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

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 <u>train_meta</u> 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 <u>train meta</u> and predict for <u>test meta</u>.

d) Holdout scheme with OOF meta-features

- 1. Split train data into two parts: partA and partB.
- Split <u>partA</u> into K folds. Iterate though each fold: retrain N diverse **models** on all folds except current fold, predict for the current fold. After this step for each object in <u>partA</u> we will have N <u>meta-features</u> (also known as <u>out-of-fold predictions</u>, <u>OOF</u>). Let's call them <u>partA meta</u>.
- 3. Fit **models** to whole <u>partA</u> and predict for <u>partB</u> and <u>test_data</u>, getting <u>partB meta</u> and <u>test_meta</u> respectively.
- 4. Fit a **meta-model** to a <u>partA_meta</u>, using <u>partB_meta</u> to validate its hyperparameters.
- 5. When the **meta-model** is validated basically do 2. and 3. without dividing <u>train_data</u> into parts and then train a **meta-model**. That is, first get *out-of-fold predictions* <u>train_meta</u> for the <u>train_data</u> using **models**. Then train **models** on <u>train_data</u>, predict for <u>test_data</u>, getting <u>test_meta</u>. Train **meta-model** on the <u>train_meta</u> and predict for <u>test_meta</u>.

e) KFold scheme with OOF meta-features

- 1. To validate the model we basically do **d.1 -- d.4** but we divide <u>train data</u> into parts <u>partA</u> and <u>partB</u> 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 \mathbf{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.

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