Lecture 12

Model Evaluation 5:
Performance Metrics

STAT 479: Machine Learning, Fall 2019

Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat479-fs2019/

Some Announcements

The Undergraduate Statistics Club + the Data Science Club present...

An Interview Skills Workshop

By Amy Yang from SuccessWorks

When: Tuesday November 12 from 6-7pm

Where: Service Memorial Institute Room 133

Why: To learn how to nail that interview!

The Undergraduate Statistics Club + the Data Science Club present...

An Alumni Panel

With UW-Madison alumni focused in Technology, Data, and Analytics

When: Thursday November 21 from 6:30-7:30pm

Where: Genetics-Biotechnology Center Building Room 1441

Why: To get advice from professionals in the field!

Lecture 12

Model Evaluation 5:
Performance Metrics

STAT 479: Machine Learning, Fall 2019

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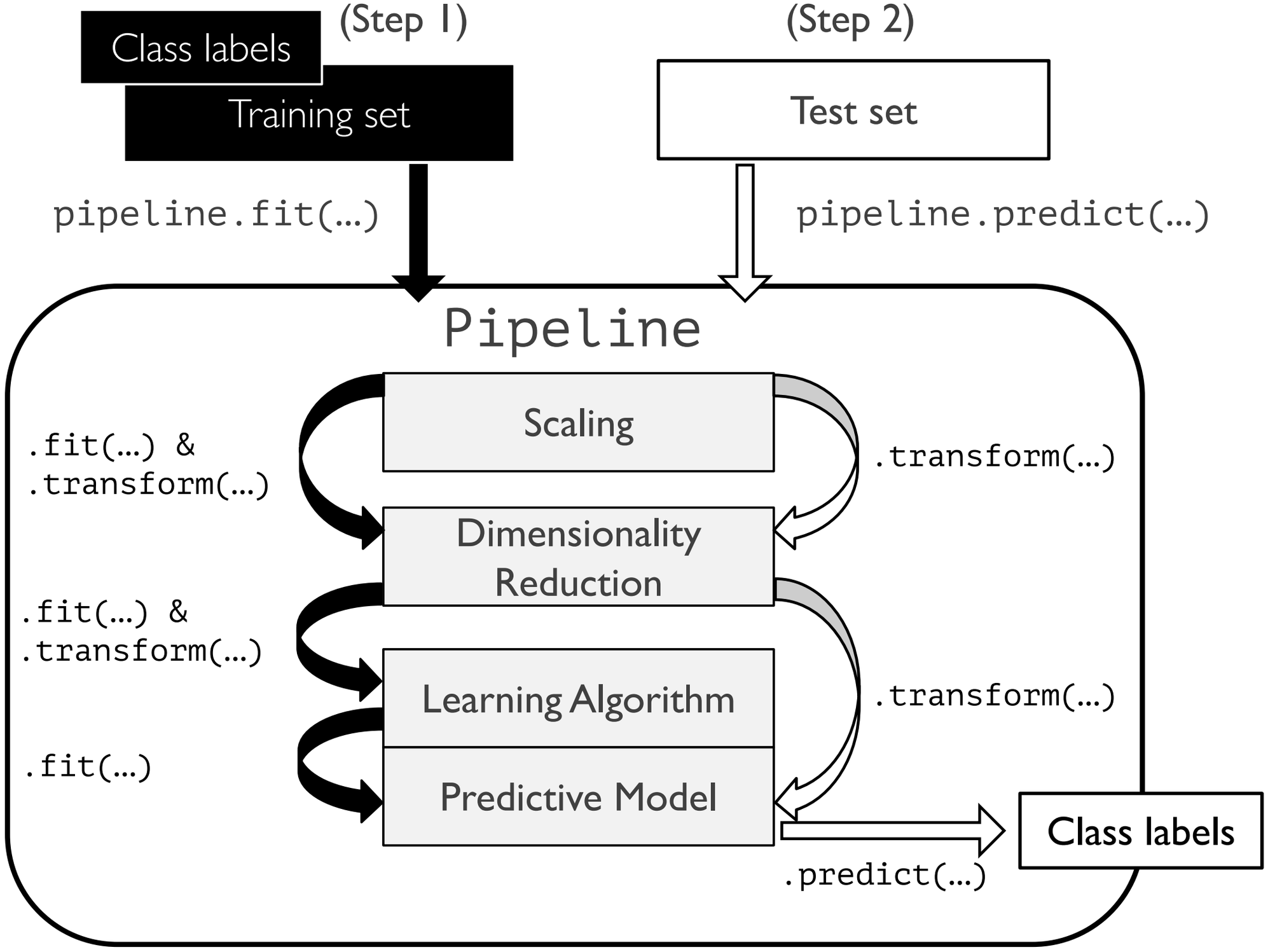
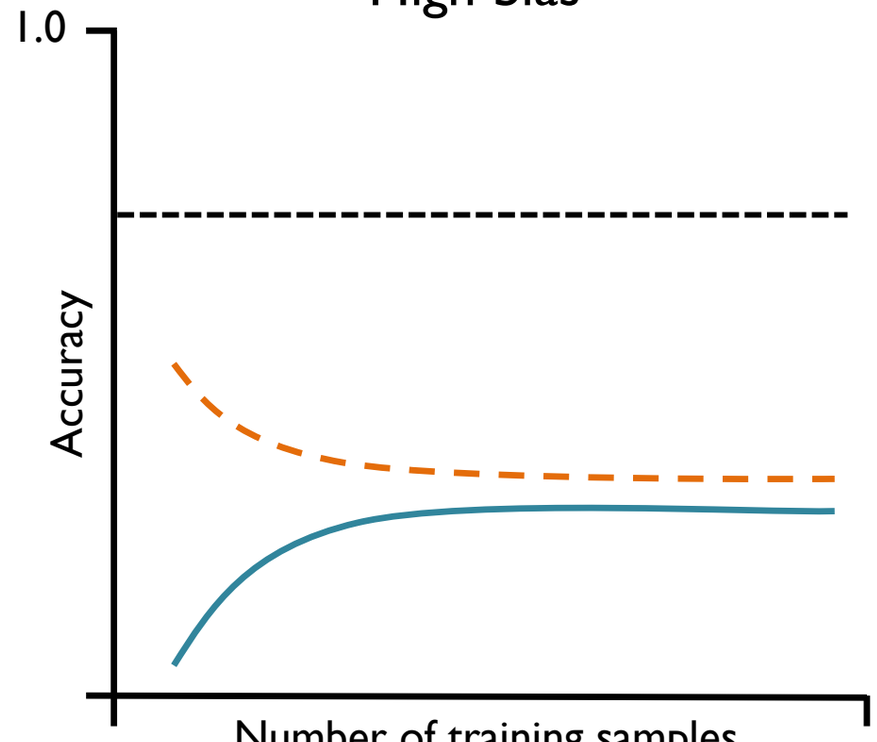
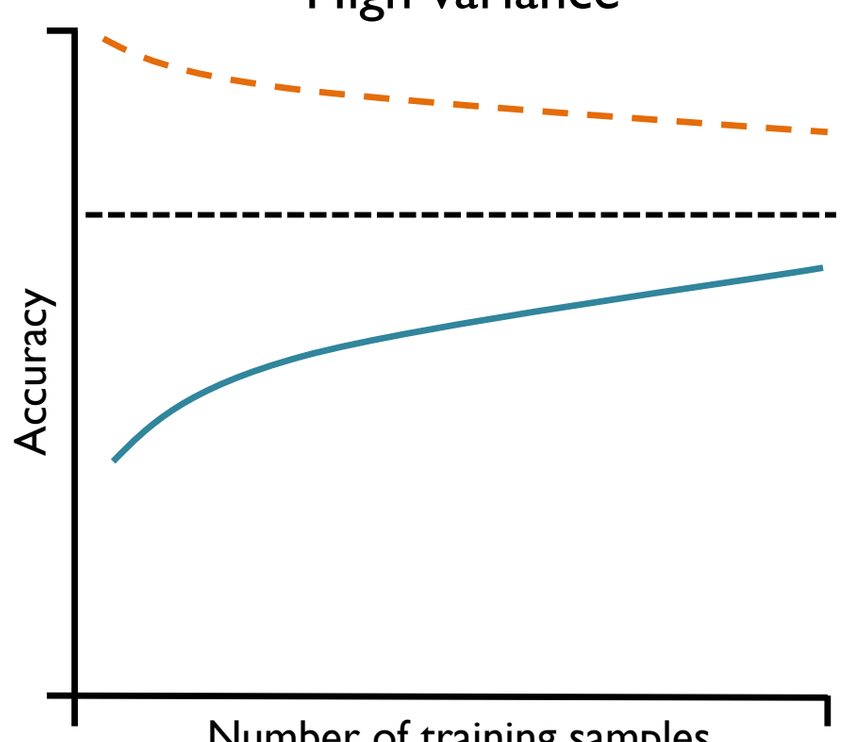
Recap

