Implementation Notes

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January 5, 2019

Notation

The data is represented by the design matrix (a.k.a data matrix) $\mathbf{X} \in \mathbb{R}^{N \times p}$ where N is the number of observations and p is the number of features. For simplicity, we assume that the target vector $\mathbf{y} \in \mathbb{R}^{N}$ represents a learning problem in the regression setting. All the the dicsussions below can be applied to the classification setting with appropriate modifications.

For stacking, the data is split over k-folds: $F_1, F_2, \ldots, F_k$. Each F_j represent the indices of the observations in the j^{th} fold. Namely,

$$X_{F_j} = X[F_j, :]$$

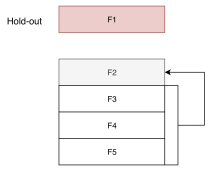
in a numpy-like notation. Negative indices $-F_j$ represent all the folds expect the j^{th}.

During fitting/training, the model parameters are optmized. We denote the folds over which the parameters are optimized in subscripts. For example

$$\mathbf{W}_{-F_i}$$

denotes that the weights $\mathbf{W}$ are optimized over all the folds expect the i^{th} fold (this would be the case when the regressor is a linear function of the data, i.e. $f(\mathbf{X}) = \mathbf{W} \cdot \mathbf{X}$).

The figure below shows a single step in stacking: The fold F_1 is kept as hold-out, and the folds F_3, F_4, F_5 are used for the fit. Predictions on the fold F_2 are obtained from the fitted model.



Stacking a single model over k-folds

For illustration, we consider a case of 5-folds stacking procedure. There are 5 out-of-sample (OOS) predictions that are to be stacked, where each fold is once kept as hold-out (HO). In the illustrative linear regression model, the target vector $\mathbf{y}$ is predicted by the linear function

$$f(X) = \mathbf{X} \cdot \mathbf{W} + \mathbf{b}$$

where $\mathbf{W} \in \mathbb{R}^p$ and $\mathbf{b} \in \mathbb{R}$. The optimal values of $\mathbf{W}$, $\mathbf{b}$ are obtained by minimizing the loss function:

$$L(\mathbf{W}, \mathbf{b}; \lambda) = (\mathbf{X} \cdot \mathbf{W} + \mathbf{b} - \mathbf{y})^2 + \lambda |\mathbf{W}|^2 \qquad , \qquad \mathbf{W}, \mathbf{b} \leftarrow \text{argmin}_{W,b}\, L(\mathbf{W}, \mathbf{b}; \lambda)$$

where λ is the hyper-parameter for the regularization term. In the initial implementation of stacking, we assume λ to be a fixed parameter. 5 fits for $\mathbf{W}, \mathbf{b}$ are performed by minimizing the loss function across folds and OOS predictions are collected. For instance, the OOS predictions for the splits pictured above are obtained by

$$\hat{y}^{OOS}_{-F_1} = \begin{bmatrix} \hat{y}_{F_2} \\ \hat{y}_{F_3} \\ \hat{y}_{F_4} \\ \hat{y}_{F_5} \end{bmatrix}$$

where each $\hat{y}_{F_j}$ is a column vector whose length is equal to the number of observations in the j^{th} fold. In the above equation, $\hat{y}_{F_2}$ is obtained by optimizing the loss function on the data $X_{-(F_1+F_2)}$, which results in $\mathbf{W}_{-(F_1+F_2)}, \mathbf{b}_{-(F_1+F_2)}$ and predicting on the fold F_2. Namely,

$$\hat{y}_{F_2} = \mathbf{X}_{F_2} \cdot \mathbf{W}_{(-F_1+F_2)} + \mathbf{b}_{-(F_1+F_2)}$$

The rest of the predictions $\hat{y}_3, \hat{y}_4, \hat{y}_5$ are obtained following a similar set of computations. The predictions on the HO fold are instead obtained by simply fitting the model on all the four folds, and predicting on the HO fold. Namely,

$$\hat{y}_{F_1}^{HO} = \mathbf{X}_{F_1} \cdot \mathbf{W}_{-F_1} + \mathbf{b}_{-F_1}$$

Since the HO fold can be any of the 5 folds, we have the following set of OOS-HO predictions:

$$\left[(\hat{y}_{-F_1}^{OOS}, \hat{y}_{F_1}^{HO}), \ldots, (\hat{y}_{-F_5}^{OOS}, \hat{y}_{F_5}^{HO})\right]$$

As will be shown below, this set of OOS and HO predictions provide an automatic way to train the stacker models by 5-folds cross-validation.

