PROGRAMMING IN PYTHON II

Model Evaluation for Classification Tasks

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Outline

MOTIVATION

Motivation

- We have already learned about the loss function
  - Computes a loss given our model output and the target
  - The higher the loss, the farther away our output is to our target
  - We want to minimize the loss of our model during training

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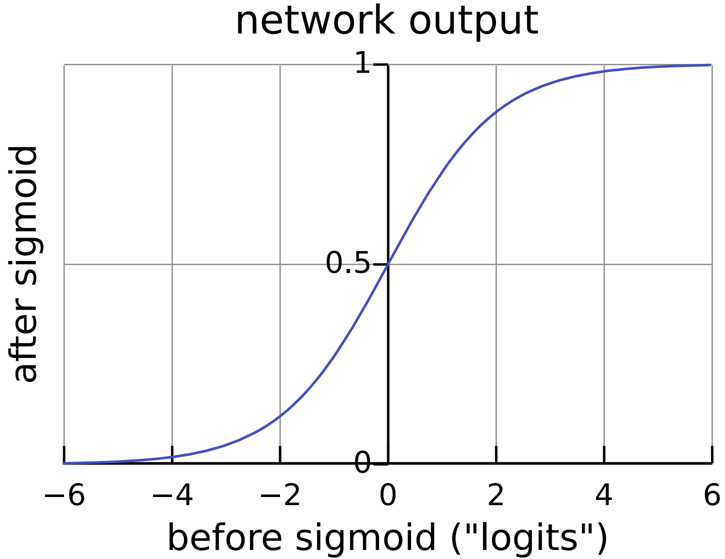
  - Computes a loss given our model output and the target
  - The higher the loss, the farther away our output is to our target
  - We want to minimize the loss of our model during training
- In this Unit we will learn about some common methods for evaluation of (binary) classifiers
  - Typically not used for training (require complete dataset to compute scores)
  - Well suited for comparison of classification performance with different goals

Recap: Classification tasks and NNs

- Different classification tasks exist (see Unit 07)
- Binary classification task: Predict whether sample is in positive or negative class
- Typically done using a sigmoid activation function (aka logistic function) in the output layer
  - sigmoid function maps network output (“logit”) from range $(-\infty, \infty)$ to range $(0, 1)$
  - Activation after sigmoid can be interpreted as probability for belonging to positive class
  - Threshold to “classify” sample as positive or negative (threshold 0.5 is common):
    predicted_class = positive if sigmoid(logit) ≥ 0.5, otherwise
    predicted_class = negative
  - Generalization to multiple classes via softmax function

Sigmoid activation function



CONFUSION MATRIX

Confusion matrix

- The confusion matrix is a central piece for many evaluation methods
- Assume a binary classification task with samples belonging to either positive (P) or negative (N) class
- The confusion matrix illustrates the number of samples being
  - True positive (TP): correctly classified as positive (aka “hit”)
  - True negative (TN): correctly classified as negative (aka “correct rejection”)
  - False positive (FP): wrongly classified as positive (aka “false alarm”, “Type I error”)
  - False negative (FN): wrongly classified as negative (aka “miss”, “Type II error”)

Confusion matrix for binary classification

		predicted class		
		positive	negative	total
true class	positive	TP	FN	P
	negative	FP	TN	N

TRUE POSITIVE RATE AND TRUE NEGATIVE RATE

True positive rate and true negative rate

- True positive rate (TPR) (aka “sensitivity”, “recall”)
  - Proportion of true positives that are correctly classified
  - $TPR = \frac{TP}{P} = \frac{TP}{TP+FN}$
  - E.g. % of diseased people that are correctly classified as being diseased
- True negative rate (TNR) (aka “specificity”)
  - Proportion of true negatives that are correctly classified
  - $TNR = \frac{TN}{N} = \frac{TN}{TN+FP}$
  - E.g. % of healthy people that are correctly classified as not being diseased
- False negative rate (FNR) (aka “miss rate”)
  - $FNR = \frac{FN}{P} = 1 - TPR$
- False positive rate (FPR) (aka “fall-out”)
  - $FPR = \frac{FP}{N} = 1 - TNR$

