PROGRAMMING IN PYTHON II

Model Evaluation

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Outline

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2. Confusion matrix
3. True positive rate and true negative rate
4. Balanced Accuracy
5. Receiver Operating Characteristic (ROC)
6. Implementation
7. Excursion: Cross Validation
8. Additional Measures: Binary Classifiers
9. Additional Measures: Regression
10. Additional Evaluation Strategies

MOTIVATION

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- 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
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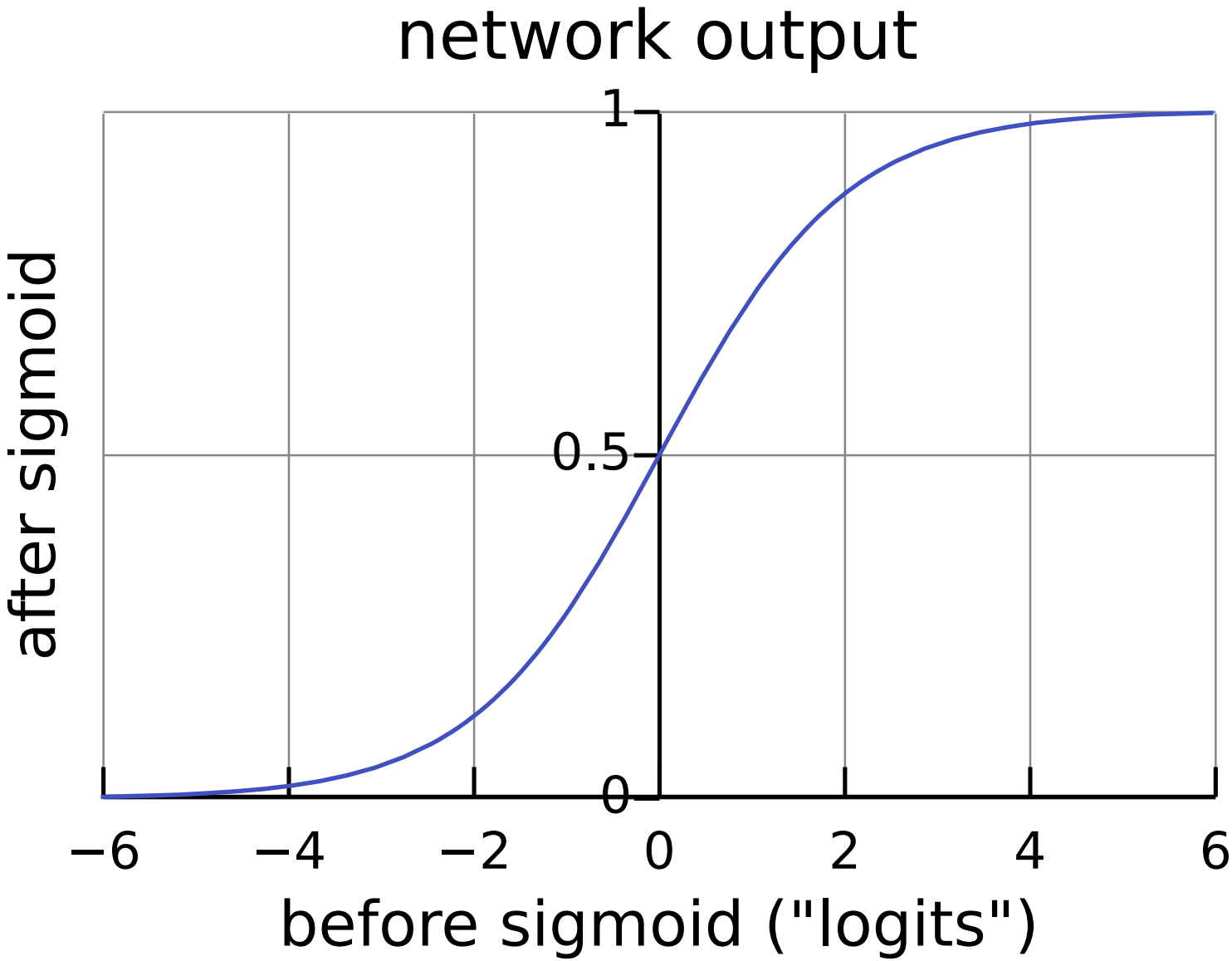
  - Computes a loss given our model output and the target
  - The higher the loss, the farther away our output is to our target
  - We want to minimize the loss of our model during training
- In this Unit we will learn about some common methods for evaluation of our models
  - Typically not used for training (bad gradients or complete dataset required 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

