

pystacked: Stacking generalization and machine learning in Stata

Achim Ahrens (ETH Zürich)

Mark E Schaffer (Heriot-Watt University, IZA)

Christian B Hansen (University of Chicago)

Package website: <https://statalasso.github.io/>

Latest version available [here](#)

November 18, 2022

Swiss Stata Group Meeting

Introduction: Stacking

- ▶ The machine learning (ML) toolbox includes a rich set of flexible methods: regularized regression, random forests, SVM, boosting, neural nets.

Introduction: Stacking

- ▶ The machine learning (ML) toolbox includes a rich set of flexible methods: regularized regression, random forests, SVM, boosting, neural nets.
- ▶ When faced with a new prediction or classification task, it is *a priori* rarely obvious which machine learner is best suited for a particular task.
- ▶ *Typical approach:*
 - ▶ Validating learner based on hold-out sample
 - ▶ Cross-validation (K -fold, Leave-one-out, One-step ahead)

The underlying idea: Select *one* learner as the best.

Introduction: Stacking

This approach seems incomplete: combining several different learners could improve performance.

The idea of *stacking generalization*, or simply *stacking*, is to combine learners (Wolpert, 1992; Breiman, 1996).

Introduction: Stacking

This approach seems incomplete: combining several different learners could improve performance.

The idea of *stacking generalization*, or simply *stacking*, is to combine learners (Wolpert, 1992; Breiman, 1996).

General idea:

- ▶ Combine a set of “base” (or “level-0”) learners using a “final” (or “level-1”) estimator.
- ▶ It is advisable to include a relatively large and diverse set of base learners to capture different types of pattern in the data.
- ▶ Stacking also provides an effective framework for hyper-parameter tuning.

Introduction: Stata's ML tools

There is a growing number of programs for ML in Stata:

- ▶ `lassopack` for regularized regression (Ahrens, Hansen, and Schaffer, 2020)
- ▶ `rforest` for random forests (Schonlau and Zou, 2020)
- ▶ `svmmachines` for support vector machines (Guenther and Schonlau, 2018)
- ▶ Cerulli (2021) and Droste (2020) provide an interface to *scikit-learn* (Pedregosa et al., 2011; Buitinck et al., 2013)
- ▶ `mlrtime` allows Stata users to make use of R's *parsnip* machine learning library (Huntington-Klein, 2021)

Our contribution: We complement these programs by offering a package that can be used to fit a wide range of machine learners, and for *stacking*.

Introducing pystacked

We introduce `pystacked` for stacking regression and binary classification in Stata.

- ▶ `pystacked` allows to fit multiple machine learning algorithms via Python's *scikit-learn* (Pedregosa et al., 2011; Buitinck et al., 2013)¹ and *combine these into one final prediction* as a weighted average of individual predictions.
- ▶ `pystacked` can also be used to *fit a single machine learner* and thus provides an easy-to-use and versatile API to *scikit-learn's* machine learning algorithms.
- ▶ Our main motivation for developing `pystacked`: Use it in combination with Double-Debiased Machine Learning (Chernozhukov et al., 2018)
⇒ **Second talk**

¹We stress that `pystacked` relies on *scikit-learn* and the on-going work of the *scikit-learn* contributors. We thus suggest that users cite *scikit-learn* along with this article when using `pystacked`.

Stacking regression

Which machine learner should we use?

We don't know whether we have a sparse or dense problem; linear or non-linear; etc.

Stacking is an ensemble method that combines multiple base learners into one model. As the default, we use *constrained least squares*:

$$\mathbf{w} = \arg \min_{w_j} \sum_{i=1}^n \left(y_i - \sum_{j=1}^J w_j \hat{y}_i^{(j)} \right)^2, \quad w_j \geq 0, \quad \sum_j w_j = 1$$

where $\hat{y}_i^{(j)}$ are cross-validated predictions of base learner j .

Voting regression is a special case with unweighted (or user-specified) weights.

