pystacked: Stacking generalization and machine learning in Stata

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Package website: `https://statalasso.github.io/`

Latest version available here

September 7, 2023

Introduction: Stacking

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- The machine leaning (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). Goes under various names: super learner, model averaging, etc.

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). Goes under various names: super learner, model averaging, etc.

General idea:

- Combine a set of "base" (or "level-0", "candidate") 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)
- `svmachines` 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)
- ...and Stata's own built-in learners

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)
- Forthcoming `pystacked` paper in *The Stata Journal* (working paper version: Ahrens, Hansen, and Schaffer (2022))

[1] We 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 *non-negative least squares*:

$$\min_{w_1,\dots,w_J} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{J} w_j \hat{y}_{(j),i}^{-k(i)} \right)^2 \qquad \text{s.t.} \quad w_j \geq 0, \quad \sum_{j=1}^{J} w_j = 1$$

where $\hat{y}_{(j),i}^{-k(i)}$ are the 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 sample $I = \{1, \ldots, n\}$ randomly into K partitions ('folds') of approximately equal size. Denote the set of observations in fold $k = 1, \ldots, K$ as I_k, and its complement as I_k^c such that $I_k^c = I \setminus I_k$. I_k constitutes the step-k validation set and I_k^c the step-k training sample.

Stacking regression

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

Stacking regression

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   1.2 For each fold $k = 1, \ldots, K$ and each base learner $j = 1, \ldots, J$, fit the supervised machine learner j to the training data I_k^c and obtain out-of-sample predicted values $\hat{y}_{(j),i}^{-k}$ for $i \in I_k$.
2. *Final learner:* Fit the final learner to the full sample. The default choice is NNLS:

$$\min_{w_1,\ldots,w_J} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{J} w_j \hat{y}_{(j),i}^{-k(i)} \right)^2 \qquad \text{s.t.} \quad w_j \geq 0, \quad \sum_{j=1}^{J} w_j = 1$$

   The stacking predicted values are defined as $\hat{y}_i^\star = \sum_j \hat{w}_j \hat{y}_{(j),i}$ where $\hat{w}_j$ is the estimated stacking weight corresponding to learner j and $\hat{y}_{(j),i}$ are the predicted values from re-fitting learner j on the full sample I.

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 machining learning algorithms 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
- Various options for the final learner (ridge, least squares)

(Base) Machine learners

`method()`	`type()`	*Machine learner description*
ols	*regress*	Linear regression
logit	*class*	Logistic regression
lassoic	*regress*	Lasso with AIC/BIC penalty
lassocv	*regress*	Lasso with CV penalty
	class	Logistic lasso with CV penalt
ridgecv	*regress*	Ridge with CV penalty
	class	Logistic ridge with CV penalty
elasticcv	*regress*	Elastic net with CV penalty
	class	Logistic elastic net with CV
svm	*regress*	Support vector regression
	class	Support vector classification
gradboost	*regress*	Gradient boosting regressor
	class	Gradient boosting classifier
rf	*regress*	Random forest regressor
	class	Random forest classifier
linsvm	*class*	Linear SVC
nnet	*regress*	Neural net
	class	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` *depvar predictors* [*if*] [*in*] [`,` `methods(`*string*`)` `cmdopt1(`*string*`)` `cmdopt2(`*string*`)` ... `cmdopt10(`*string*`)` `pipe1(`*string*`)` `pipe2(`*string*`)` ... `xvars1(`*predictors*`)` `xvars2(`*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*`)`, ...
- `pipe*(`*string*`)` are for pipelines; `xvars*(`*predictors*`)` allows to specify a learner-specific variable lists of predictors.

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-preprocess 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

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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*`)`

General options I

A full list of general options is provided in the `pystacked` help file. We list only the most important general options here:

`type(`*string*`)` allows *reg(ress)* for regression problems or *class(ify)* for classification problems. The default is regression.