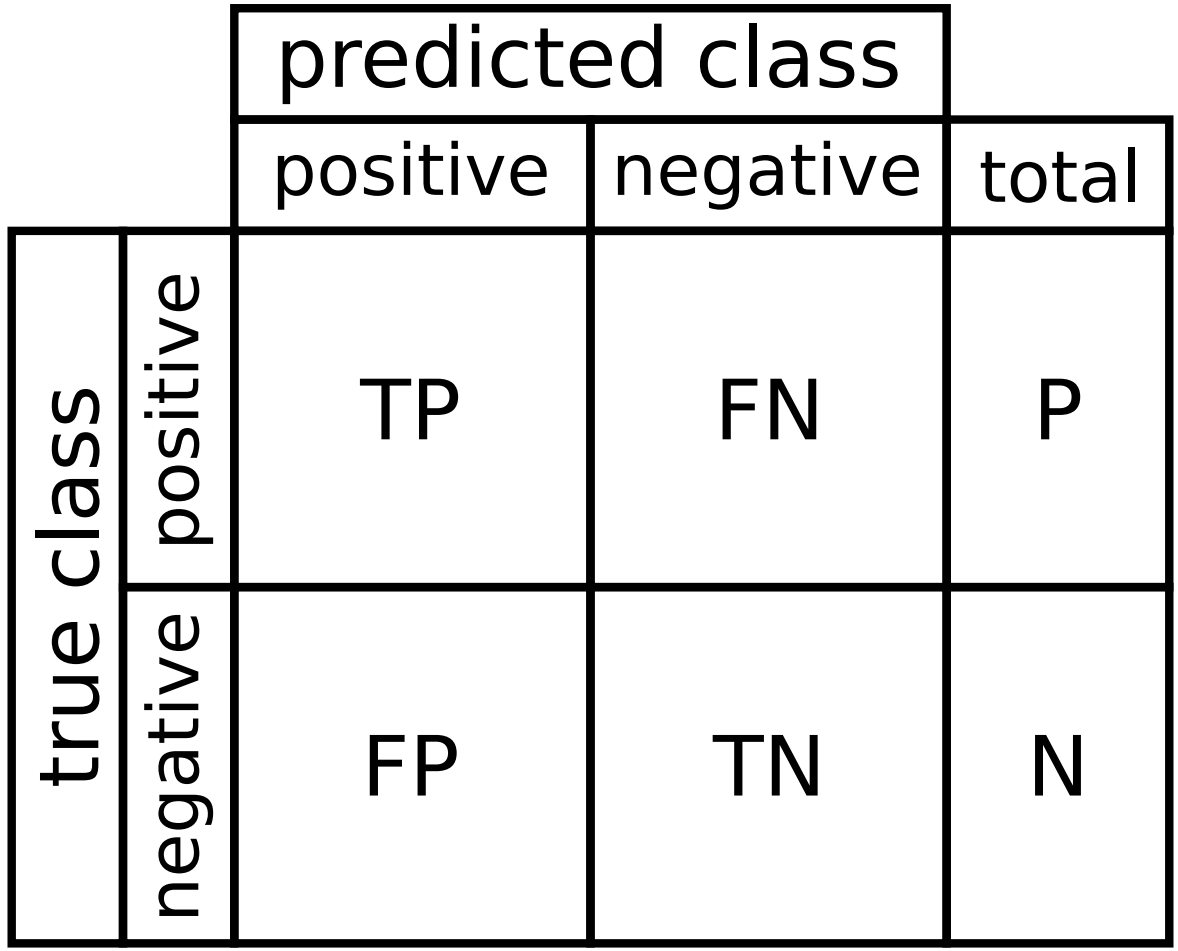


CONFUSION MATRIX

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



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

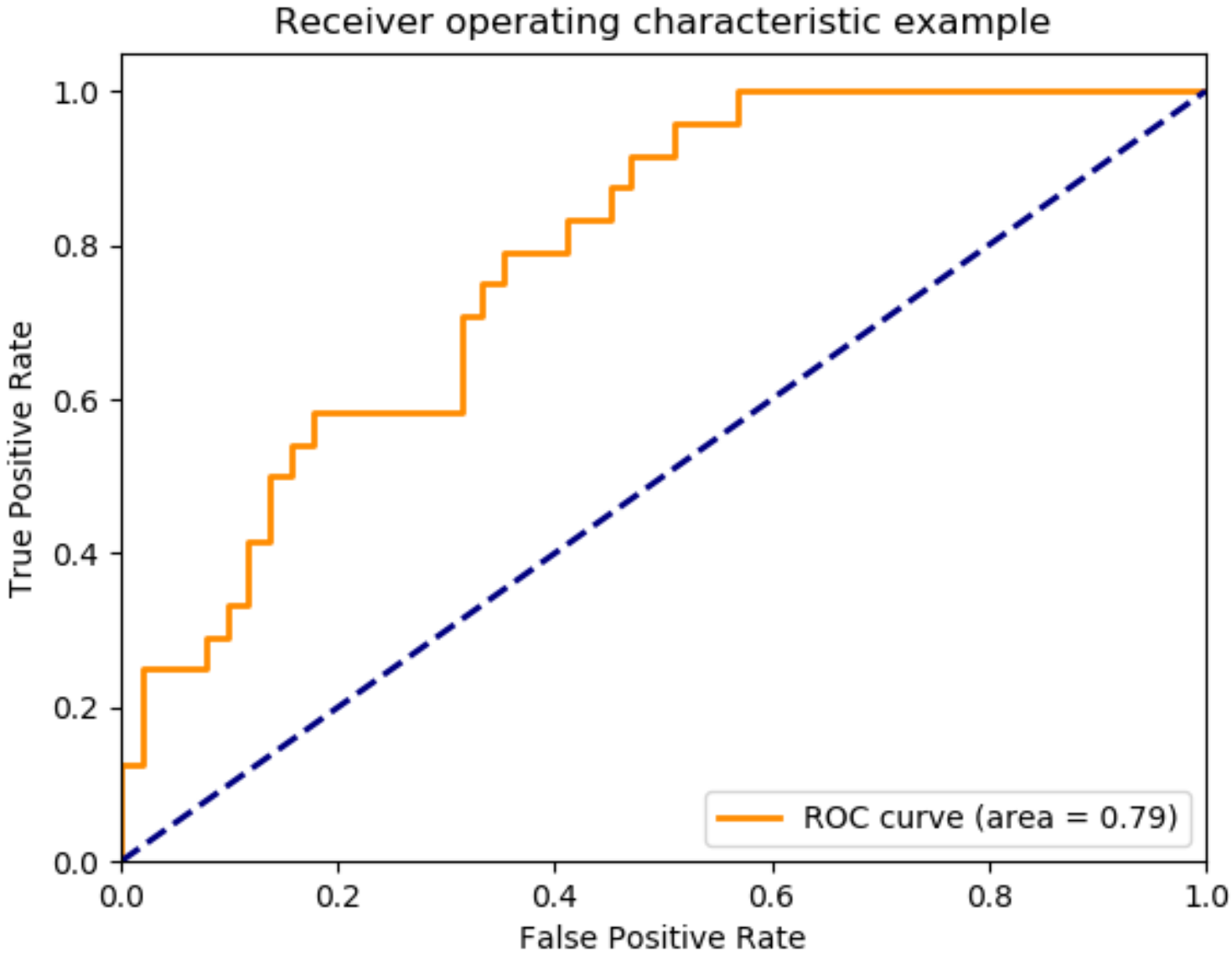
- Accuracy (ACC) (aka “fraction correct (FC)”)
  - Proportion of correctly classified samples
  - $ACC = \frac{TP+TN}{P+N} = \frac{TP+TN}{TP+TN+FP+FN}$
  - Simple measure but bad with imbalanced classes
- Balanced accuracy (BACC)
  - Normalizes TP and TN by the number of positive and negative samples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