Stacking regression

1. *Cross-validation*:

- 1.1 Split the data randomly into K partitions of approximately equal size. These partitions are referred to as *folds*. Denote the set of observations in fold k as I_k , and its complement as I_k^c such that $I_k^c = \{1, \dots, n\} / I_k$. I_k constitutes the validation set and I_k^c the training sample.

Stacking regression

1. *Cross-validation*:

- 1.1 Split the data randomly into K partitions of approximately equal size. These partitions are referred to as *folds*. Denote the set of observations in fold k as I_k , and its complement as I_k^c such that $I_k^c = \{1, \dots, n\} / I_k$. I_k constitutes the validation set and I_k^c the training sample.
- 1.2 For each fold $k = 1, \dots, K$ and each base learner $j = 1, \dots, J$, fit machine learner j to the training data I_k^c and obtain out-of-sample predicted values $\hat{y}_i^{(j)}$ for $i \in I_k$.

Stacking regression

1. Cross-validation:

1.1 Split the data randomly into K partitions of approximately equal size. These partitions are referred to as *folds*. Denote the set of observations in fold k as I_k , and its complement as I_k^c such that $I_k^c = \{1, \dots, n\} / I_k$. I_k constitutes the validation set and I_k^c the training sample.

1.2 For each fold $k = 1, \dots, K$ and each base learner $j = 1, \dots, J$, fit machine learner j to the training data I_k^c and obtain out-of-sample predicted values $\hat{y}_i^{(j)}$ for $i \in I_k$.

2. *Final learner*: Fit the final learner to the full sample. The default choice is *constrained least squares*:

$$\mathbf{w} = \arg \min_{\mathbf{w}_j} \sum_{i=1}^n \left(y_i - \sum_{j=1}^J w_j \hat{y}_i^{(j)} \right)^2, \quad w_j \geq 0, \quad \sum_j w_j = 1$$

The stacking predicted values are defined as $\hat{y}_i^* = \sum_j \hat{w}_j \hat{y}_i^{(j)}$.

pystacked overview

pystacked implements stacking regression (Wolpert, 1992) via [scikit learn](#)'s `StackingRegressor` and `StackingClassifier`.

pystacked overview

pystacked implements stacking regression (Wolpert, 1992) via [scikit learn](#)'s `StackingRegressor` and `StackingClassifier`.

Main features:

- ▶ Two alternatives syntaxes
- ▶ 10+ different machine learners supported that can be used stand-alone or as base learners in combination with stacking
- ▶ Regression+classification
- ▶ Graphing and plotting features
- ▶ Supports central *scikit-learn* learn pipelines
- ▶ Supports sparse matrices and parallelization

(Base) Machine learners

<code>method()</code>	<code>type()</code>	<i>Machine learner description</i>
<code>ols</code>	<code>regress</code>	Linear regression
<code>logit</code>	<code>class</code>	Logistic regression
<code>lassoic</code>	<code>regress</code>	Lasso with AIC/BIC penalty
<code>lassocv</code>	<code>regress</code>	Lasso with CV penalty
	<code>class</code>	Logistic lasso with CV penalt
<code>ridgecv</code>	<code>regress</code>	Ridge with CV penalty
	<code>class</code>	Logistic ridge with CV penalty
<code>elasticcv</code>	<code>regress</code>	Elastic net with CV penalty
	<code>class</code>	Logistic elastic net with CV
<code>svm</code>	<code>regress</code>	Support vector regression
	<code>class</code>	Support vector classification
<code>gradboost</code>	<code>regress</code>	Gradient boosting regressor
	<code>class</code>	Gradient boosting classifier
<code>rf</code>	<code>regress</code>	Random forest regressor
	<code>class</code>	Random forest classifier
<code>linsvm</code>	<code>class</code>	Linear SVC
<code>nnet</code>	<code>regress</code>	Neural net
	<code>class</code>	Neural net

Note: The first two columns list all allowed combinations of `method(string)` and `type(string)`, which are used to select base learners. Column 3 provides a description of each machine learner. 'CV penalty' indicates that the penalty level is chosen to minimize the cross-validated MSPE. 'AIC/BIC penalty' indicates that the penalty level minimizes either either the Akaike or Bayesian information criterion. SVC refers to support vector classification.

