Machine Learning

Supervised Learning. Features. Loss Functions. Cross-validation

Aleksandr Petiushko

ML Research

SOFIA UNIVERSITY

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1. Supervised Learning Setting
2. Objects' features
3. Model outputs
4. Loss functions

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Machine Learning Paradigms: reminder

Definitions

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

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- Reinforcement
  — Action generation based on interaction with the environment

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

How objects are defined

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- Numerical (or Quantitative) attribute

How answers are given

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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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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

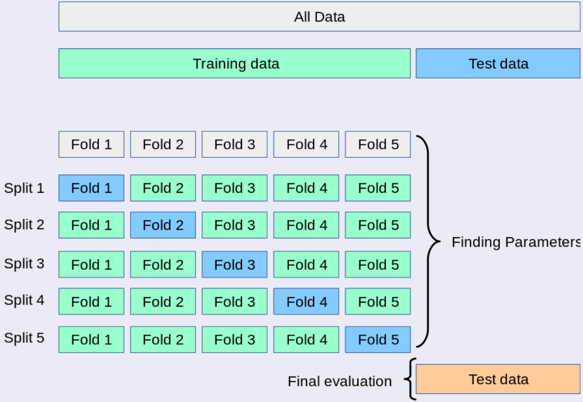
Special cases

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

Cross Validation

Special cases

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



[1] Image source: `https://scikit-learn.org/`

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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

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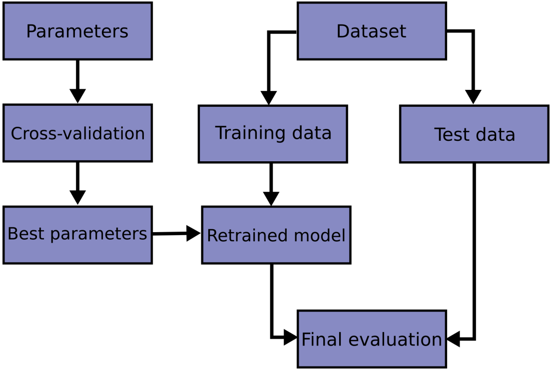
General scheme[2]:



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  - Grid Search: to traverse a predefined range of hyperparameters
  - Randomized Search: to generate hyperparameters randomly (according to their given distributions)
  - Usually there is no big 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

Mandatory external links to read

1. Read the sections 1.2.1, 2.6, (1.3 optionally), 4.1, 5.1, 5.3, 5.7 from "**The Hundred-Page Machine Learning Book**"(see "*References*" course page)
   - Please don't be afraid: all these sections are 1-2 pages max! After you read it, the items below are to increase your understanding on it
2. Read the reminder about Supervised Learning: IBM article
   - This set of readings will remind the main concepts of Supervised Learning
3. Read the section about How Supervised Learning algorithms work
   - This will provide the insight on the machinery behind simple ML algorithms
4. Read the page about what is a feature for an ML algorithm
   - This will provide the high-level understanding of how feed the inputs into ML algorithms
5. Read the introduction into loss functions
   - This will share with you the overview of one of the main concept in ML

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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!