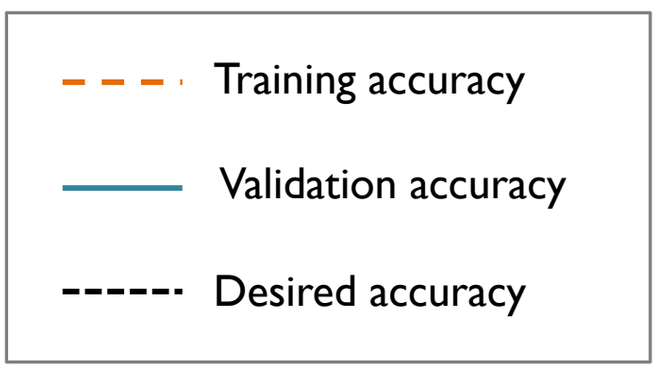


Source: *Python Machine Learning, 2nd Edition*

Recap







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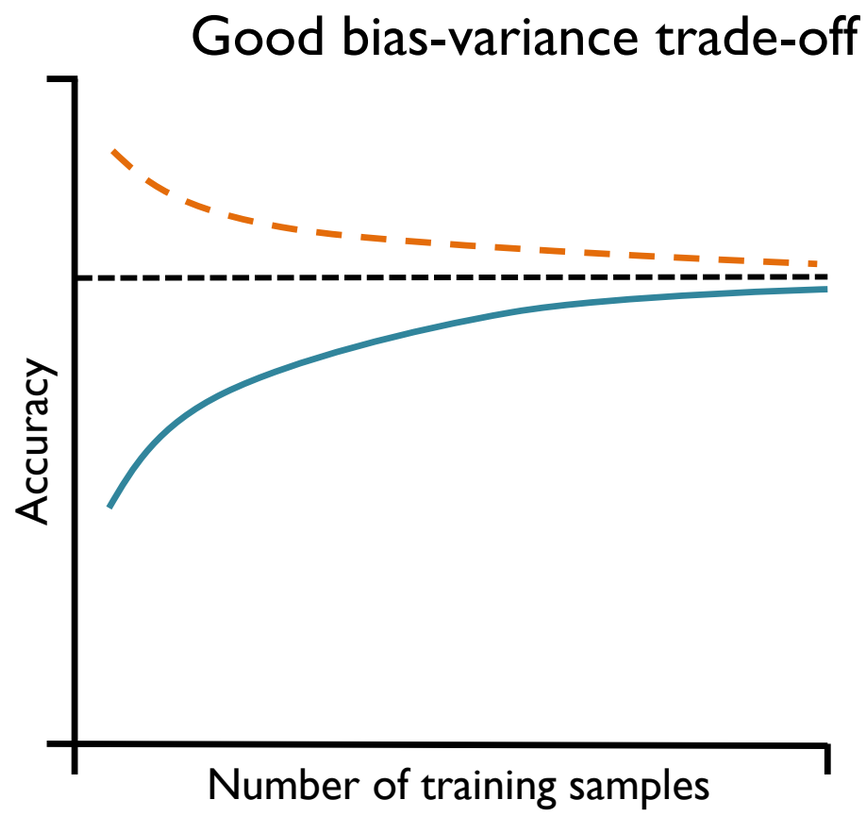
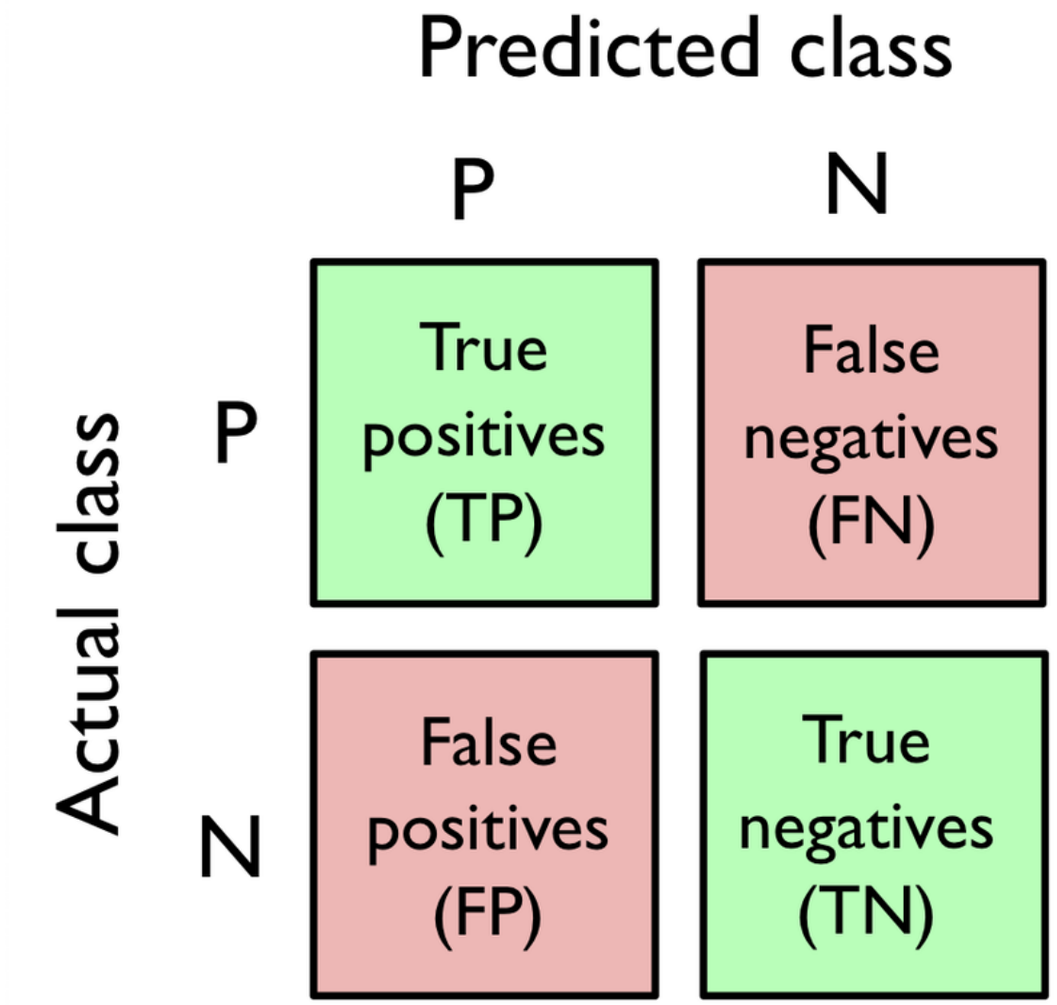