Stacking multiple models over k folds

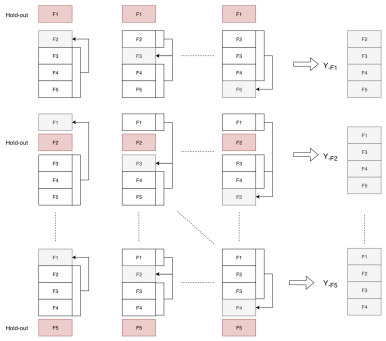
Suppose we have M models that we would like to stack. For each model (assuming fixed hyper-parameters), we will repeat the above procedure to get OOS and HO predictions and construct new data matrices by column-stacking. For example, when F_1 is the HO fold, we have

$$\mathbf{X}_{-F_1}^{OOS} = \begin{bmatrix} | & \cdots & | \\ \hat{y}_{-F_1}^{(1)\,OOS} & \cdots & \hat{y}_{-F_1}^{(M)\,OOS} \\ | & \cdots & | \end{bmatrix} \quad , \quad \mathbf{X}_{F_1}^{HO} = \begin{bmatrix} | & \cdots & | \\ \hat{y}_{F_1}^{(1)\,HO} & \cdots & \hat{y}_{F_1}^{(M)\,HO} \\ | & \cdots & | \end{bmatrix}$$

Peforming the same for other HO folds, we end up with the following set of 5 pairs:

$$\left[(\mathbf{X}_{-F_1}^{OOS}, \mathbf{X}_{F_1}^{HO}), \ldots, (\mathbf{X}_{-F_5}^{OOS}, \mathbf{X}_{F_5}^{HO})\right]$$

which can be used to train the stacker models by optimizing their hyper-parameters by 5-folds cross validation. The whole procedure of obtaining training/validation folds from OOS/HO pairs is decpicted in the figure below



Once the hyper-parameters of the stacker model are determined, the final predictions can be obtained. For the sake of simplicity, let's assume that the stacker is also a linear model. The stacker model uses the OOS predictions to train and predict on the HO folds. The predictions on the first HO fold F_1 are obtained by

$$\hat{Y}_{F_1} = X^{HO}_{F_1} \cdot \Omega_{-F_1} + \beta_{-F_1}$$

where Ω and β are parameters of the stacker model optimized during fitting:

$$\Omega_{-F_1}, \beta_{-F_1} \leftarrow \text{argmin}_{\Omega,\beta} \left[((\mathbf{X}^{OOS}_{-F_1} \cdot \Omega + \beta) - \mathbf{y}_{-F_1})^2 + \Lambda \left| \Omega \right|^2 \right]$$

After performing the same set of computations for other HO folds and a grid of values for Λ, we can train the stacker model. Λ is determined across 5-folds by minimizing the mean-squared-error (MSE) between $\hat{y}_{F_j}$ and $\mathbf{y}_{F_j}$ for $j = 1, \ldots, 5$. More precisely, the value of Λ is the one that results in the lowest average MSE across folds:

$$\Lambda \leftarrow \text{argmin}_{\Lambda} \left[\sum_{i=1}^{5} (\mathbf{y}_{F_i} - \hat{Y}_{F_i})^2 \right]$$

Here $\hat{Y}_{F_i}$ has an implicit dependence on Λ by the above equations.