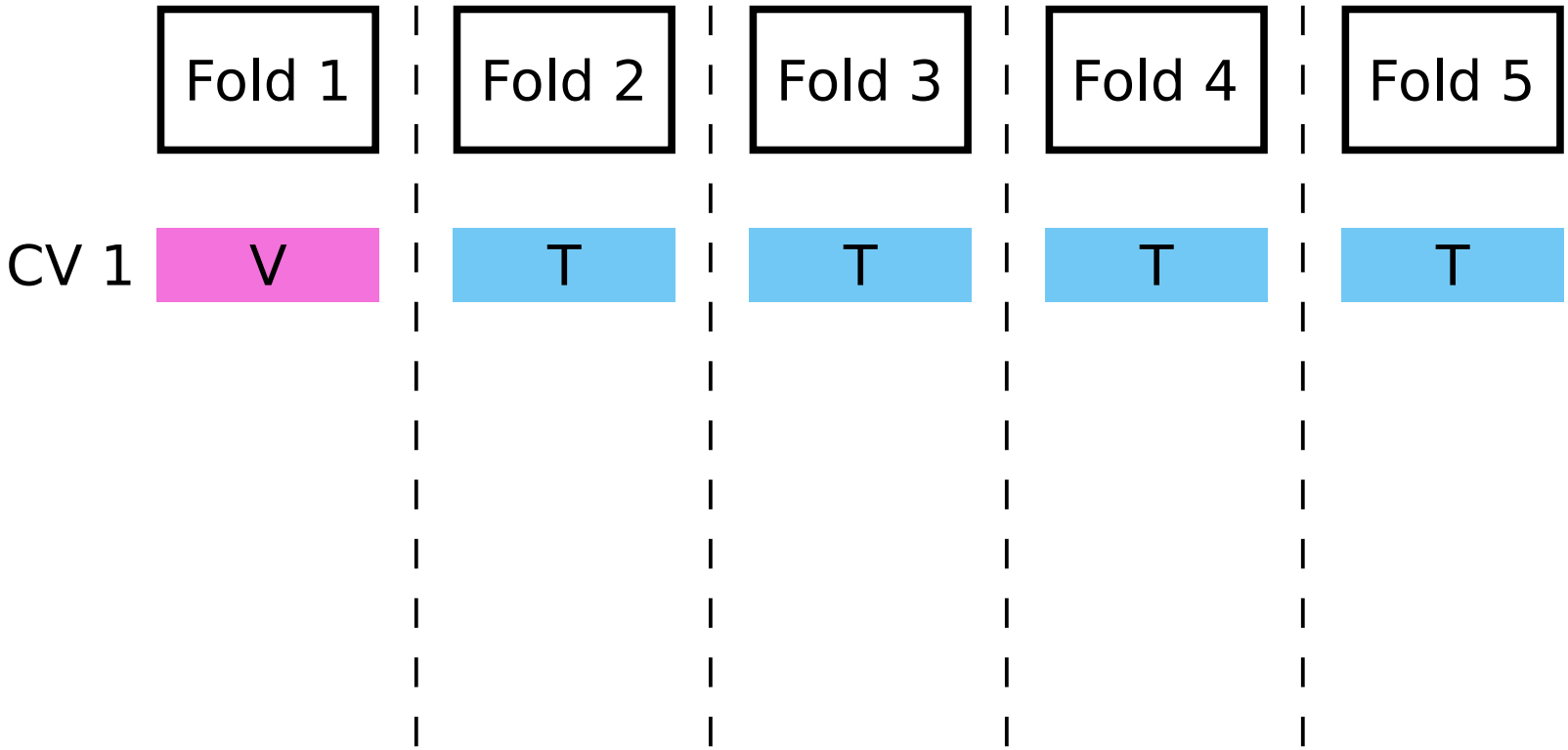
  `https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics`
- For examples, see the code part of this Unit