2x2 Confusion Matrix



$$ERR = \frac{FP + FN}{FP + FN + TP + TN} = 1 - ACC \tag{1}$$

$$ACC = \frac{TP + TN}{FP + FN + TP + TN} = 1 - ERR \tag{2}$$

Confusion Matrix for Multi-Class Settings

Predicted Labels

True Labels

	Class 0	Class 1	Class 2
Class 0	T(0,0)		
Class 1		T(1,1)	
Class 2			T(2,2)

Confusions matrices are traditionally for binary class problems but we can be readily generalized it to multi-class settings

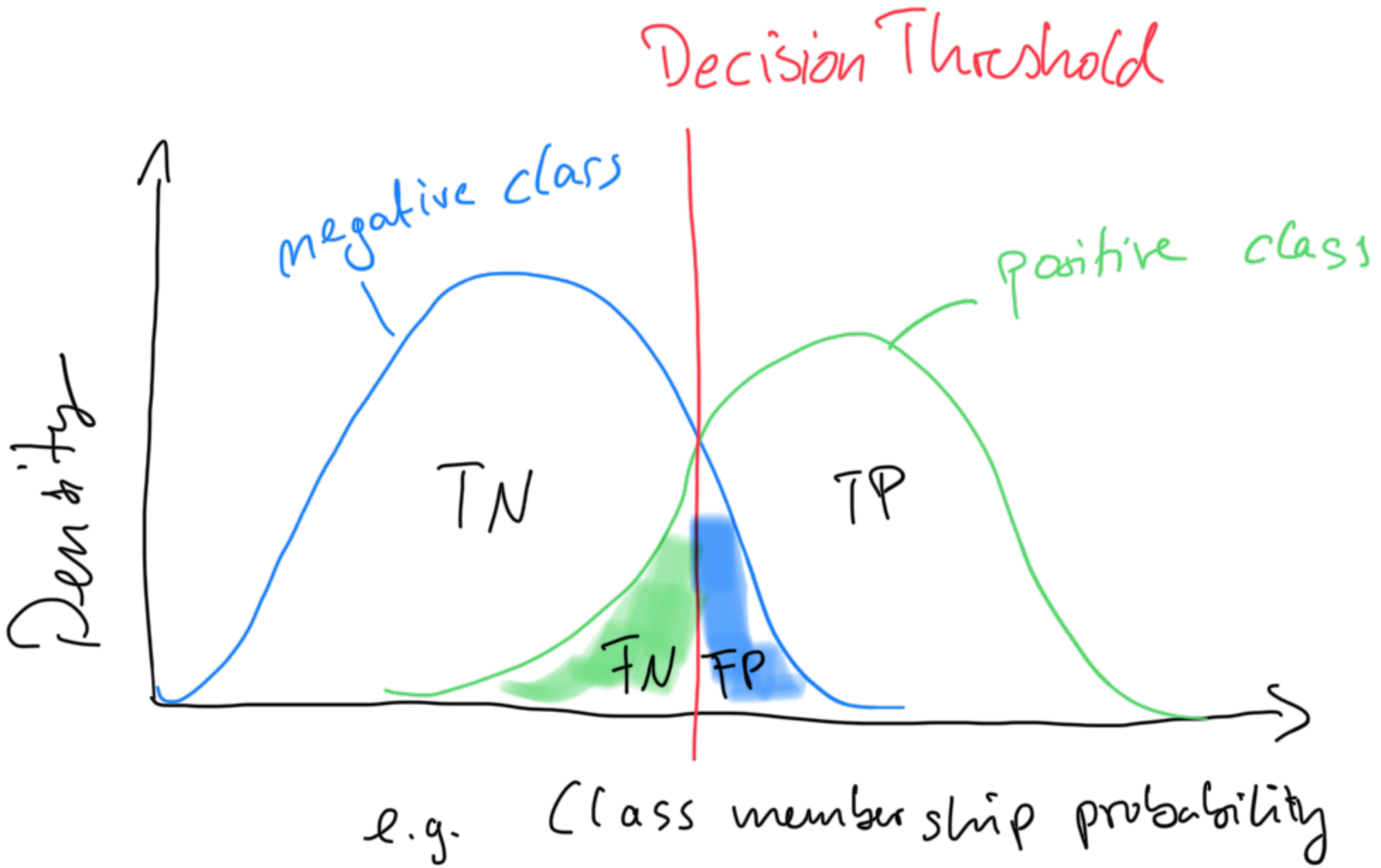
False Positive Rate and False Negative Rate

$$FPR = \frac{FP}{N} = \frac{FP}{FP + TN} \tag{3}$$

$$TPR = \frac{TP}{P} = \frac{TP}{FN + TP} \tag{4}$$

- Think of it in a spam classification problem (what are true positives, and if you had to pick one at the expense of the other: would you rather decrease the FPR or increase the TPR?)