Final fit on training data

After the stacker model is trained (i.e. Λ is determined), the final fit is obtained by using all the 5 folds in X^{OOS} instead of leaving one folds for HO. Namely,

$$\hat{y}^{OOS} = \begin{bmatrix} \hat{y}_{F_1} \\ \hat{y}_{F_2} \\ \hat{y}_{F_3} \\ \hat{y}_{F_4} \\ \hat{y}_{F_5} \end{bmatrix}$$

where $\hat{y}_{F_i}$ is determined as follows:

$$\hat{y}_{F_i} = \mathbf{X}_{F_i} \cdot \mathbf{W}_{-F_i} + \mathbf{b}_{-F_i} \qquad , \qquad \mathbf{W}_{-F_i}, \mathbf{b}_{-F_i} \leftarrow \text{argmin}_{W,b} \left[(\mathbf{X}_{-F_i} \cdot \mathbf{W} + \mathbf{b} - \mathbf{y}_{-F_i})^2 + \lambda |\mathbf{W}|^2 \right]$$

Column-stacking theese column vectors for M models results in $\mathbf{X}^{OOS}$. With Λ determined by the 5-fold cross validation procedure from above, the final predictions are provided by the stacker model:

$$\hat{Y} = \mathbf{X}^{OOS} \cdot \Omega + \beta \qquad , \qquad \Omega, \beta \leftarrow \text{argmin}_{\Omega,\beta} \ \left[(\mathbf{X}^{OOS} \cdot \Omega + \beta - \mathbf{y})^2 + \Lambda |\Omega|^2 \right]$$

Final fit on test data

The test data contains a completely new set of observations that need to go through the stacking procedure as well. In the first step, we also need to split the test data on 5-folds and predict using the 5 different sets of parameters $\mathbf{W}_{-F_i}, \mathbf{b}_{-F_i}$. Unlike the training set where it is clear which fold is predicted by which model parameters (i.e. F_1 is predicted by the model that uses $\mathbf{W}_{-F_1}, \mathbf{b}_{-F_1}$), for the test set there is no natural one-to-one correspondance. We therefore predict on each test fold by each model, resulting in a 5×5 set of predictions for **each model!**

Let's assume that we are stacking a single model's predictions. We construct the following matrix for this purpose:

$$\mathbf{Z}^{(1)} = \begin{bmatrix} \mathbf{X}^{\text{test}}_{F_1} \cdot \mathbf{W}_{-F_1} + \mathbf{b}_{-F_1} & \mathbf{X}^{\text{test}}_{F_1} \cdot \mathbf{W}_{-F_2} + \mathbf{b}_{-F_2} & \dots & \mathbf{X}^{\text{test}}_{F_1} \cdot \mathbf{W}_{-F_5} + \mathbf{b}_{-F_5} \\ \mathbf{X}^{\text{test}}_{F_2} \cdot \mathbf{W}_{-F_1} + \mathbf{b}_{-F_1} & \mathbf{X}^{\text{test}}_{F_2} \cdot \mathbf{W}_{-F_2} + \mathbf{b}_{-F_2} & \dots & \mathbf{X}^{\text{test}}_{F_2} \cdot \mathbf{W}_{-F_5} + \mathbf{b}_{-F_5} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{X}^{\text{test}}_{F_5} \cdot \mathbf{W}_{-F_1} + \mathbf{b}_{-F_1} & \mathbf{X}^{\text{test}}_{F_5} \cdot \mathbf{W}_{-F_2} + \mathbf{b}_{-F_2} & \dots & \mathbf{X}^{\text{test}}_{F_5} \cdot \mathbf{W}_{-F_5} + \mathbf{b}_{-F_5} \end{bmatrix}$$

We need one column vector from $\mathbf{Z}^{(1)}$, which we choose to pick by taking the row averages:

$$\hat{y}^{\text{test,OOS}} = \frac{1}{5} \begin{bmatrix} \sum_j Z_{1j}^{(1)} \\ \vdots \\ \sum_j Z_{5j}^{(1)} \end{bmatrix}$$

Column-stacking the test OOS predictions into $\mathbf{X}^{\text{test,OOS}}$ for M models, we can then predict the test data using the stacker model (with Ω, β determined from the training set).

Training models to be stacked in addition to stacker

Up to this point we have assumed that the hyper-parameters (λ) of all the initial models are fixed. This led to 5 models characterized by parameters $\mathbf{W}_{-F_i}, \mathbf{b}_{-F_i}$, for $i = 1, \ldots, 5$. Instead, for each HO fold an internal 4-fold cross-validation can be performed to optimize the hyper-parameters of each input model during training. While this procedure leads to an increased computational time, it usually results in better generalizability. This results in 5 fits per model with differing hyper-parameters.