MADS-ML – Machine Learning

Classification II

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Outline

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Note: Implementations like SVC already implement such strategies (SVC implements OVO).

Outline

"All models are wrong, but some are useful."

"For optimization problems, the performance of two algorithms, averaged over all problems is identical."

Very rough summary of the "No-free-lunch" theorem by David Wolpert.

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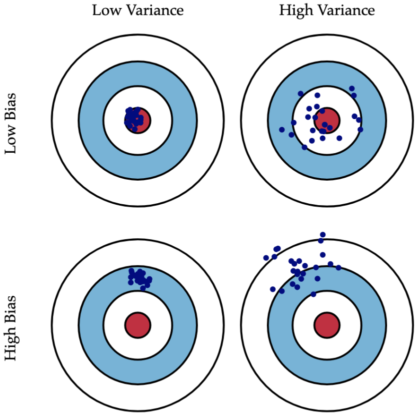
- test and compare algorithms on your dataset

The Problem

Repeatedly learn model using different sets of training data. Each time, predict for the same, new data instance:



Source: [1]

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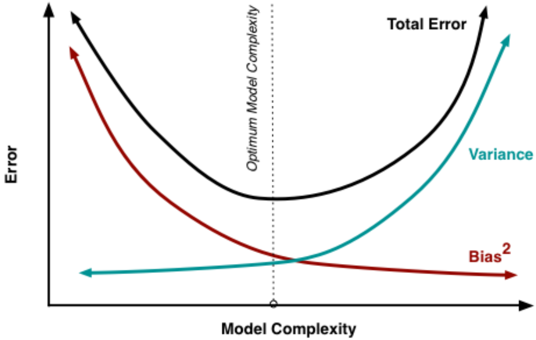
  - model is too complex, has too many degrees of freedom (parameters)

Bias-Variance-Tradeoff



Source: [1]

Combatting overfitting is one of the main tasks in ML.

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Solutions

- Use several splits of the data → cross validation

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- 10-fold CV has been suggested to yield a good balance between bias and variance.

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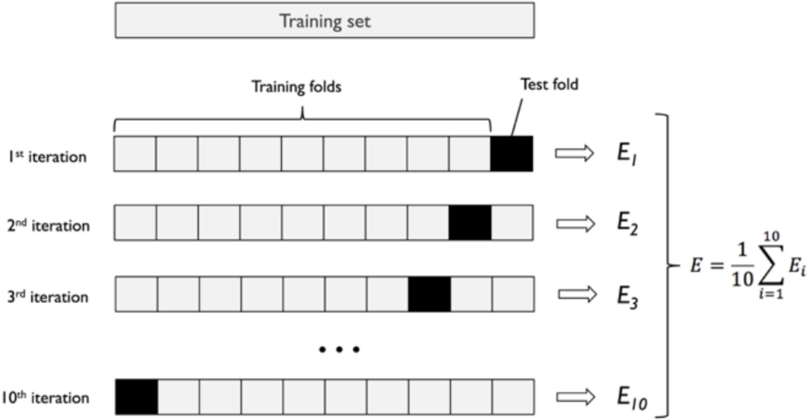

Source: [2], p. 192

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In Python, k-fold and stratified k-fold setups are available.

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- Simulated Annealing: borrows from physics, starts with random point, then checks neighbors, gets out of local optima by allowing moves to worse solutions with decreasing probabilities (e.g. module `simulated_annealing`)

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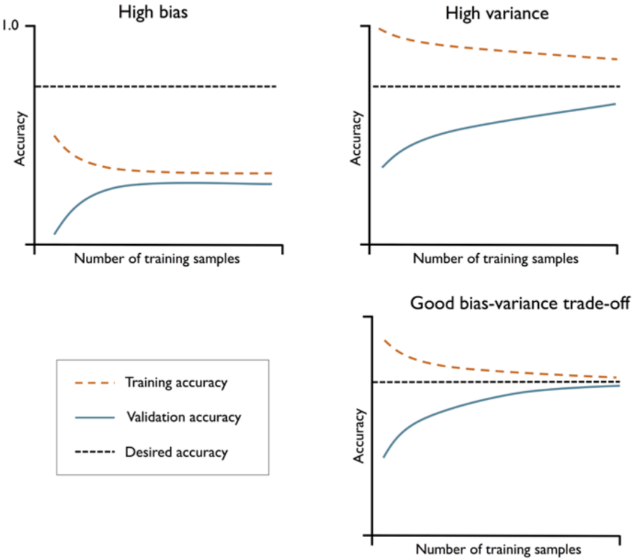

Source: [2], p. 196

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Evaluation with Imbalanced Data

Problem: With imbalanced data, accuracy might be very high, even though we miss all the elements of the small class.
Solutions:

- evaluation measures like balanced accuracy, weighted accuracy, recall/precision/f1, area under the roc curve
- penalize missclassification during training harder for smaller (more expensive) classes
- upsampling: copy instances of the smaller class to make it larger
- downsampling: drop instances of the larger class to make it smaller
- create artificial instances of the smaller class

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Solution: **Stratification** – enforce the same class distribution in all subsets (as far as possible)

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Notebook 06_1_evaluation_metrics

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- the choice of the evaluation measure should be domain-driven
- often it is reasonable to compute and visualize more than one measure

Outline

Pipelines

Idea Collect multiple steps of the ML process into one pipeline.

Components E.g.:

- imputing missing values
- preprocessing steps
- scaling
- encoding of values

Exercises 1–2

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"Shit in – Shit out."

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Imputation Fill in the gap. Most common: Mean imputation. Replace missing value by the features mean (total or per class). Alternatively, use a fix constant (zero, one, ...)

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Flagging For categorical values, impute using a new category "Missing". For continous values, impute and add a feature with the values missing.

Missing Values

Detection (in tabular data): In pandas: `df.isnull().sum()` yields missing values per column

Elimination `df.dropna(axis=x)`

- x=0: drop rows with missing values
- x=1: drop columns with missing values

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Cleanup Data Extraction Investigate and debug the data creation process, remove errors that cause the missing values!

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Sometimes, data contains categorical values, but the algorithms handle only continouus data. ➔ Turn them into numerical variables, using dummies.

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  - might be acceptable e.g. for medical conditions

"Biased data
leads to
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General rule

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