False Positive Rate and False Negative Rate



Precision, Recall, and F1 Score

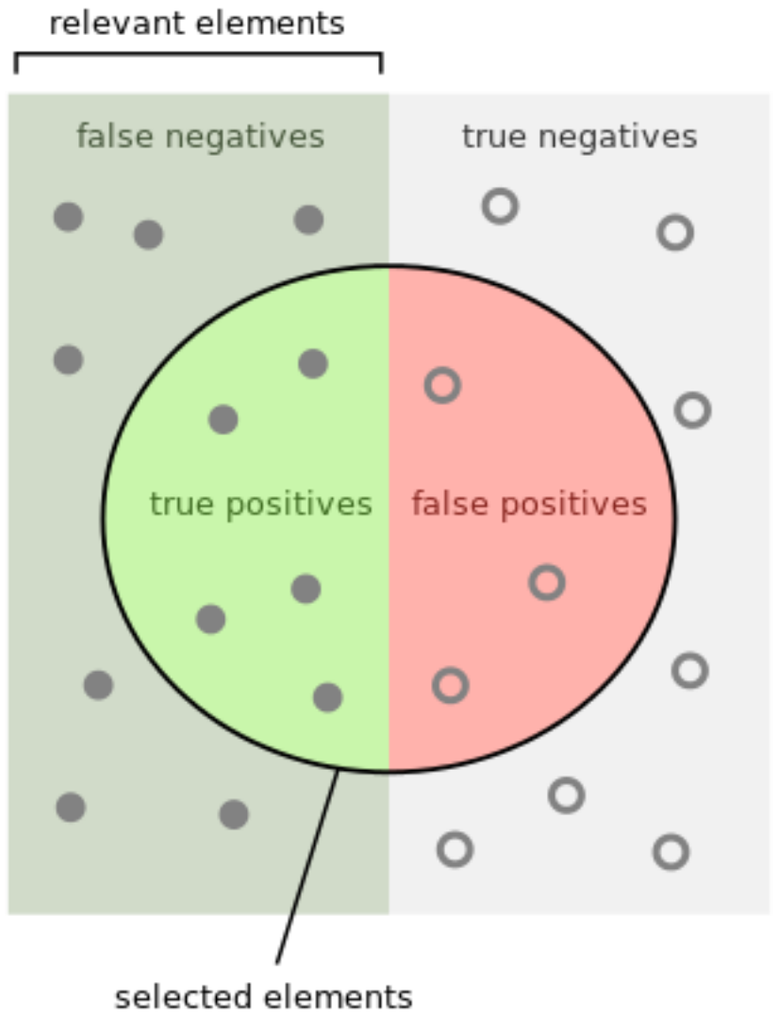
$$PRE = \frac{TP}{TP + FP} \tag{5}$$

$$REC = TPR = \frac{TP}{P} = \frac{TP}{FN + TP} \tag{6}$$

$$F_1 = 2 \cdot \frac{PRE \cdot REC}{PRE + REC} \tag{7}$$

- Terms that are more popular in Information Technology
- Recall is actually just another term for True Positive Rate (or "sensitivity")

Precision and Recall



How many selected items are relevant?

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

https://en.wikipedia.org/wiki/Precision_and_recall

Sensitivity and Specificity

$$SEN = TPR = REC = \frac{TP}{P} = \frac{TP}{FN + TP} \tag{8}$$

$$SPC = TNR = \frac{TN}{N} = \frac{TN}{FP + TN} \tag{9}$$

Sensitivity (SEN) measures the recovery rate of the Positives and complimentary, *Specificity (SPC)* measures the recovery rate of the Negatives.

Matthew's Correlation Coefficient

- Matthews correlation coefficient (MCC) was first formulated by Brian W. Matthews [1] in 1975 to assess the performance of protein secondary structure predictions
- The MCC can be understood as a specific case of a linear correlation coefficient (Pearson r) for a binary classification setting
- Considered as especially useful in unbalanced class settings
- The previous metrics take values in the range between 0 (worst) and 1 (best)
- The MCC is bounded between the range 1 (perfect correlation between ground truth and predicted outcome) and -1 (inverse or negative correlation) — a value of 0 denotes a random prediction.

$$MCC = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \tag{10}$$

[1] Brian W Matthews. Comparison of the predicted and observed secondary structure of T4 phage lysozyme. Biochimica et Biophysica Acta (BBA)- Protein Structure, 405(2):442–451, 1975.

Balanced Accuracy / Average Per-Class (APC) Accuracy

Predicted Labels

True Labels

	Class 0	Class 1	Class 2
Class 0	T(0,0)		
Class 1		T(1,1)	
Class 2			T(2,2)

