

Generalization Error

ML Instruction Team, Fall 2022

CE Department
Sharif University of Technology

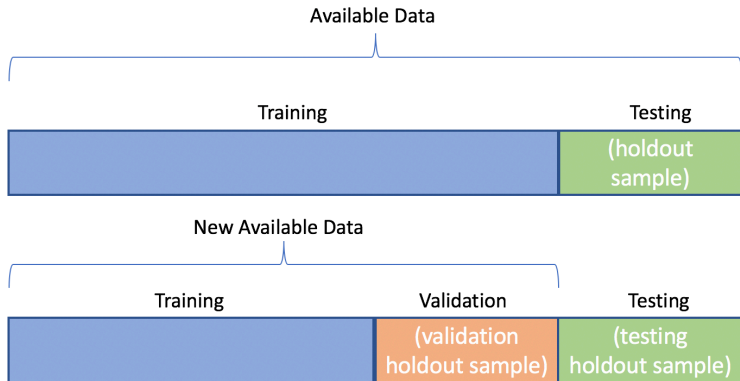
Why Evaluation?

- Estimation of the generalization error
- Increasing of the predictive performance
- Selecting best-suited ML algorithm for our problem

Why Validation?

- Training set error is an optimistically biased estimator of the generalization error
- Test set error is an unbiased estimator of the generalization error

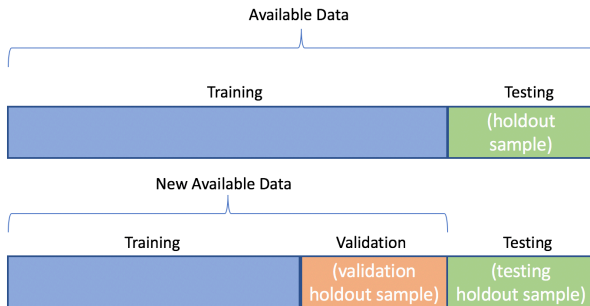
Validation



Types of Validation

- Holdout Validation
- LOOCV (Leave One Out Cross Validation)
- K-Fold Cross Validation

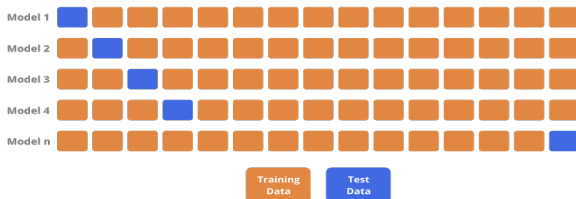
Holdout Validation



- Pros
 - ▶ Fully independent of data
 - ▶ Lower computational costs
- Cons
 - ▶ higher variance

LOOCV

Leave-One-Out Cross Validation



Pros

- ▶ Lower bias

Cons

- ▶ Higher computational cost

K-Fold Cross Validation



Pros

- ▶ Lower computational compared to LOOCV
- ▶ Lower variance compared to Holdout
- ▶ Reducing both Bias and Variance

Cons

- ▶ Higher computational costs in big data state
- ▶ Impact model in imbalanced data state

Hyperparameter Optimization

- Hyperparameter optimization or tuning is the problem of choosing a set of optimal hyperparameters for a learning algorithm.
- A hyperparameter is a parameter whose value is used to control the learning process.
- By contrast, the values of other parameters of the model are learned.
- Hyperparameter optimization finds a tuple of hyperparameters that yields an optimal model which minimizes a predefined loss function on given independent data.

Various algorithms of hyperparameter optimization:

- ▶ Grid search
 - ▶ Random Search
 - ▶ Bayesian Optimization
 - ▶ Gradient-based optimization
 - ▶ Population-based optimization
- Important hyperparameter tuning packages:
 - ▶ Hyperopt
 - ▶ Optuna
 - ▶ Skopt

Thank You!

Any Question?