`finalest(`*string*`)` selects the final estimator used to combine base learners. The default is non-negative least squares without an intercept and the additional constraint that weights sum to 1 (*nnls1*). Alternatives are *nnls0* (non-negative least squares without an intercept and without the sum-to-one constraint), *singlebest* (use the base learner with the minimum MSE), *ls1* (least squares without an intercept and with the sum-to-one constraint), *ols* (ordinary least squares) or *ridge* for (logistic) ridge, which is the *scikit-learn* default.

`folds(`*integer*`)` specifies the number of folds used for cross-validation. The default is 5.

`foldvar(`*varname*`)` is the integer fold variable for cross-validation.

`bfolds(`*integer*`)` sets the number of folds used for base learners that use cross-validation (e.g. cross-validated lasso); the default is 5.

General options II

`pyseed(`*integer*`)` sets the Python seed. Note that since `pystacked` uses Python, we also need to set the Python seed to ensure replicability. There are three options:

1. `pyseed(`*-1*`)` draws a number between 0 and 10^8 in Stata which is then used as a Python seed; this is `pystacked`'s default behavior. This way, one only needs to deal with the Stata seed. For example, `set seed 42` is sufficient, as the Python seed is generated automatically.
2. Setting `pyseed(`*x*`)` with any positive integer *x* allows to control the Python seed directly.
3. `pyseed(`*0*`)` sets the seed to `None` in Python.

`njobs(`*integer*`)` sets the number of jobs for parallel computing. The default is 0 (no parallelization), –1 uses all available CPUs, –2 uses all CPUs minus 1.

`backend(`*string*`)` backend used for parallelization. The default is ‘threading’.

`voting` selects voting regression or classification which uses pre-specified weights. By default, voting regression uses equal weights; voting classification uses a majority rule.

General options III

`voteweights(`*numlist*`)` defines positive weights used for voting regression or classification. The length of *numlist* should be the number of base learners – 1. The last weight is calculated to ensure that the sum of weights equals 1.

`sparse` converts predictor matrix to a sparse matrix. This conversion will only lead to speed improvements if the predictor matrix is sufficiently sparse. Not all learners support sparse matrices and not all learners will benefit from sparse matrices in the same way. One can also use the sparse pipeline to use sparse matrices for some learners but not for others.

`printopt` prints the default options for specified learners. Only one learner can be specified. This is for information only; no estimation is done.

`showopt` prints the options passed on to Python.

`showpy` prints Python messages.

`showcoefs` (*new*) shows, for each base learner, the coefficient estimates (in the case of ols, logit, regularized regression) or variable importance measures (random forests and gradient boosting).

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)
```

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

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Stacking weights:
───────────────────────────────────────
  Method               │      Weight
───────────────────────┼───────────────
  gradboost            │      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

We use lasso with cross-validated penalty and display the coefficients using `showcoef`:

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

Stacking weights:
────────────────────────────────────────
  Method           │       Weight
───────────────────┼────────────────────
  lassocv          │       1.0000000
Coefficients lassocv:
─────────────────────────────────────────
  Predictor          │        Value
─────────────────────┼───────────────────
  longitude          │       -8.4494974
  latitude           │       -8.9253902
  houseage           │        1.4741459
  rooms              │       -1.7358155
  bedrooms           │        4.8881583
  population         │       -3.9955915
  households         │        1.3265723
  medinc             │        7.6752298
  _cons              │       20.7432595
```

Demonstration 1: Single base learner

`showcoef` displays variable importance for non-parametric learners (if available).

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

Stacking weights:
─────────────────┬────────────────────
  Method         │      Weight
─────────────────┼────────────────────
  gradboost      │      1.0000000
Variable importance gradboost:
──────────────────┬────────────────────
  Predictor       │      Value
──────────────────┼────────────────────
  longitude       │      0.1429768
  latitude        │      0.1454391
  houseage        │      0.0496290
  rooms           │      0.0034422
  bedrooms        │      0.0217799
  population      │      0.0232365
  households      │      0.0092332
  medinc          │      0.6042632
```

Demonstration 1: Single base learner

Here, we compare lasso with and without the *poly2* pipeline, which creates 2nd-order polynomials and interaction effects:

