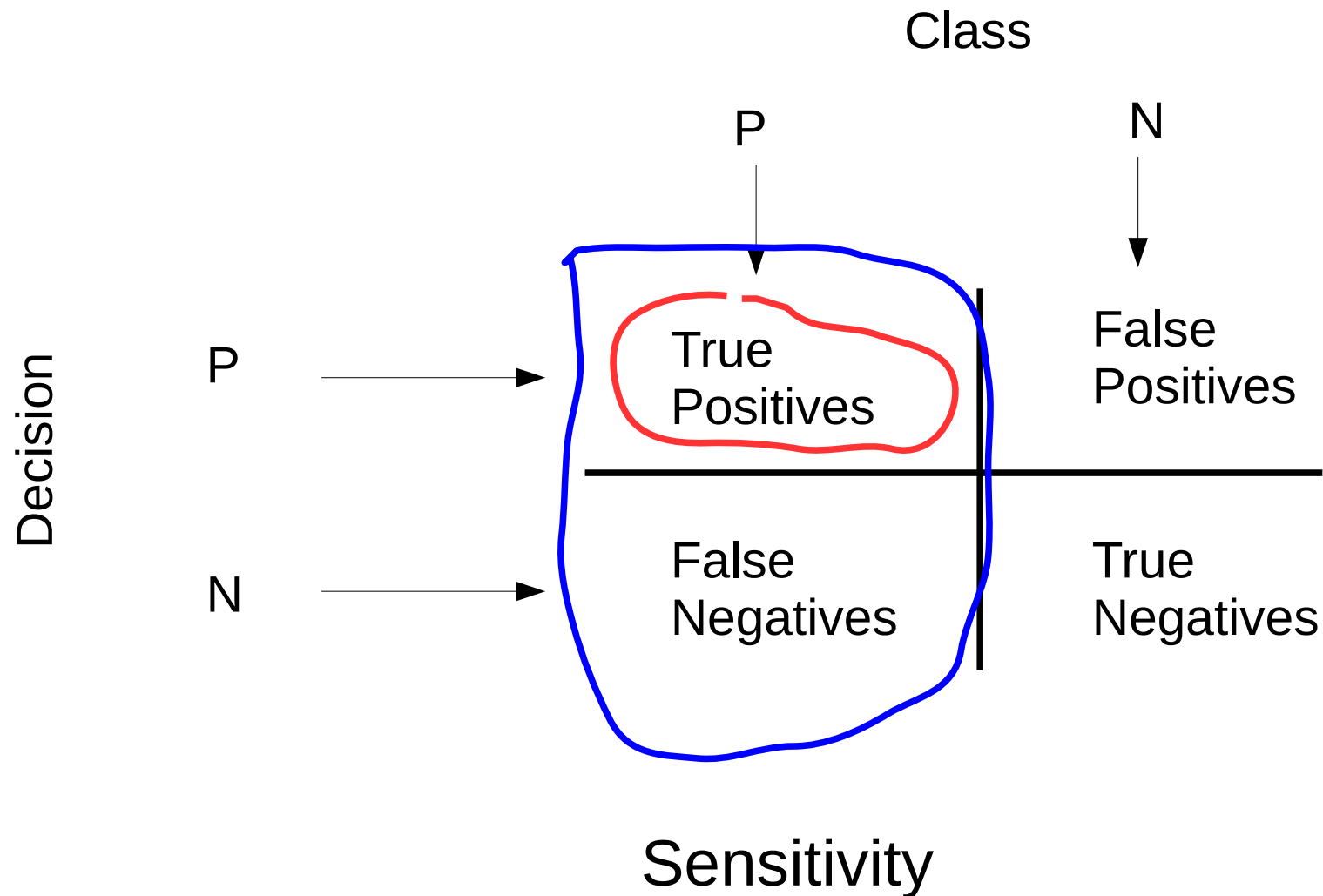
Accuracy on a binary classifier



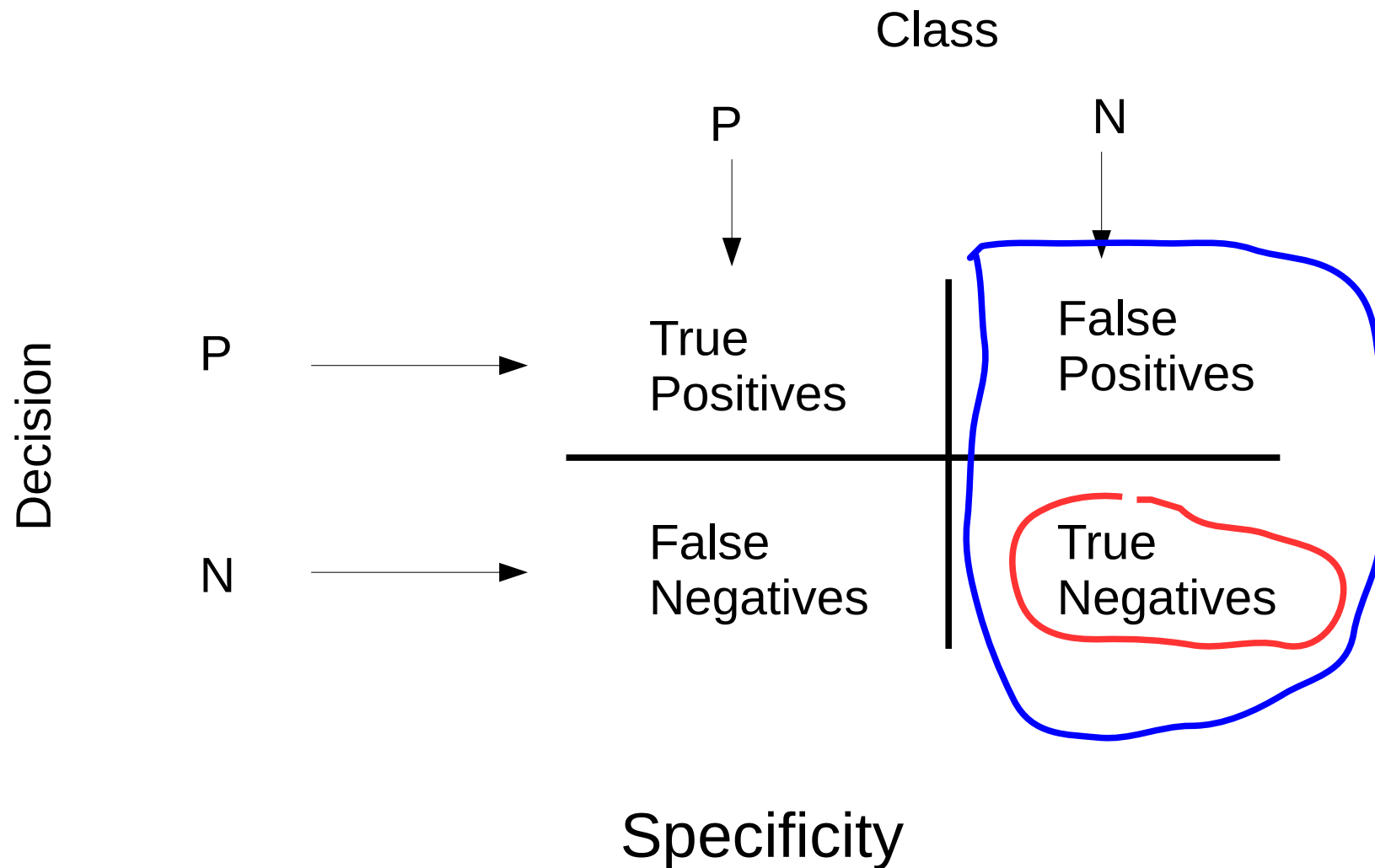
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Accuracy on a binary classifier



