

Validation schemes for 2-nd level models

There are a number of ways to validate **second level models (meta-models)**. In this reading material you will find a description for the most popular ones. If not specified, we assume that the data does not have a time component. We also assume we already validated and fixed hyperparameters for the **first level models (models)**.

a) Simple holdout scheme

1. Split train data into three parts: partA and partB and partC.
2. Fit N diverse **models** on partA, predict for partB, partC, test data getting *meta-features* partB_meta, partC_meta and test_meta respectively.
3. Fit a **metamodel** to a partB_meta while validating its hyperparameters on partC_meta.
4. When the **metamodel** is validated, fit it to [partB_meta, partC_meta] and predict for test_meta.

b) Meta holdout scheme with OOF meta-features

1. Split train data into K folds. Iterate through each fold: retrain N diverse **models** on all folds except current fold, predict for the current fold. After this step for each object in train data we will have N *meta-features* (also known as *out-of-fold predictions*, *OOF*). Let's call them train_meta.
2. Fit **models** to whole train data and predict for test data. Let's call these features test_meta.
3. Split train_meta into two parts: train_metaA and train_metaB. Fit a **meta-model** to train_metaA while validating its hyperparameters on train_metaB.
4. When the **meta-model** is validated, fit it to train_meta and predict for test_meta.

c) Meta KFold scheme with OOF meta-features

1. Obtain *OOF predictions* train_meta and test metafeatures test_meta using **b.1** and **b.2**.
2. Use KFold scheme on train_meta to validate hyperparameters for **meta-model**. A common practice to fix seed for this KFold to be the same as seed for KFold used to get *OOF predictions*.
3. When the **meta-model** is validated, fit it to train_meta and predict for test_meta.

d) Holdout scheme with OOF meta-features

1. Split train data into two parts: partA and partB.
2. Split partA into K folds. Iterate through each fold: retrain N diverse **models** on all folds except current fold, predict for the current fold. After this step for each object in partA we will have N *meta-features* (also known as *out-of-fold predictions*, *OOF*). Let's call them partA_meta.
3. Fit **models** to whole partA and predict for partB and test data, getting partB_meta and test_meta respectively.

4. Fit a **meta-model** to a partA_meta, using partB_meta to validate its hyperparameters.
5. When the **meta-model** is validated basically do 2. and 3. without dividing train_data into parts and then train a **meta-model**. That is, first get *out-of-fold predictions* train_meta for the train_data using **models**. Then train **models** on train_data, predict for test_data, getting test_meta. Train **meta-model** on the train_meta and predict for test_meta.

e) KFold scheme with OOF meta-features

1. To validate the model we basically do **d.1 -- d.4** but we divide train_data into parts partA and partB M times using KFold strategy with M folds.
2. When the meta-model is validated do **d.5**.

Validation in presence of time component

f) KFold scheme in time series

In time-series task we usually have a fixed period of time we are asked to predict. Like day, week, month or arbitrary period with duration of **T**.

1. Split the train data into chunks of duration **T**. Select first **M** chunks.
2. Fit N diverse models on those **M** chunks and predict for the chunk **M+1**. Then fit those models on first **M+1** chunks and predict for chunk **M+2** and so on, until you hit the end. After that use all train data to fit models and get predictions for test. Now we will have *meta-features* for the chunks starting from number **M+1** as well as *meta-features* for the test.
3. Now we can use *meta-features* from first **K** chunks [**M+1, M+2, ..., M+K**] to fit level 2 models and validate them on chunk **M+K+1**. Essentially we are back to step 1. with the lesser amount of chunks and *meta-features* instead of features.

g) KFold scheme in time series with limited amount of data

We may often encounter a situation, where scheme **f)** is not applicable, especially with limited amount of data. For example, when we have only years 2014, 2015, 2016 in train and we need to predict for a whole year 2017 in test. In such cases scheme **c)** could be of help, but with one constraint: KFold split should be done with the respect to the time component. For example, in case of data with several years we would treat each year as a fold.