

Machine Learning

Supervised Learning. Features. Loss Functions. Cross-validation

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① Supervised Learning Setting

Content

- ➊ Supervised Learning Setting
- ➋ Objects' features

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- ③ Model outputs

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- ➍ Loss functions
- ➎ Cross-validation
- ➏ Hyperparameters tuning

Machine Learning Paradigms: reminder

Definitions

- X — set of objects
- Y — set of (correct) answers/labels
- $y : X \rightarrow Y$ — the unknown dependency

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- Reinforced
 - Action generation based on interaction with the environment

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 - How answers are given
 - What does it mean that one dependency approximates another

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Regression Tasks

$Y = \mathbb{R}$ or $Y = \mathbb{R}^n$

Loss Function

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Loss functions for regression problems

$L(a, x) = (a(x) - y)^2$ — squared error

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- Even within the same model, there can be many (hyper)parameters to choose from

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Naive approach

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So... what to do?

In order not to implicitly learn from test data — you need to use **cross-validation**

Cross Validation

General idea

The main idea of cross-validation is to split the training set into two non-overlapping sets (possibly multiple times):

$$X^{learn} = X^{train} \sqcup X^{val}$$

On one of them, training takes place, and on the other, the model is validated.

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Why validate?

Usually, any machine learning algorithm contains a whole set of so-called “**hyperparameters**” (i.e. parameters that are not learned, but set initially): dimension, various weighting factors, etc.

And in order to select these parameters “fairly”, without using any test data at all, a validation procedure is carried out.

Cross Validation

Special cases

- ① The simplest cross-validation is **hold-out** control, in which the set is split once:



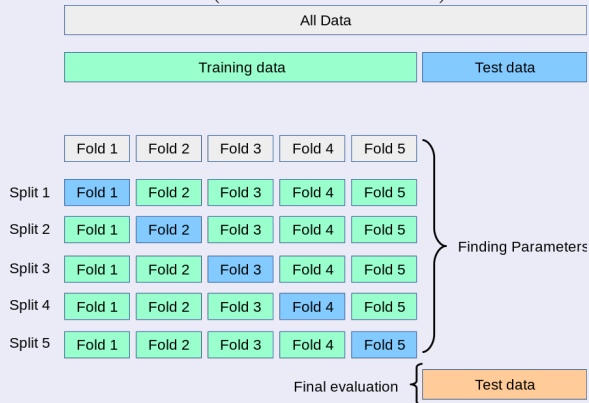
Train

Validation

Cross Validation

Special cases

② k block control (**k-fold** validation)¹:



¹Image source: <https://scikit-learn.org/>

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- ③ Control by individual objects (**leave-one-out**, or LOO validation) — a special case of k -fold validation, if k is equal to the cardinality of the training set
- ④ **Multiple k -fold** validation — repeat k -fold validation several times with different splits.

Cross-validation: the main stages of correct training

- 1 We come up with a model and hyperparameter space

²Image source: <https://scikit-learn.org/>

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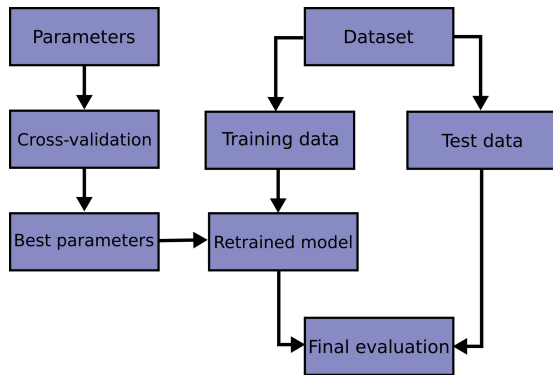
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General scheme²:



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- Usually two approaches are used:
 - ▶ Grid Search: to traverse a predefined range of hyperparameters
 - ▶ Randomized Search: to generate hyperparameters randomly (according to their given distributions)
 - ▶ Usually there is not much difference — and if you do not need to check **specific** values of hyperparameters in advance, then it is better to limit yourself to a random search

Takeaway notes

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- 3 Cross-validation can be of the very different types, but the main goal is the same: to test the generalization ability of the ML model (generalization means performance on an independent data set)
- 4 Hyperparameters tuning is needed for almost every ML model

Thank you!