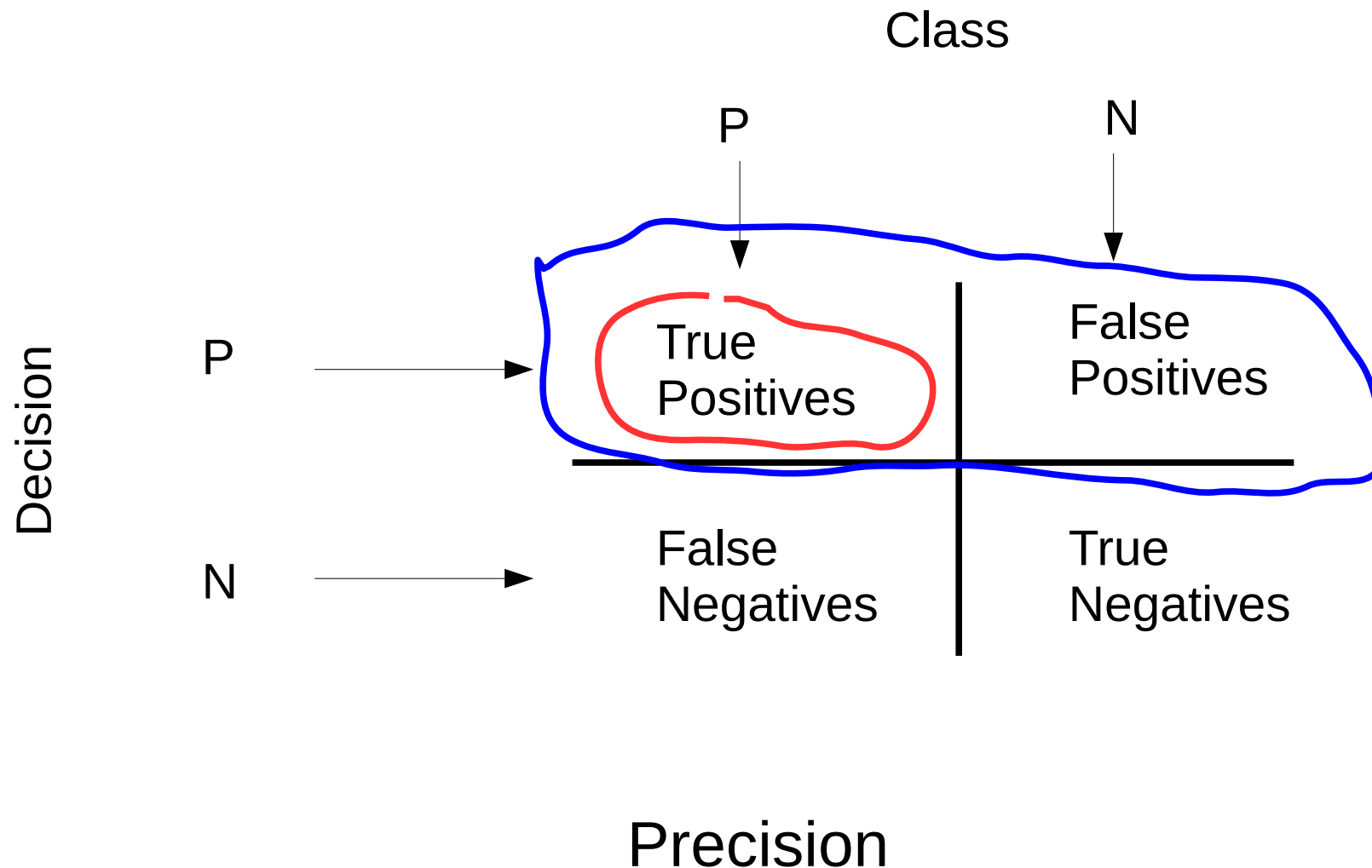
Accuracy on a binary classifier



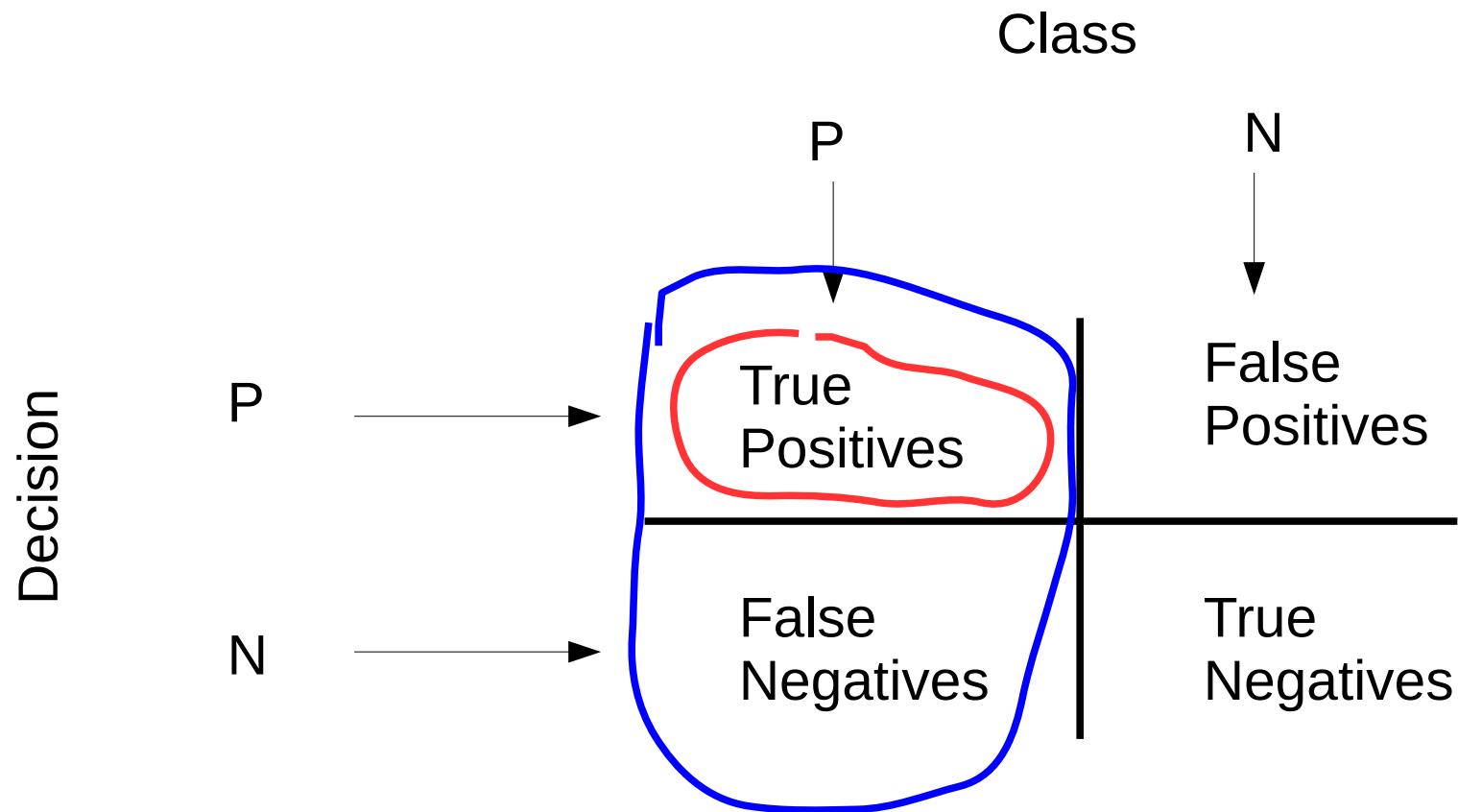
Accuracy on a binary classifier



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Accuracy on a binary classifier



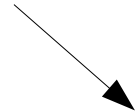
Recall (same as sensitivity)

Accuracy metrics



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TN!



