Stanford University

CS 329P : Practical Machine Learning (2021 Fall)

4.3 Model Validation

Qingqing Huang, Mu Li, Alex Smola

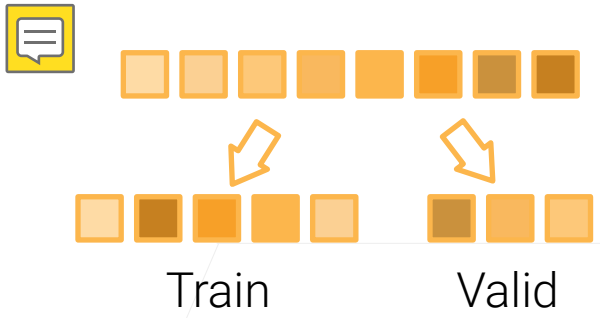
https://c.d2l.ai/stanford-cs329p

Generalization Error

- Approximated by the error on a holdout test dataset, which has never been seen by the model and can be only used **once**
  - Your midterm exam score
  - The final price of a pending house sale
  - Dataset used in private leaderboard in Kaggle
- Validation dataset:
  - Often a subset of the dataset, not used for model training
  - Can be used multiple times for hyper param tuning
  - "test error" usually refers to error on "validation" dataset

Hold Out Validation

- Split your data into "train" and "valid" sets (often calls "test")
  - Train your model on the train set, use the error on the valid set to approximate the generalization error
- Often randomly select n % examples as the valid set
  - Typical choices $n = 50, 40, 30, 20, 10$



Split non I.I.D. data

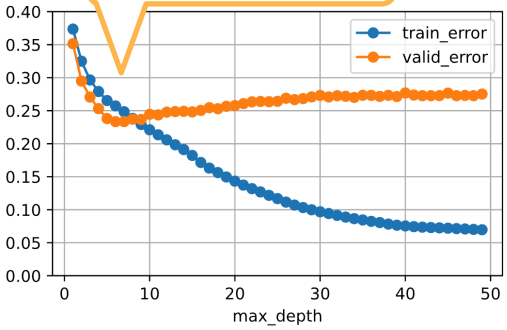
- Random data splitting may lead to underestimate of generalization error
- Sequential data
  - e.g. house sales, stock prices
  - Valid set should not overlap with train set in time
- Examples are highly clustered
  - e.g. photos of the same person, clips of the same video
  - Split clusters instead of examples
- Highly imbalanced label classes
  - Sample more from minor classes

Case Study on House Sales Data

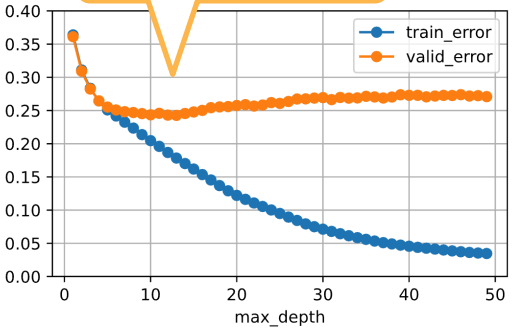
- Split by 50%, test both random and sequential splittings

Decision tree

Sequential, best $d = 6$



Random, best $d = 13$

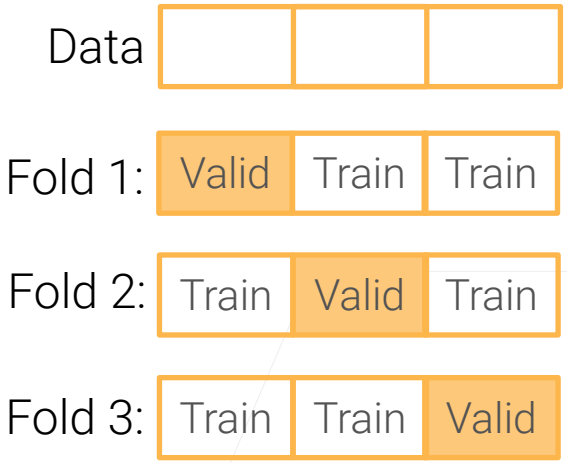


Linear regression

Split	Train	Valid
Random	0.126	0.136
Sequential	0.109	995901.7

K-fold Cross Validation

- Useful when not sufficient data
- Algorithm:
  - Partition the training data into *K* parts
  - For *i* = *1*, …, *K*
    - Use the *i*-th part as the validation set, the rest for training
  - Report the validation error averaged over K rounds
- Popular choices: *K = 5 or 10*



Common Mistakes

- If your ML model performance is too good to be true, very likely there is a bug, and contaminated valid set is the #1 reason.
- Valid set has duplicated examples from train set
  - Often happens when integrating multiple datasets
    - Scrape images from search engine to evaluate models trained on ImageNet
- Information leaking from train set to valid set
  - Often happens for non I.I.D data
    - use future to predict past, see a person's face before
- Excessive use of valid set for hyper param tuning is cheating

Summary

- The test data is used once to evaluate your model
- One can hold out a validation set from the training data to estimate the test data
  - You can use valid set multiple times for model selections and hyper param tuning
  - Validation data should be close to the test data
  - Improper valid set is a common mistake that lead to over estimate of the model performance