$$ACC = \frac{T}{n}$$

Predicted Labels

True Labels

	Class 0	Class 1	Class 2
Class 0	3	0	0
Class 1	7	50	12
Class 2	0	0	18

$$ACC = \frac{3 + 50 + 18}{90} \approx 0.79$$

$$APC\ ACC = \frac{83/90 + 71/90 + 78/90}{3} \approx 0.86$$

Balanced Accuracy / Average Per-Class Accuracy

Predicted Labels

True Labels	Class 0	Neg Class
Class 0	3	0
Neg Class	7	80

Predicted Labels

True Labels	Class 1	Neg Class
Class 1	50	19
Neg Class	0	21

Predicted Labels

True Labels	Class 2	Neg Class
Class 2	18	0
Neg Class	12	60

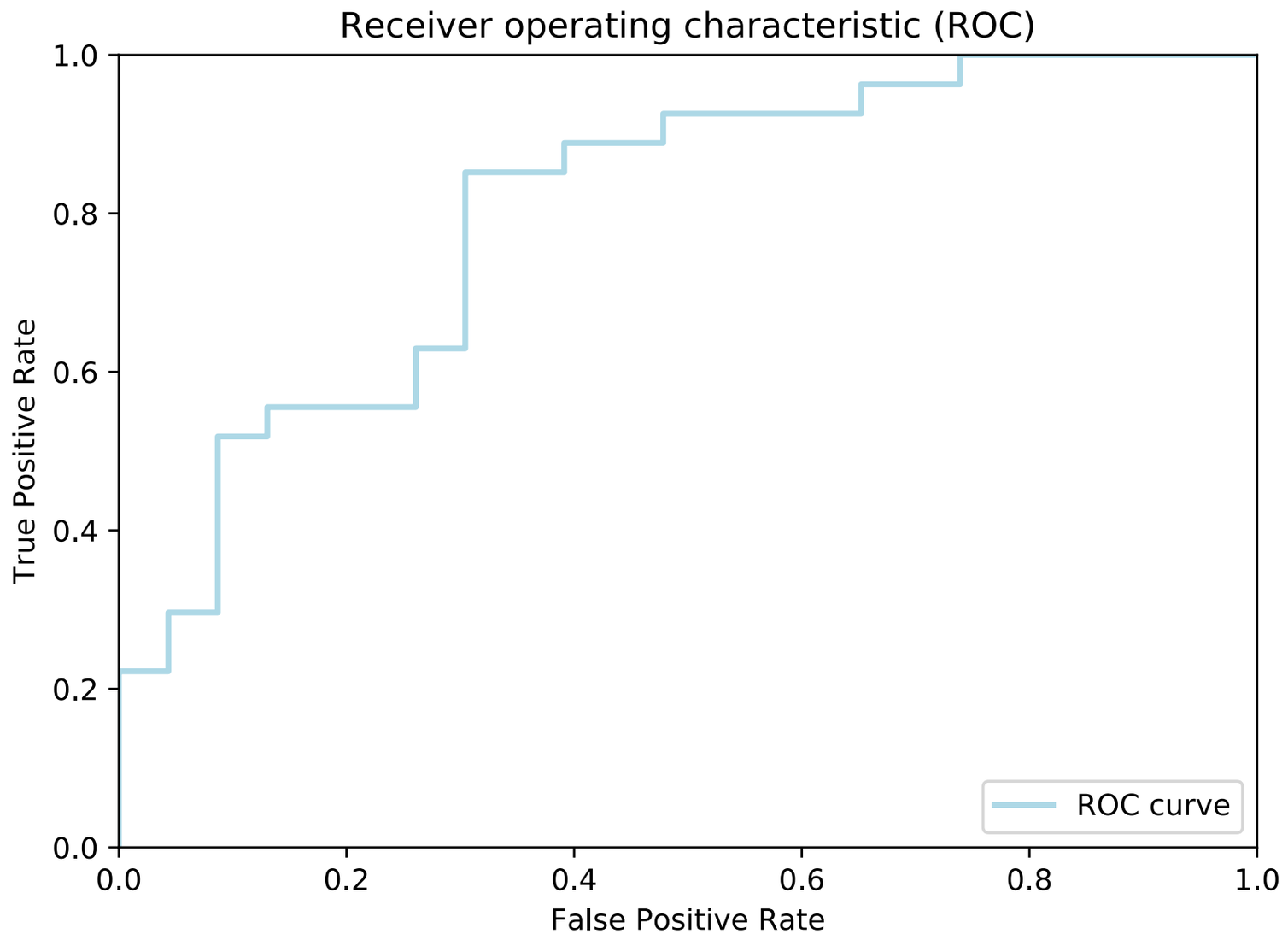
Predicted Labels

True Labels	Class 0	Class 1	Class 2
Class 0	3	0	0
Class 1	7	50	12
Class 2	0	0	18

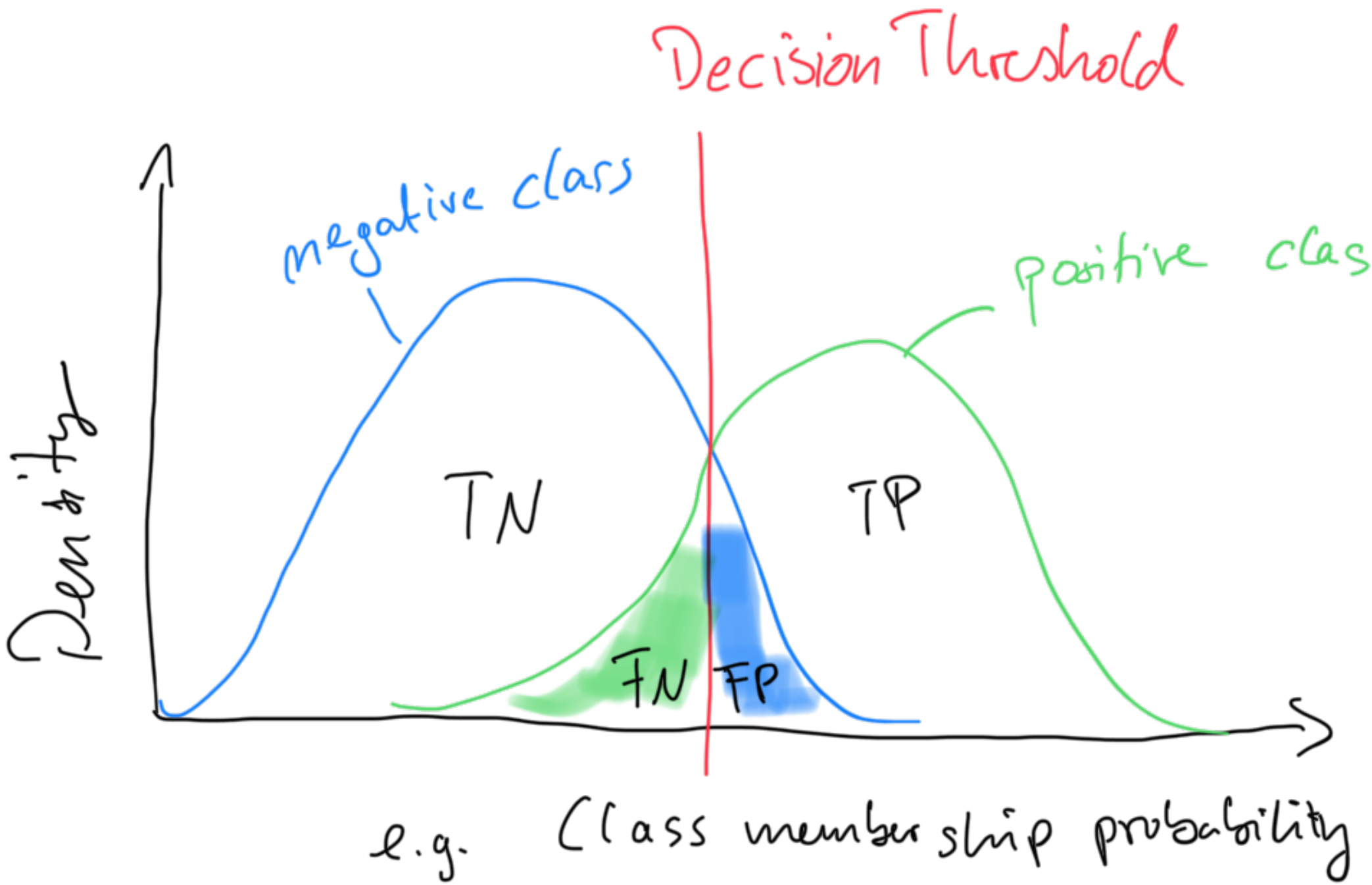
$$APC\ ACC = \frac{83/90 + 71/90 + 78/90}{3} \approx 0.86$$

Receiver Operating Characteristic curve (ROC curve)

- Trade-off between True Positive Rate and False Positive Rate
- ROC can be plotted by changing the prediction threshold
- ROC term comes from "Radar Receiver Operators"
  (analysis of radar [**RA**dio **D**irection **A**nd **R**anging] images)