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

$$\text{Sensitivity} = \frac{\#TP}{\#TP + \#FN}$$

$$\text{Specificity} = \frac{\#TN}{\#TN + \#FP}$$

$$\text{Precision} = \frac{\#TP}{\#TP + \#FP}$$

$$\text{Recall} = \frac{\#TP}{\#TP + \#FN}$$

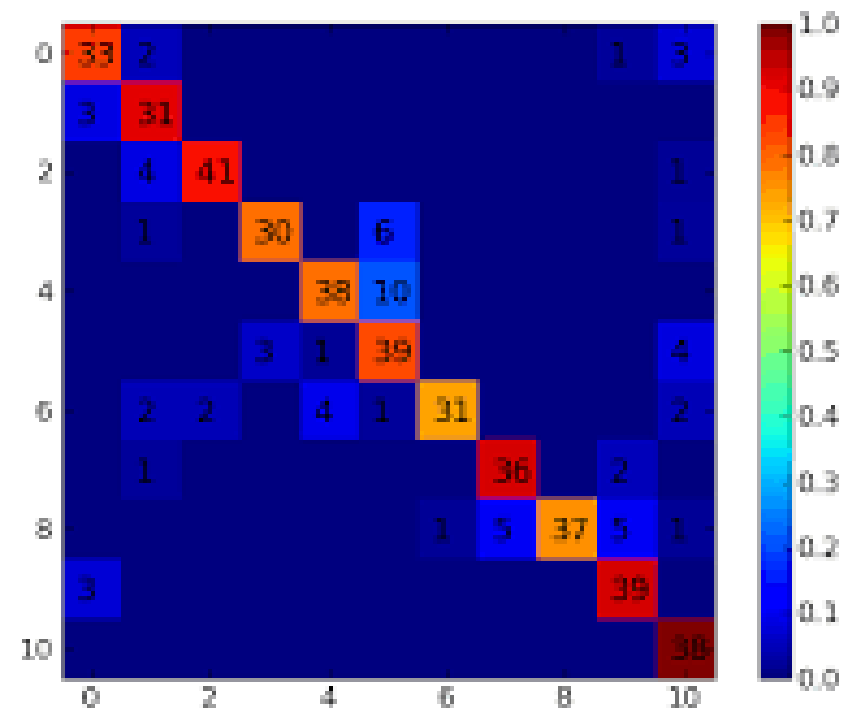
True Positives	False Positives
False Negatives	True Negatives

$$F_1 = 2 \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \quad 0 \leq F_1 \leq 1$$

$$MCC = \frac{\#TP \times \#TN - \#FP \times \#FN}{\sqrt{(\#TP + \#FP)(\#TP + \#FN)(\#TN + \#FP)(\#TN + \#FN)}}$$