BALANCED ACCURACY

Balanced Accuracy

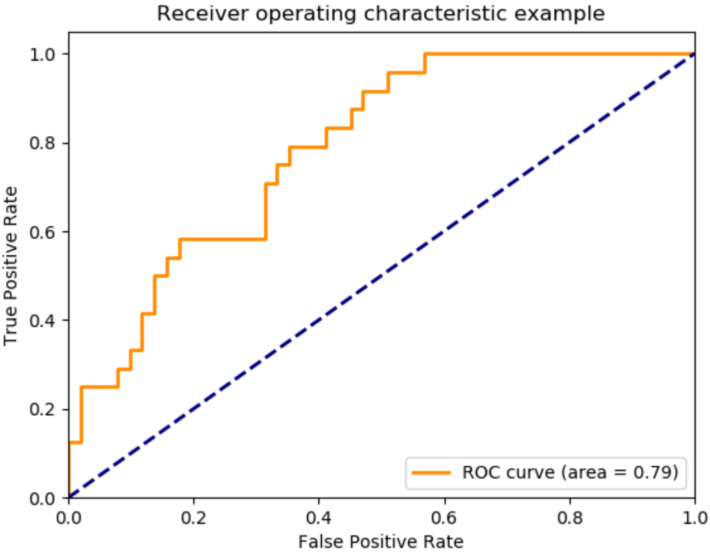
- Accuracy (ACC) (aka “fraction correct (FC)”)
  - Proportion of correctly classified samples
  - $ACC = \frac{TP+TN}{P+N} = \frac{TP+TN}{TP+TN+FP+FN}$
  - Simple measure but bad with imbalanced classes
- Balanced accuracy (BACC)
  - Normalizes TP and TN by the number of positive and negative samples
  - $BACC = \frac{TPR+TNR}{2}$
  - Suited for imbalanced classes

RECEIVER OPERATING CHARACTERISTIC (ROC)

Receiver Operating Characteristic (ROC)

- Receiver operating characteristic (ROC) curve
  - Shows TPR and FPR while varying classification threshold
  - Classification performance w.r.t. FN and FP costs
- Area under the receiver operating characteristic curve (AUC)
  - Reduces ROC curve to single value (the area under the curve)
  - Probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one
  - Ranges from 0 to 1, with 1 being perfect and 0.5 being random
  - Suitable for imbalanced classes

Receiver Operating Characteristic (ROC)



[Source: `https://scikit-learn.org/stable/auto_examples/model_selection/plot_roc.html`]

IMPLEMENTATION

Implementation

- Many more evaluation methods exist, some of which with generalizations to tasks with multiple classes
- The scikit-learn (`sklearn.metrics`) module provides a vast selection of evaluation methods

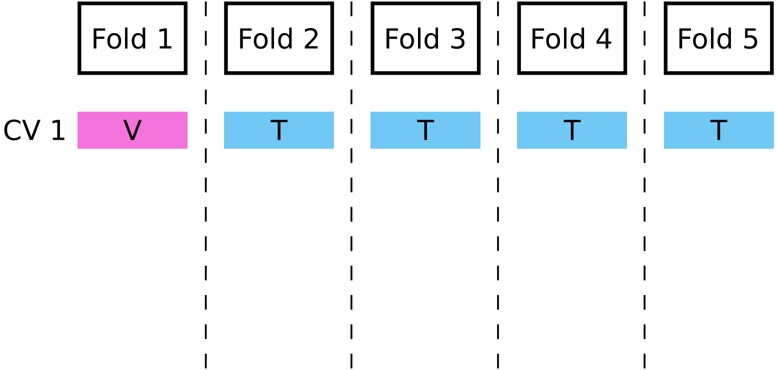
  `https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics`
- For examples, see the code part of this Unit

EXCURSION: CROSS VALIDATION

Excursion: Cross Validation

- To get an estimate for the model performance on future data, we have to use the test set to compute the scores
- For small datasets, the requirement that training and test set must not overlap is painful
- Solution: Cross Validation (CV)
  - Split dataset into n disjoint folds
  - Use $n-1$ folds as training set, left-out fold as test set
  - Train n times, every time leaving out a different fold as test set
  - Average over n estimated risks on test sets to get better estimate of generalization capability

Cross Validation (1)



5-fold Cross Validation

T: Training set; V: Test set

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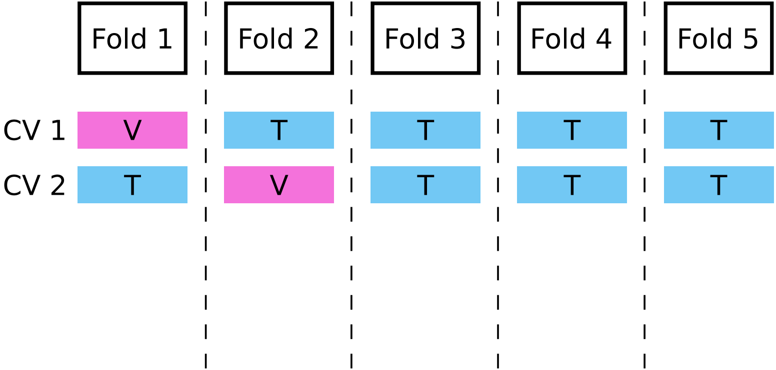

5-fold Cross Validation

T: Training set; V: Test set

Cross Validation (1)

	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
CV 1	V	T	T	T	T
CV 2	T	V	T	T	T
CV 3	T	T	V	T	T
CV 4	T	T	T	V	T
CV 5	T	T	T	T	V

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- Nested Cross Validation
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  1. Apply cross validation on training set (withhold test set)
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- Getting a risk estimate on selected model:
  1. Apply cross validation on training set (withhold test set)
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- In practice, the found model is often trained further or re-trained on complete dataset for best performance