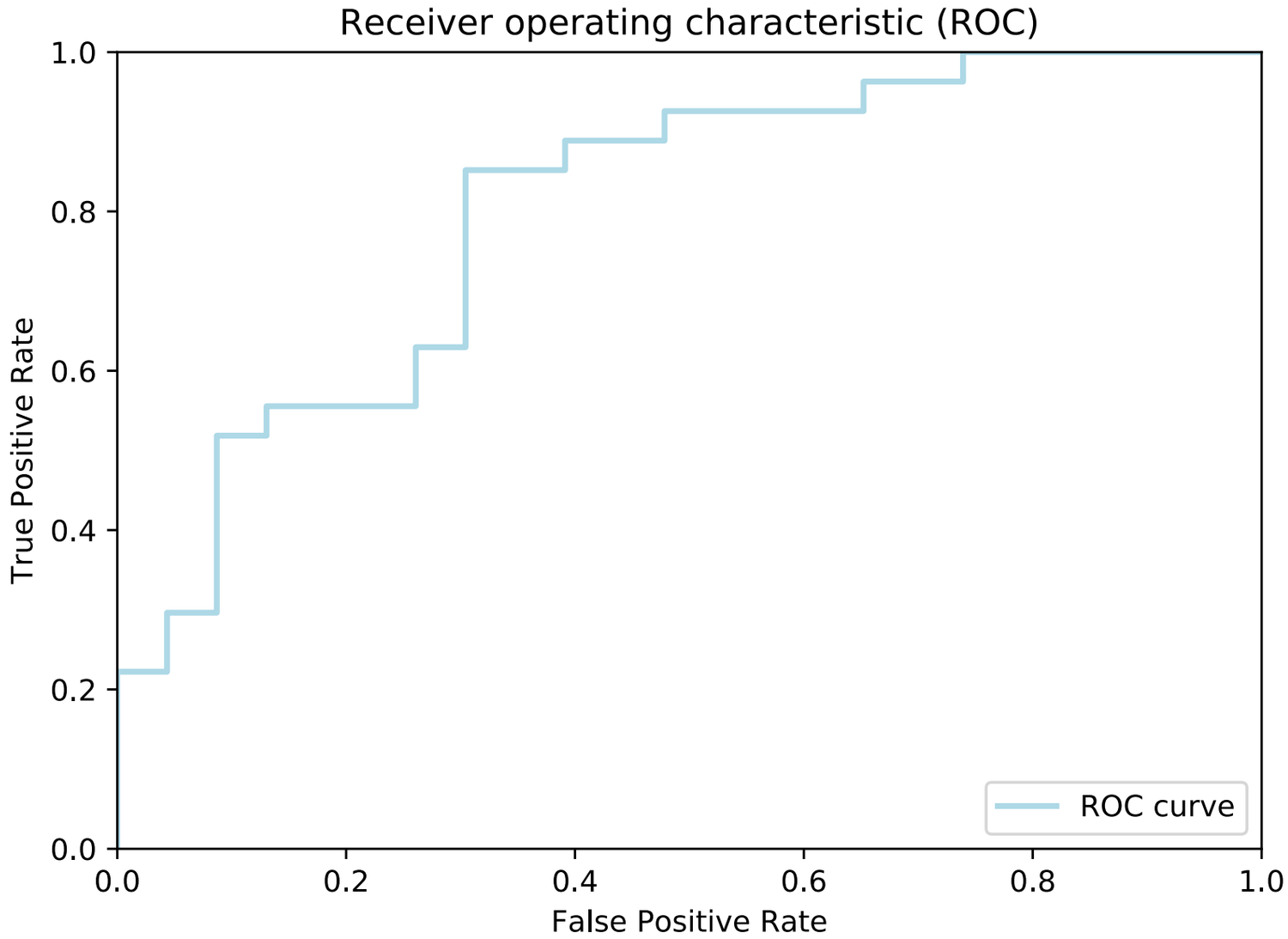


RECAP: False Positive Rate and False Negative Rate

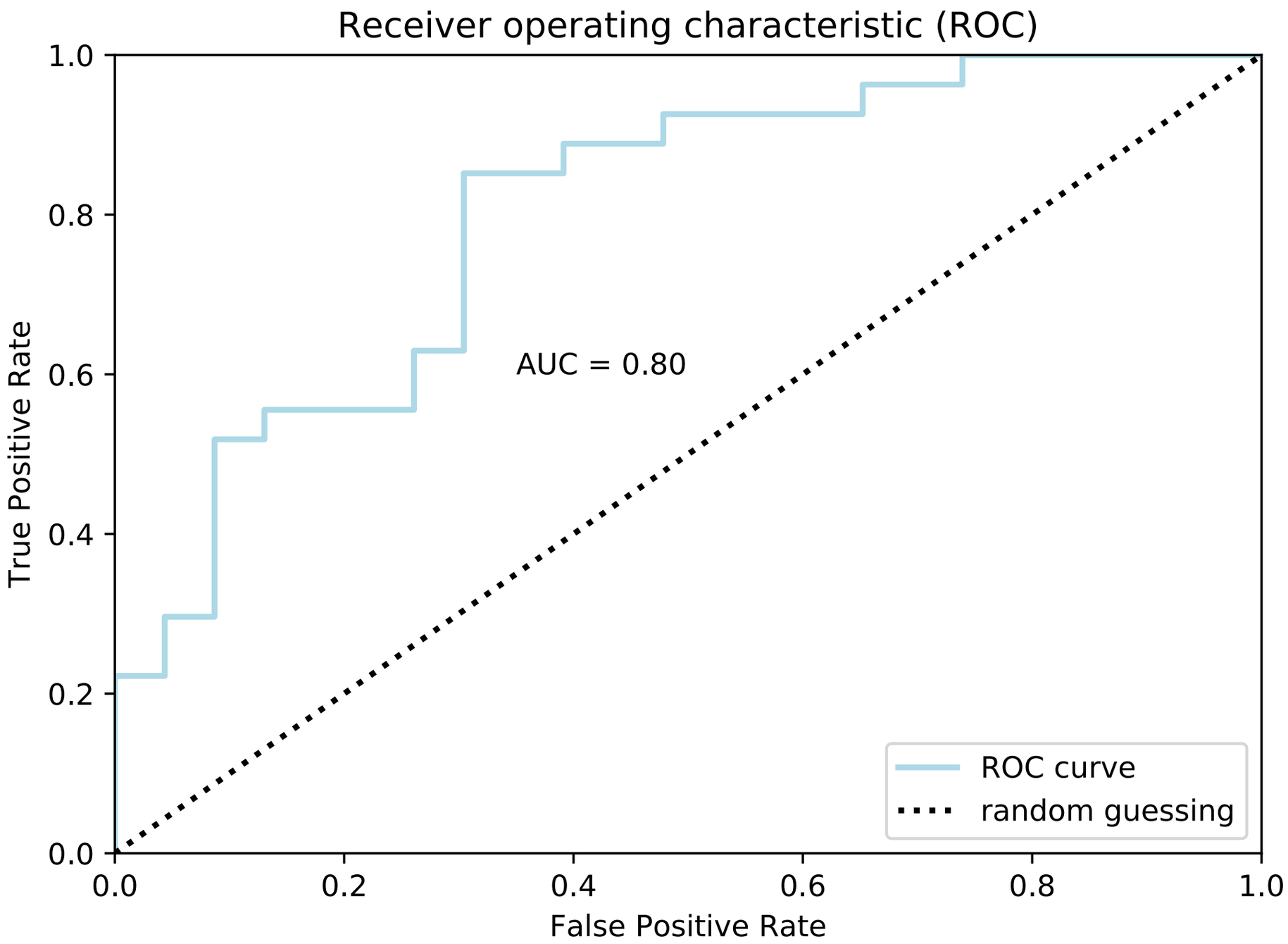


Receiver Operating Characteristic curve (ROC curve)