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

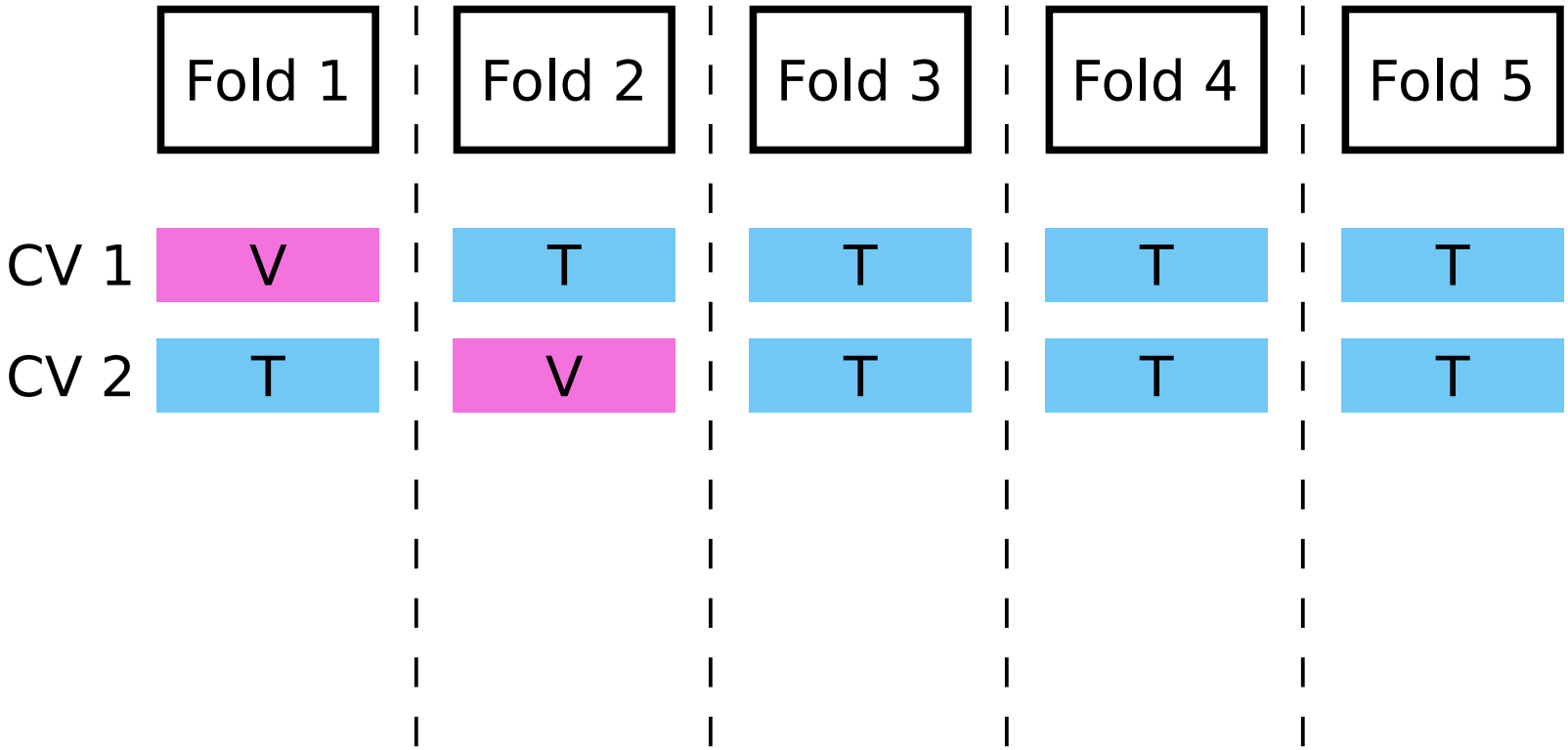
Cross Validation (1)



5-fold Cross Validation

T: Training set; V: Test set

Cross Validation (1)