$$-1 \leq MCC \leq 1$$

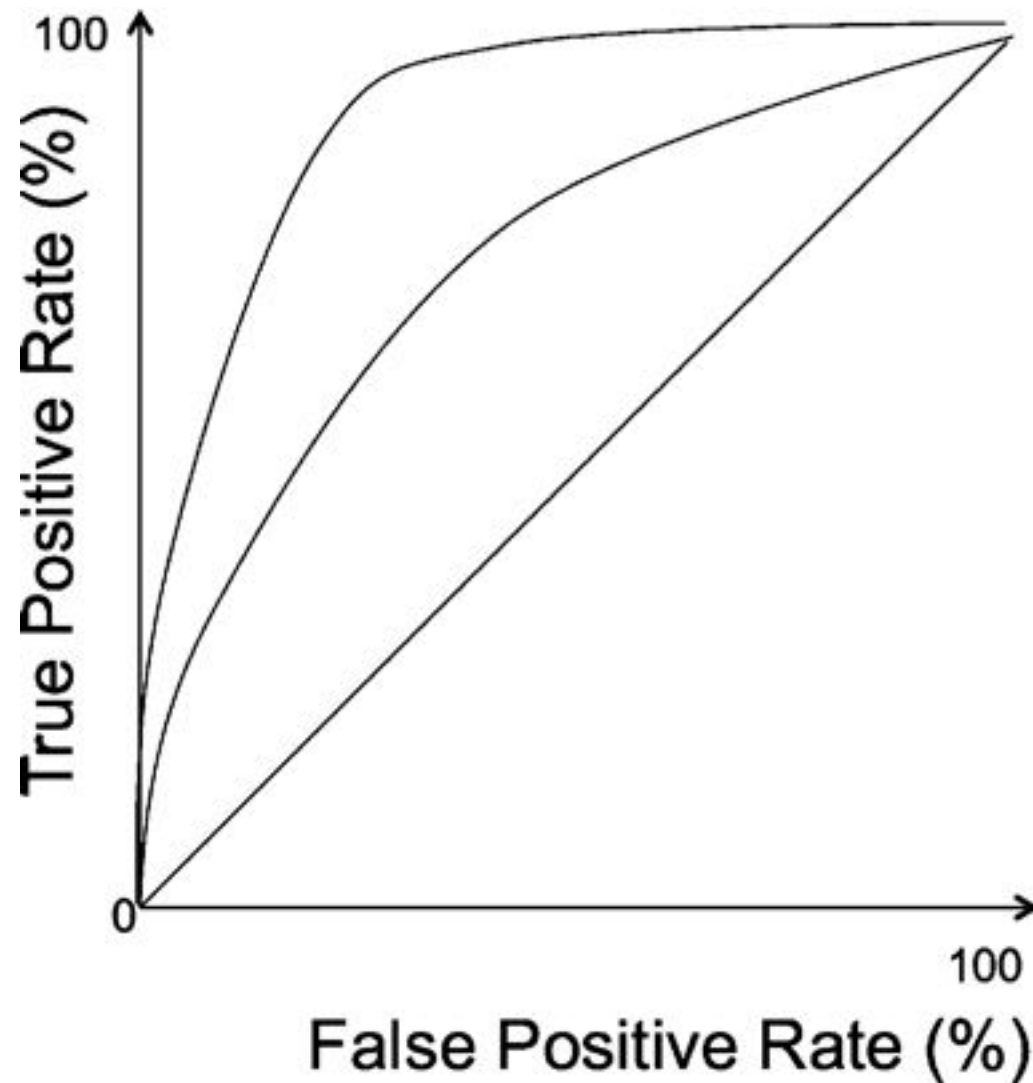
Confusion Matrix



ROC curve

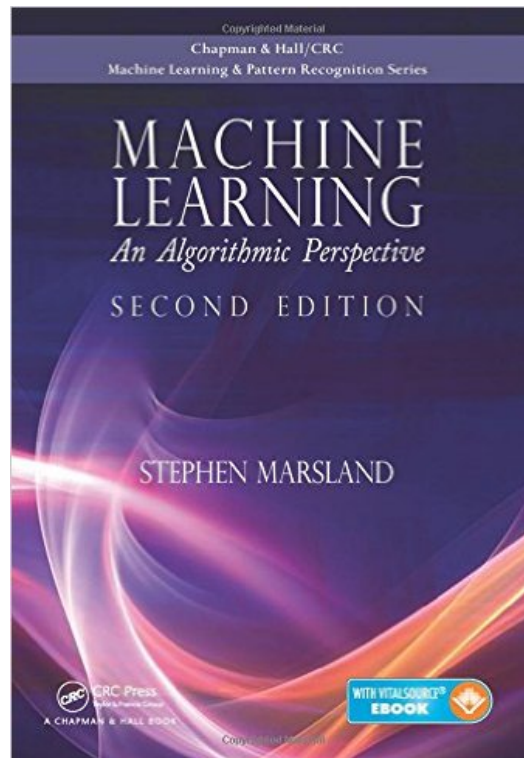


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Conclusion



Chapter 2, up to 2.2