Main syntax

Syntax 1:

```
pystacked deivar predictors [if] [in] [, methods(string)  
cmdopt1(string) cmdopt2(string) ... cmdopt10(string)  
pipe1(string) pipe2(string) ... pipe10(string)  
xvars1(predictors) xvars2(predictors) ... xvars10(predictors)  
general_options ]
```

Notes:

- ▶ `methods(string)` is used to select base learners, where *string* is a list of base learners.
- ▶ Options are passed on to base learners via `cmdopt1(string)`, `cmdopt2(string)` to `cmdopt10(string)`.
- ▶ `pipe*(string)` are for pipelines; `xvars*(predictors)` allows to specify a learner-specific variable lists of predictors.
- ▶ *Limitation*: only 10 base learners supported.

Main syntax

Syntax 2:

```
pystacked depvar [indepvars] || method(string) opt(string)  
pipe(string) xvars(predictors) [ || method(string) opt(string)  
pipe(string) xvars(predictors) ... || ] [if] [in] [ ,  
general_options ]
```

Notes:

Base learners are added before the comma using method(*string*) along with further learner-specific settings and separated by '||'.

Pipelines and learner-specific predictors

Pipelines

scikit-learn uses pipelines to pre-process input data on the fly. In `pystacked`, pipelines can be used to impute missing values, create polynomials and interactions, and to standardize predictors.

Pipelines and learner-specific predictors

Pipelines

scikit-learn uses pipelines to pre-process input data on the fly. In *pystacked*, pipelines can be used to impute missing values, create polynomials and interactions, and to standardize predictors.

Learner-specific predictors

- ▶ By default, *pystacked* uses the same set of predictors for each base learner.
- ▶ This is often not desirable: For example, when using linear machine learners such as the lasso adding polynomials, interactions and other transformations of the base set of predictors might greatly improve out-of-sample prediction performance.
- ▶ *Solution*: Use pipelines or `xvars*(predictors)`

Demonstration 1: Single base learner

We import the California house price data from Pace and Barry (1997), and split the sample randomly into training and validation partition using a 75/25 split. The aim of the prediction task is to predict median house prices (`medhousevalue`) using a set of house price characteristics

```
. clear all
. use https://statalasso.github.io/dta/cal_housing.dta, clear
. set seed 42
. gen train=runiform()
. replace train=train<.75
(20,640 real changes made)
. replace medh = medh/10e3
variable medhousevalue was long now double
(20,640 real changes made)
. label var medh
```

Demonstration 1: Single base learner

The option `method(gradboost)` selects gradient boosting. We will later see that we can specify more than one learner in `methods()`, and that we can also fit gradient boosted classification trees.

```
. pystacked medh longi-medi if train, type(reg) methods(gradboost)
Single base learner: no stacking done.
```

```
Stacking weights:
```

Method	Weight
gradboost	1.0000000

```
. predict double yhat_gb1 if !train
```

Demonstration 1: Single base learner

The option `method(gradientboost)` selects gradient boosting. We will later see that we can specify more than one learner in `methods()`, and that we can also fit gradient boosted classification trees.

```
. pystacked medh longi-medi if train, type(reg) methods(gradientboost)
Single base learner: no stacking done.
```

```
Stacking weights:
```

Method	Weight
gradientboost	1.0000000

```
. predict double yhat_gb1 if !train
```

The output shows the stacking weights associated with each base learner. Since we only consider one method, the output is not particularly informative and simply shows a weight of one for gradient boosting. Yet, `pystacked` has fitted 100 boosted trees (the default) in the background!