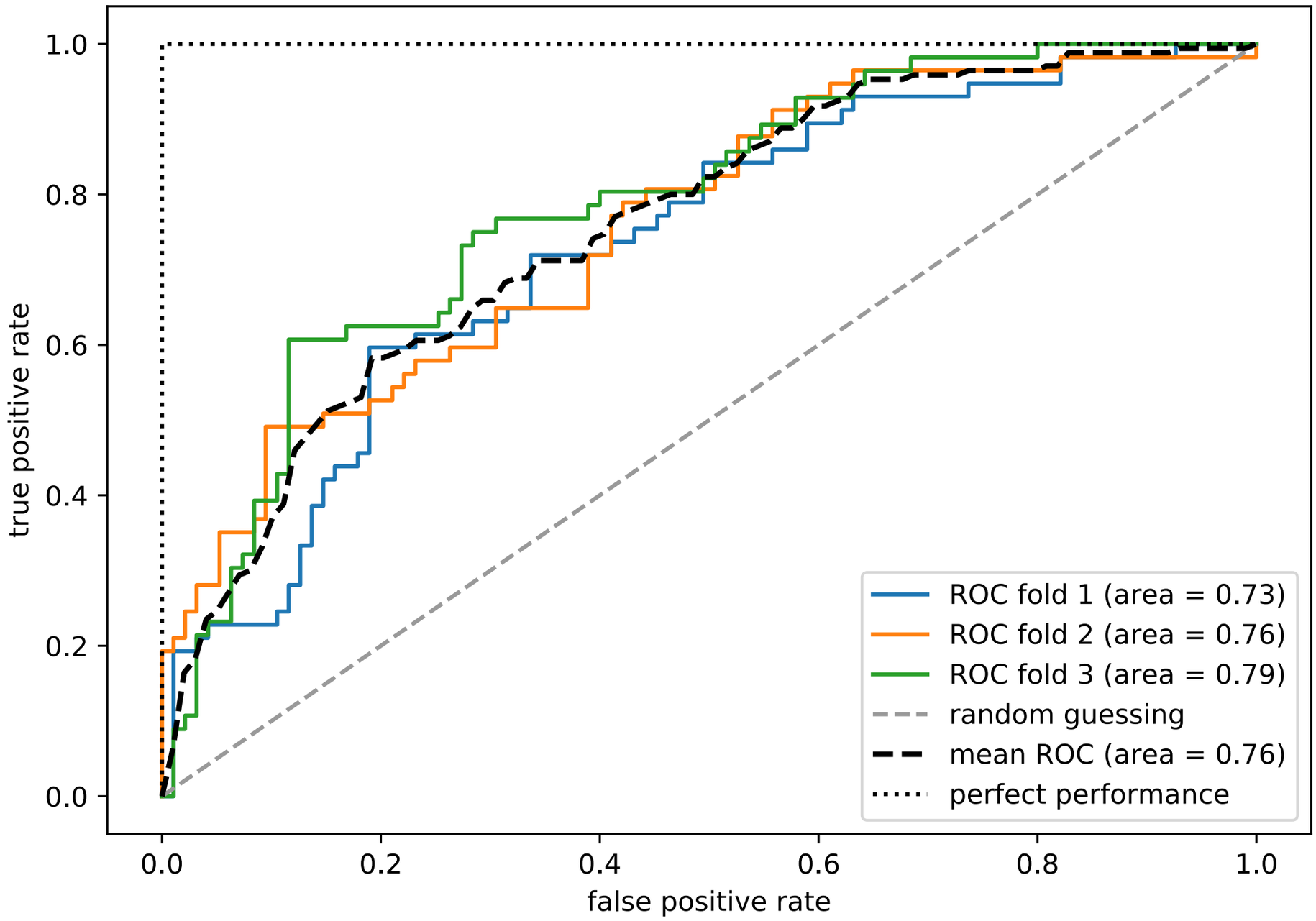
- ?.? = Perfect Prediction
- ?.? = Random Prediction



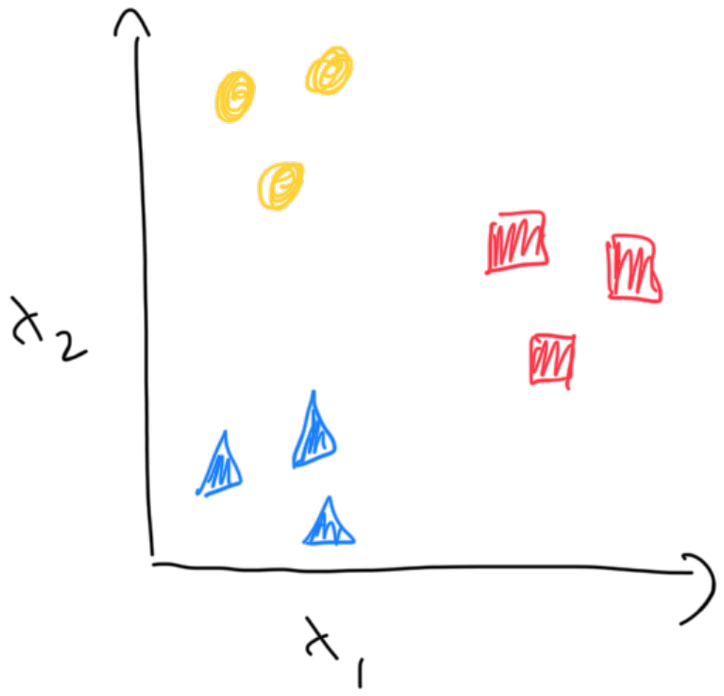
ROC Area Under the Curve (AUC)