```
. 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 lassocv lassocv rf gradboost)                      ///
>     pipe3(poly2) cmdopt5(learning_rate(0.01)                       ///
>     n_estimators(1000))

Stacking weights:
---------------------------------------
  Method            |      Weight
--------------------+------------------
  ols               |      0.0000000
  lassocv           |      0.0000000
  lassocv           |      0.0000000
  rf                |      0.8382714
  gradboost         |      0.1617286
```

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          │      0.0000000
  rf               │      0.8382714
  gradboost        │      0.1617286
```

Demonstration 2: Stacking regression

`pystacked` supports alternative final estimators. Here, we select the best-performing individual candidate learner.

```
. set seed 42

. pystacked medh longi-medi if train,                                   ///
>     type(regress)                                                     ///
>     methods(ols lassocv lassocv rf gradboost)                         ///
>     pipe3(poly2) cmdopt5(learning_rate(0.01)                          ///
>     n_estimators(1000)) finalest(singlebest)

Stacking weights:
─────────────────┬────────────────────
  Method         │      Weight
─────────────────┼────────────────────
  ols            │      0.0000000
  lassocv        │      0.0000000
  lassocv        │      0.0000000
  rf             │      1.0000000
  gradboost      │      0.0000000
```

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 `basexb` option:

```
. predict double yhat, xb

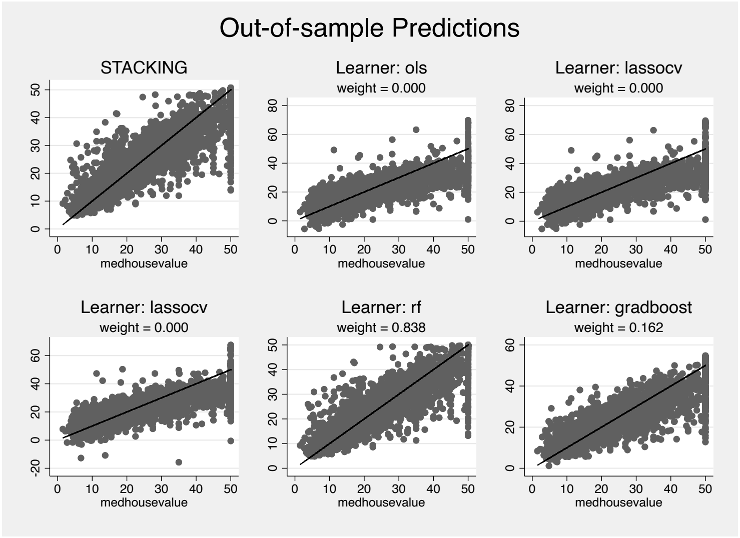
. predict double ybase, basexb

. list yhat ybase* if _n <= 5

     +-----------------------------------------------------------------------+
     |      yhat      ybase1      ybase2      ybase3      ybase4      ybase5 |
     |-----------------------------------------------------------------------|
  1. | 42.875233   41.315834   41.193417    40.02005   43.160831   41.394928 |
  2. | 38.736641    41.45306   41.421459   44.443344   38.289108    41.05629 |
  3. | 40.683311   38.212036   38.154835   37.796288   41.268902   37.648071 |
  4. | 33.559086   32.332497   32.266319   32.546425     33.4869   33.933231 |
  5. | 24.190615   25.382839   25.369064   25.269325   23.859699   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

RMSPE: In-Sample, CV, Holdout
─────────────────┬───────────────────────────────────────────────────────
  Method         │ Weight   In-Sample        CV           Holdout
─────────────────┼───────────────────────────────────────────────────────
  STACKING       │    .         2.313        4.980          4.939
  ols            │ 0.000        6.986        7.008          6.853
  lassocv        │ 0.000        6.987        7.008          6.857
  lassocv        │ 0.000        6.696        6.699          6.606
  rf             │ 0.838        1.847        5.001          4.963
  gradboost      │ 0.162        5.312        5.523          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 and unregularized 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.

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