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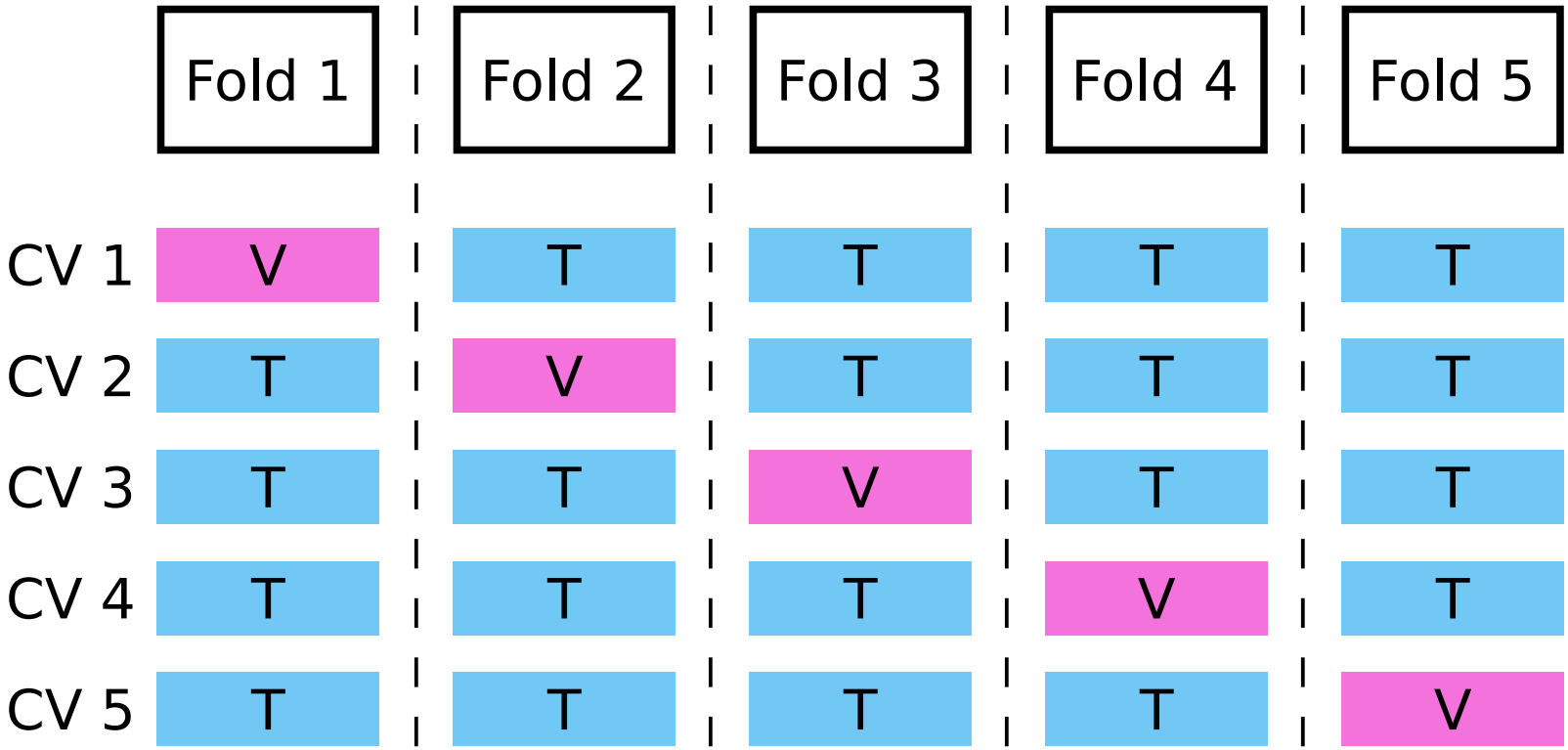

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Cross Validation (2)

- Nested Cross Validation
  - We can apply another (inner) CV procedure within each training-set of the original (outer) CV

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- Nested Cross Validation
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  - $\rightarrow$ allows for evaluation of model selection procedure
- Getting a risk estimate on selected model:
  1. Apply cross validation on training set (withhold test set)
  2. Use test set to estimate risk for the model selected via CV
- In practice, the found model is often trained further or re-trained on complete dataset for best performance

