$h2oml \ postestimation$ — Postestimation tools for h2oml gbm and h2oml rf⁺

⁺This command includes features that are part of StataNow.

Postestimation commands h2omlpredict Remarks and examples References Also see

Postestimation commands

The following postestimation commands are of special interest after h2oml gbm and h2oml rf:

Command	Description
Estimation results and postestimation frame	
h2omlest	store and restore estimation results
h2omlpostestframe	specify frame for postestimation analysis
Tuning and estimation summaries	
h2omlestat metrics	display performance metrics
h2omlgraph scorehistory	produce score history plot
h2omlestat cvsummary	display cross-validation summary
h2omlestat gridsummary	display grid-search summary
h2omlexplore	explore models after grid search
h2omlselect	select model after grid search
h2omlgof	compare goodness of fit for machine learning models
Model performance after binary classification	
h2omlestat threshmetric	display threshold-based metrics
h2omlgraph prcurve	produce precision-recall curve plot
h2omlgraph roc	produce ROC curve plot
Model performance after multiclass classificat	lion
h2omlestat aucmulticlass	display AUC and AUCPR metrics
h2omlestat hitratio	display hit-ratio table
Model performance after binary and multiclass classification	
h2omlestat confmatrix	display confusion matrix
Prediction	
h2omlpredict	predict continuous responses, probabilities, and classes
Model explainability	
h2omlgraph varimp	produce variable importance plot
h2omlgraph pdp	produce partial dependence plot
h2omlgraph ice	produce individual conditional expectation plot
h2omltree	save decision tree DOT file and display rule set
Explainability after regression and binary clas	sification
h2omlgraph shapvalues	produce SHAP values plot for individual observations
h2omlgraph shapsummary	produce SHAP beeswarm plot

h2omlpredict

Description for h2omlpredict

h2omlpredict generates new variables (H2O columns) containing predictions, probabilities, and class predictions. The latter two are provided for the binary and multiclass classification problems.

Menu for h2omlpredict

Statistics > H2O machine learning

Syntax for h2omlpredict

```
After h2oml gbregress and h2oml rfregress
```

h2omlpredict *newvar* [, frame(*framename*)]

After h2oml gbbinclass and h2oml rfbinclass

h2omlpredict *stub** | *newvar* | *newvarlist* [, *binopts* frame(*framename*)]

After h2oml gbmulticlass and h2oml rfmulticlass

h2omlpredict *stub** | *newvar* | *newvarlist* [, *multopts* frame(*framename*)]

binopts	Description
Main	
class	predicted classes
pr	predicted probability of each class
<u>thres</u> hold(#)	specify threshold for predicting classes
multopts	Description
Main	2.000
class	predicted classes
pr	predicted probability of each class
outcome(<i>outcome</i>)	specify outcome level (class) for which probabilities are computed

You specify one or k new variables with pr, where k is the number of outcomes. If you specify one new variable and you do not specify outcome(), then outcome(#1) is assumed.

Options for h2omlpredict

Main

frame (framename) specifies the H2O frame in which predictions are stored.

- class computes class predictions for each observation and is the default. For h2oml gbbinclass and h2oml rfbinclass, the predicted class for each observation is determined based on a threshold value. By default, the threshold is set to maximize the F1 score. Alternatively, a custom threshold can be specified using the threshold() option. For h2oml gbmulticlass and h2oml rfmulticlass, the predicted class for each observation is based on the highest predicted probability. Only one of class or pr is allowed.
- pr computes the predicted probabilities for all outcome levels (classes) or for a specific outcome level (class) after classification. To compute probabilities for all outcome levels, you specify k new variables (H2O columns), where k is the number of classes of the response. Alternatively, you can specify *stub**, in which case pr will store predicted probabilities in variables (H2O columns) *stub1*, *stub2*, ..., *stubk*. To compute the probability for a specific outcome level, you specify one new variable (H2O column) and, optionally, the outcome value in option outcome(); if you omit outcome(), then the first outcome value, outcome(#1), is assumed. Say that you fit a model by typing h2oml *estimation_cmd* y x1 x2, and y has four classes. Then you could type h2omlpredict p1 p2 p3 p4, pr to obtain all four predicted probabilities. To compute specific probabilities one at a time, you can type h2omlpredict p1, pr outcome(#1) (or simply h2omlpredict p1, pr); h2omlpredict p2, pr outcome(#2); and so on. See the outcome() option for other ways to refer to the outcome value. Only one of pr or class is allowed.
- threshold(#) specifies the threshold for predicted classes for binary classification. The specified number should be between [0, 1]. By default, the threshold value that maximizes the F1 metric is used.