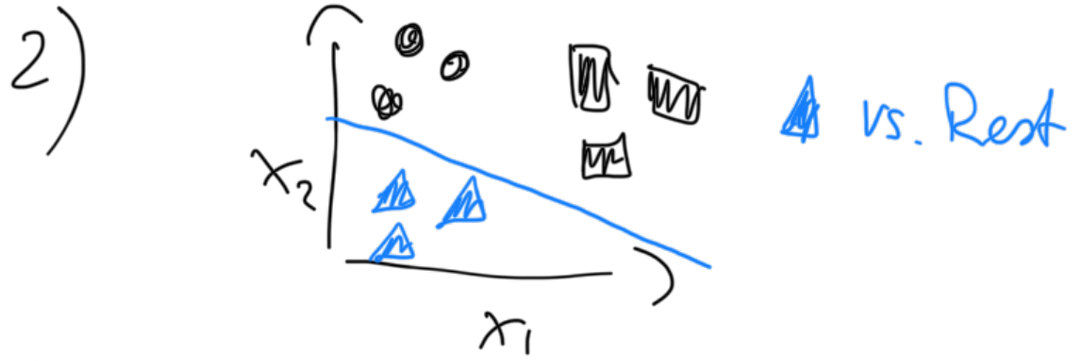


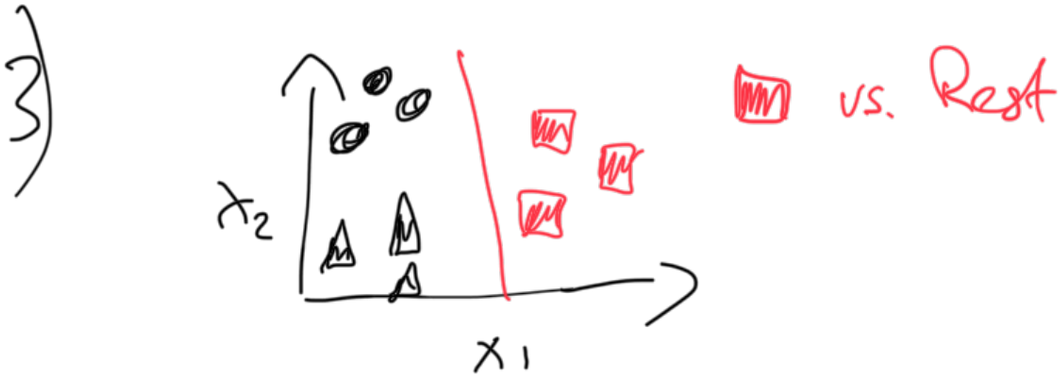
ROC and k-Fold Cross-Validation



Binary Classifiers and One-vs-Rest (OvR) / One-vs-All (OvA)

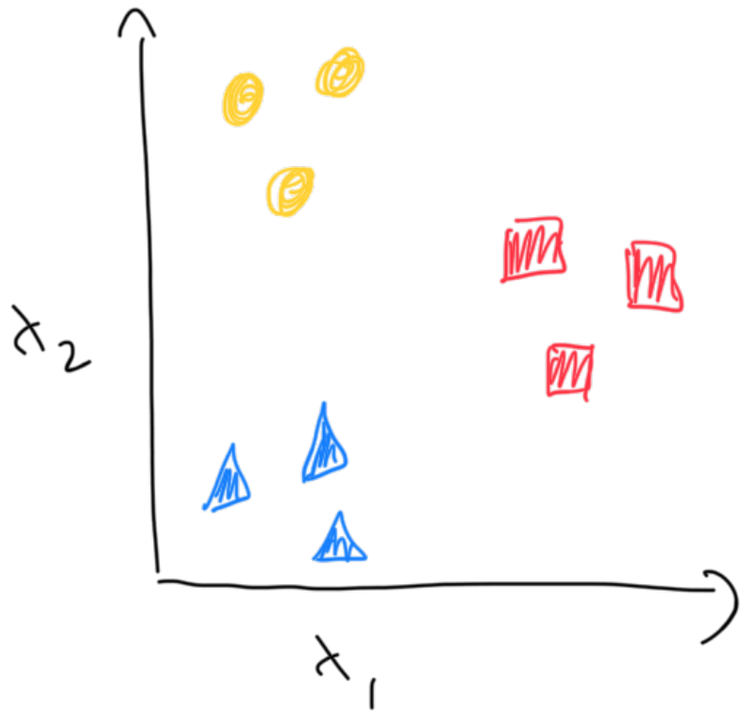


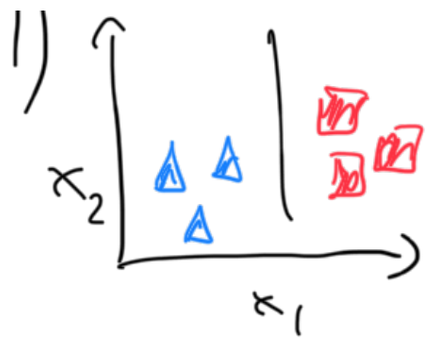


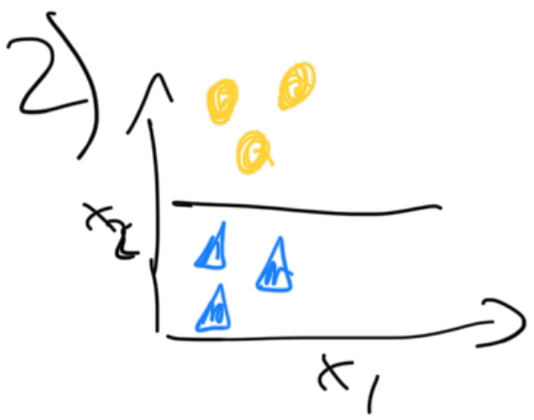


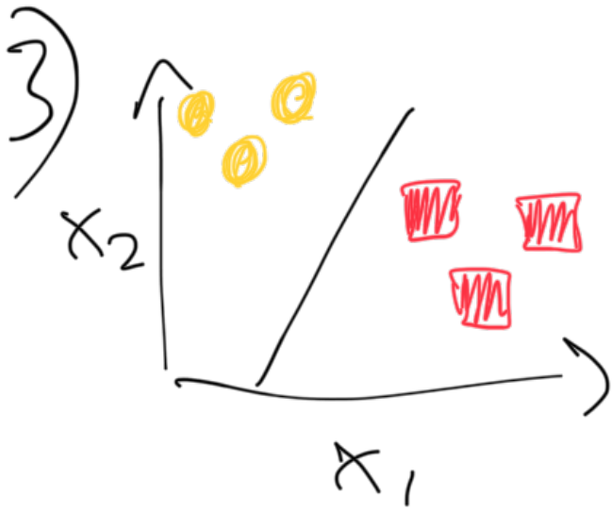
Then, choose the class with the highest confidence score

Binary Classifiers and One-vs-One (OvO) / All-vs-All (AvA)









num_classes x (num_classes - 1) / 2

Big O: O(?)

Select the class by majority vote (and use confidence score in case of ties)

Macro and Micro Averaging

$$PRE_{micro} = \frac{TP_1 + \ldots + TP_c}{TP_1 + \ldots + TP_c + FP_1 + \ldots + FP_c}$$

$$PRE_{macro} = \frac{PRE_1 + \ldots + PRE_c}{c}$$

Micro-averaging is useful if we want to weight each instance or prediction equally, whereas macro-averaging weights all classes equally to evaluate the overall performance of a classifier with regard to the most frequent class labels.

Dealing with Class Imbalance

User Guide

https://imbalanced-learn.readthedocs.io/en/stable/user_guide.html

Reading Assignment

No lecture notes, instead see

- Raschka & Mirjalili: *Python Machine Learning, 2nd Edition*
  Chapter 6: Learning Best Practices for Model Evaluation and Hyperparameter Tuning

(code notebook: https://github.com/rasbt/python-machine-learning-book-2nd-edition/blob/master/code/ch06/ch06.ipynb)

Code Examples

https://github.com/rasbt/stat479-machine-learning-fs19/tree/master/12_eval5-metrics/code