Demonstration 1: Single base learner

Here, we compare lasso with and without the *poly2* pipeline:

```
. pystacked medh longi-medi if train, type(reg) methods(lassocv)
Single base learner: no stacking done.
```

Stacking weights:

Method	Weight
lassocv	1.0000000

```
. predict double yhat_lasso1 if !train
```

```
.
```

```
. pystacked medh longi-medi if train, type(reg) methods(lassocv) ///
> pipe1(poly2)
```

```
Single base learner: no stacking done.
```

Stacking weights:

Method	Weight
lassocv	1.0000000

```
. predict double yhat_lasso2 if !train
```

Demonstration 2: Stacking regression

We now consider a stacking regression application with five base learners:

1. linear regression,
2. lasso with penalty chosen by cross-validation,
3. lasso with second order polynomials and interactions,
4. random forest with default settings,
5. gradient boosting with a learning rate of 0.01 and 1000 trees.

Demonstration 2: Stacking regression

Syntax 1:

```
. set seed 42
. pystacked medh longi-medi if train,          ///
>   type(regress)                            ///
>   methods(ols lasso cv lasso cv rf gradboost)  ///
>   pipe3(poly2) cmdopt5(learning_rate(0.01)    ///
>   n_estimators(1000))
```

Stacking weights:

Method	Weight
ols	0.0000000
lasso cv	0.0000000
lasso cv	0.4692388
rf	0.2505079
gradboost	0.2802533

Demonstration 2: Stacking regression

Syntax 2:

```
. set seed 42
. pystacked medh longi-medi      || ///
>   m(ols)                      || ///
>   m(lassocv)                  || ///
>   m(lassocv) pipe(poly2)     || ///
>   m(rf)                       || ///
>   m(gradboost) opt(learning_rate(0.01) n_estimators(1000))  ///
>   if train, type(regress)
```

Stacking weights:

Method	Weight
ols	0.0000000
lassocv	0.0000000
lassocv	0.4692388
rf	0.2505079
gradboost	0.2802533

Demonstration 2: Stacking regression

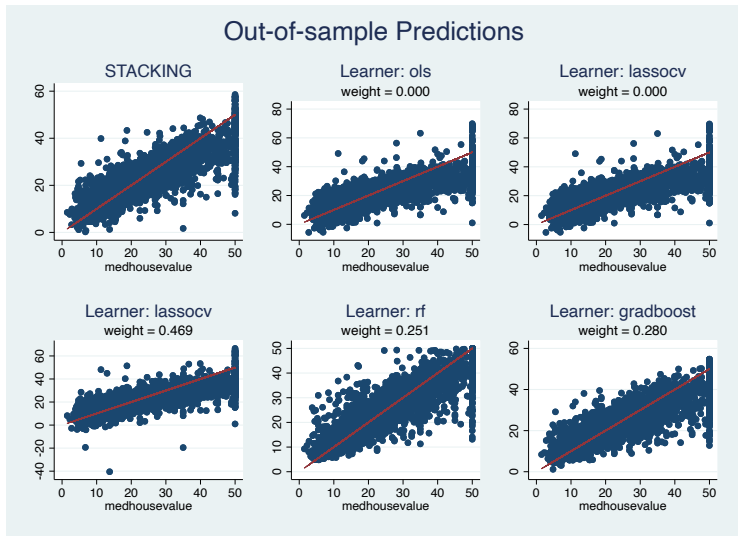
Predicted values. In addition to the stacking predicted values, we can also get the predicted values of each base learner using the transform option:

```
. predict double yhat, xb  
. predict double ytrans, transf  
. list yhat ytrans* if _n <= 5
```

	yhat	ytrans1	ytrans2	ytrans3	ytrans4	ytrans5
1.	41.357332	41.315834	41.24048	40.36963	43.16083	41.394926
2.	42.876817	41.45306	41.434102	46.420851	38.289107	41.056291
3.	39.222298	38.212036	38.176811	39.068403	41.268902	37.648071
4.	33.686191	32.332498	32.291791	33.645113	33.4869	33.933232
5.	25.253149	25.382839	25.374455	25.608601	23.8597	25.905815