outcome(outcome) specifies for which outcome level (class) the predicted probabilities are to be calculated after multiclass classification. outcome() should contain either one class of the response or one of #1, #2, ..., with #1 meaning the first class of the response, #2 meaning the second class, etc. outcome() is not allowed with class. stata.com

Remarks and examples

Remarks and examples are presented under the following headings:

Binary classification prediction Multiclass classification prediction Testing frame prediction Regression prediction

Binary classification prediction

Example 1

In this example, we show how to use the h2omlpredict command to predict probabilities and classes for binary classification.

We start by opening the 1978 automobile data (auto.dta) in Stata and then putting the data into an H2O frame. Recall that h2o init initiates an H2O cluster, _h2oframe put loads the current Stata dataset into an H2O frame, and _h2oframe change makes the specified frame the current H2O frame. For details, see Prepare your data for H2O machine learning in Stata in [H2OML] h2oml and see [H2OML] H2O setup.

```
. use https://www.stata-press.com/data/r18/auto
(1978 automobile data)
. h20 init
 (output omitted)
. _h20frame put, into(auto)
Progress (%): 0 100
. _h20frame change auto
```

We use h2oml rfbinclass to perform random forest binary classification to predict classes of the car origin.

```
. global predictors price mpg length weight
. h2oml rfbinclass foreign $predictors, ntrees(100) h2orseed(19)
Progress (%): 0 40.0 100
Random forest binary classification using H20
Response: foreign
Frame:
                                       Number of observations:
 Training: auto
                                                   Training =
                                                                 74
Model parameters
Number of trees
                    = 100
             actual = 100
Tree depth:
                                      Pred. sampling value =
                                                                  -1
           Input max = 20
                                      Sampling rate =
                                                                .632
                 min =
                       3
                                      No. of bins cat.
                                                           = 1,024
                 avg = 5.5
                                      No. of bins root
                                                           = 1.024
                max =
                                      No. of bins cont.
                                                           =
                                                                  20
                       9
Min. obs. leaf split = 1
                                      Min. split thresh.
                                                           = .00001
Metric summary
           Metric
                      Training
         Log loss
                      .3053323
 Mean class error
                      .1284965
              AUC
                      .9309441
            AUCPR
                      .8455917
 Gini coefficient
                      .8618881
             MSE
                      .1046538
             RMSE
                      .3235024
```

Next we use h2omlpredict to create a new variable (a column in the current H2O frame) containing the predicted classes.

. h2omlpredict foreignhat, class
Progress (%): 0 100

The threshold value is a cutpoint that determines the predicted classes from the predicted probabilities. In binary classification, the threshold is the value that maximizes the F1 score. We can determine this threshold value by using h2omlestat threshmetric.

Maximum or minimum metrics using H2O Training frame: auto Metric Max/Min Threshold F1 .7778 .125 F2 .0732 .8871 F0.5 .7979 .6286 .8649 .6286 Accuracy Precision 1 1 Recall 1 .0732 Specificity 1 1 Min. class accuracy .8269 .2258 .8715 .125 Mean class accuracy 52 True negatives 1 0 .0732 + False negatives 22 .0732 True positives Ο False positives 1 + True-negative rate 1 1 0 .0732 + False-negative rate True-positive rate 1 .0732 False-positive rate 0 1 + MCC .6855 .125

+ identifies minimum metrics.

. h2omlestat threshmetric

The threshold that maximizes the F1 score is 0.125. Thus, the observations with predicted probabilities greater than 0.125 are assigned to the positive class (Foreign in our example), and the remaining observations are assigned to the negative class (Domestic in our example). We can specify a different threshold with the threshold() option. For example, we can select the threshold that maximizes the true-positive rate, which is 0.0732.