ADDITIONAL MEASURES: BINARY CLASSIFIERS

F-Score

- F-score (F_1-score, F-measure)
  - F-score = $2 * \frac{Precision * Recall}{Precision + Recall}$
  - Used for binary classification models
  - Defined as the harmonic mean of Precision and Recall (TPR, Sensitivity) of a model

- F_β-score (generalized version of F-score)
  - F_β-score = $(1 + \beta^2) * \frac{Precision * Recall}{\beta^2 * Precision + Recall}$
  - Used for binary classification models
  - β indicates how much Recall is more important than Precision

Accuracy for multi-class classification

Accuracy (binary classes) (ACC)	**Balanced Accuracy (binary classes)** (BACC)
$\frac{TP+TN}{P+N} = \frac{total\ hit\ count}{total\ samples}$	$\frac{1}{2}(TPR + TNP)$
	It's suitable for imbalanced classes

Accuracy (multi-classes) (ACC)	**Balanced Accuracy (multi-classes)** (BACC)
$\frac{\sum TP_i}{\sum P_i} = \frac{total\ hit\ count}{total\ test}$	$\frac{1}{n}\sum \frac{TP_i}{P_i}$
	It's suitable for imbalanced classes

- TP_i and P_i are respectively the numbers of true positive and actual positive examples for class i
- n is the number of classes
- Not suitable for multi-label classification

ADDITIONAL MEASURES: REGRESSION

Measures for Regression Models

- Mean Absolute Error (MAE): $\frac{\sum_{i=1}^{n} |y_i - y'_i|}{n}$
- Mean Squared Error (MSE): $\frac{\sum_{i=1}^{n} (y_i - y'_i)^2}{n}$ $\rightarrow$this measure exaggerates the presence of outliers
- Root Mean Squared Error (RMSE): Square root of MSE
- Relative Absolute Error: $\frac{\sum_{i=1}^{n} |y_i - y'_i|}{\sum_{i=1}^{n} |y_i - \overline{y}_i|}$
- Relative Squared Error: $\frac{\sum_{i=1}^{n} (y_i - y'_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y}_i)^2}$
- Root Relative Squared Error: Squared root of Relative Squared Error

y_i and y'_i are respectively the true and predicted value of the depending variable y in the test set; $\overline{y}_i$ is the mean value of y_i in the training set.

ADDITIONAL EVALUATION STRATEGIES

Hold-out test set

- Hold-out test set
  - Randomly partitioned a data set into a training set, (validation set,) and a test set
    - e.g. 2/3 of the data for training set, remaining 1/3 for test set
  - Training set used to train a model, test set used for performance estimate
  - Performance estimate not reliable if test set is small
  - Used for:
    - Large datasets where CV isn't feasible
    - Challenges (often with fine-tuning on full dataset for more training samples)

Bootstrapping

- Bootstrapping methods
  - A class of evaluation methods in which
    - training set is formed by randomly picking samples from the data set
    - samples in the data set may be selected more than once
  - Commonly use bootstrapping method: .632 bootstrap
    - Training set is formed by n-times randomly picking a sample from data set of n examples
    - Samples which were not picked for training set form the test set
    - If n is large, 63.2% of samples in data set form the training set and the remaining 36.8% form the test set*

*) The probability an example selected from the given data set is $\frac{1}{n}$ so the probability of not being selected is $(1 - \frac{1}{n})$. n times of selections are done so $(1 - \frac{1}{n})^n$ is the probability that an example will not be selected. If n is large, this probability approximates $\lim_{n\to\infty}(1 - \frac{1}{n})^n = e^{-1} = 0.368$

Bagging (Bootstrap Aggregation)

- Bagging (bootstrap aggregation)
  - Build k models from data set
  - Each model is learned from a training set which is formed by a bootstrapping
  - The composite (ensemble) model works based on
    - Majority votes on predicted classes of the member models in case of classification
    - The average value of predicted values of member models in case of regression
  - Properties
    - Greater predictive performance since using more training samples
    - More robust to the effects of noisy data
    - Composite model reduces variance of the individual classifiers