Demonstration 2: Stacking regression

Plotting. The graph option creates a scatter plot of predicted versus observed values for stacking and each base learner:



Demonstration 2: Stacking regression

MSPE table. The table option allows to compare stacking weights with in-sample and out-of-sample MSPE. As with the graph option, we can use table as a post-estimation command:





```
. pystacked, table holdout
Number of holdout observations: 5192
MSPE: In-Sample and Out-of-Sample
```

Method	Weight	In-Sample	Out-of-Sample
STACKING	.	4.795	5.473
ols	0.000	6.986	6.853
lassocv	0.000	6.986	6.855
lassocv	0.469	6.613	6.564
rf	0.251	1.847	4.963
gradboost	0.280	5.312	5.511





Summary

- ▶ `pystacked` implements *stacked generalization* (Wolpert, 1992) for regression and binary classification via Python's *scikit-learn*.
- ▶ Stacking combines multiple supervised machine learners—the “base” or “level-0” learners—into a single learner.
- ▶ The currently *supported (base) machine learners* include regularized regression, random forest, gradient boosting, support vector machines and feed-forward neural nets (multi-layer perceptron).
- ▶ `pystacked` can also be used with as a ‘regular’ machine learning program to fit a single base learner and, thus, provides an easy-to-use API for *scikit-learn*'s machine learning algorithms.





References I

-  Ahrens, Achim, Christian B. Hansen, and Mark E. Schaffer (2020). “lassopack: Model selection and prediction with regularized regression in Stata”. In: *The Stata Journal* 20.1, pp. 176–235. URL: <https://doi.org/10.1177/1536867X20909697>.
-  Breiman, Leo (July 1996). “Stacked regressions”. en. In: *Machine Learning* 24.1, pp. 49–64. URL: <http://link.springer.com/10.1007/BF00117832> (visited on 12/04/2021).
-  Buitinck, Lars et al. (2013). “API design for machine learning software: experiences from the scikit-learn project”. In: *ECML PKDD Workshop: Languages for Data Mining and Machine Learning*, pp. 108–122.
-  Cerulli, Giovanni (2021). *Machine Learning using Stata/Python*.

References II

-  Chernozhukov, Victor et al. (2018). “Double/debiased machine learning for treatment and structural parameters”. In: *The Econometrics Journal* 21.1. tex.ids= Chernozhukov2018a publisher: John Wiley & Sons, Ltd (10.1111), pp. C1–C68. URL: <https://onlinelibrary.wiley.com/doi/abs/10.1111/ectj.12097>.
-  Droste, Michael (2020). *pylearn*. <https://github.com/mdroste/stata-pylearn/>. [Online; accessed 02-December-2021].
-  Guenther, Nick and Matthias Schonlau (Nov. 2018). *SVMACHINES: Stata module providing Support Vector Machines for both Classification and Regression*. Statistical Software Components, Boston College Department of Economics. URL: <https://ideas.repec.org/c/boc/bocode/s458564.html>.
-  Huntington-Klein, Nick C. (2021). *mlrtime*. <https://github.com/NickCH-K/MLRtime/>. [Online; accessed 02-December-2021].

References III

-  Pace, R. Kelley and Ronald Barry (1997). “Sparse spatial autoregressions”. In: *Statistics & Probability Letters* 33.3, pp. 291–297. URL: <https://www.sciencedirect.com/science/article/pii/S016771529600140X>.
-  Pedregosa, F. et al. (2011). “Scikit-learn: Machine Learning in Python”. In: *Journal of Machine Learning Research* 12, pp. 2825–2830.
-  Schonlau, Matthias and Rosie Yuyan Zou (2020). “The random forest algorithm for statistical learning”. In: *The Stata Journal* 20.1, pp. 3–29. URL: <https://doi.org/10.1177/1536867X20909688>.
-  Wolpert, David H. (1992). “Stacked generalization”. In: *Neural Networks* 5.2, pp. 241–259. URL: <https://www.sciencedirect.com/science/article/pii/S0893608005800231>.