. h2omlpredict foreignhat_tpr, class threshold(0.0732)

If we want to obtain predicted probabilities, we can use the pr option.

. h2omlpredict foreignpr1 foreignpr2, pr
Progress (%): 0 100

We can get the predictions and the rest of the data in the H2O frame back into Stata by using the _h2oframe get command.

. clear

. _h2oframe get auto

Multiclass classification prediction

Example 2

In this example, we show how to use the h2omlpredict command to predict probabilities and classes for multiclass classification.

For this example, we will use a well-known iris dataset, where the goal is to predict a class of iris plant. This dataset was used in Fisher (1936) and originally collected by Anderson (1935). We start by initializing a cluster, opening the dataset in Stata, and importing the dataset as an H2O frame. We then use the _h2oframe split command to randomly split the iris frame into a training frame (80% of observations) and a testing frame (20% of observations), which we name train and test, respectively. We also change the current frame to train.

```
. use https://www.stata-press.com/data/r18/iris
(Iris data)
. h2o init
 (output omitted)
. _h2oframe put, into(iris)
Progress (%): 0 100
. _h2oframe split iris, into(train test) split(0.8 0.2) rseed(19)
. h2oframe change train
```

Next, we use h2oml rfmulticlass to perform random forest multiclass classification.

```
. global predictors seplen sepwid petlen petwid
. h2oml rfmulticlass iris $predictors, ntrees(100) h2orseed(19)
Progress (%): 0 100
Random forest multiclass classification using H2O
Response: iris
                                      Number of classes
                                                                  3
                                      Number of observations:
Frame:
                                                  Training =
                                                                125
 Training: train
Model parameters
Number of trees
                    = 100
             actual = 100
                                      Pred. sampling value =
Tree depth:
                                                                 -1
          Input max = 20
                                      Sampling rate =
                                                               .632
                min =
                                     No. of bins cat.
                                                           = 1,024
                       1
                avg = 3.5
                                     No. of bins root = 1.024
                max =
                                     No. of bins cont.
                        8
                                                         =
                                                                 20
                                                           = .00001
Min. obs. leaf split =
                                      Min. split thresh.
                        1
Metric summary
          Metric
                     Training
                      .1282741
         Log loss
 Mean class error
                      .0650407
             MSE
                      .0389344
            RMSE
                       .197318
```

Now, we use h2omlpredict to obtain the predicted classes of the iris plant.

. h2omlpredict irishat, class
Progress (%): 0 100

For multiclass classification, the class is assigned based on the class with the largest predicted probability. We can use the pr option to see the predicted probabilities. The number of specified new variable names should correspond to the number of classes (or we can specify *stub**, such as irispr*).

. h2omlpredict irispr1 irispr2 irispr3, pr
Progress (%): 0 100

By default, the variables (H2O columns) corresponding to the predicted probabilities and classes are created in the current frame, which in our case is train.

Testing frame prediction

Example 3

We continue the previous example and show how to obtain predictions on the testing data. In general, there are two approaches to achieve this goal.

In the first approach, which we recommend, we use the h2omlpostestframe command.

```
. h2omlpostestframe test
(testing frame test is now active for h2oml postestimation)
. h2omlpredict irishat, class
Progress (%): 0 100
```

The above commands generate variable irishat in the frame test.

In the second approach, we use the frame() option.

. h2omlpredict irishat1, class frame(test)

Note that neither approach physically changes the working frame to the specified frame, test.

If we are interested in listing the generated variable, then we can type the following.

```
. _h2oframe change test
. _h2oframe list in 1/5
   iris seplen sepwid petlen petwid irishat irishat1
1 Setosa
         4.7
              3.2
                     1.3
                           .2
                                  Setosa
                                         Setosa
2 Setosa
          5.1
                 3.8
                       1.5
                              .3 Setosa
                                           Setosa
3 Setosa
         5.1
               3.7
                      1.5
                              .4 Setosa Setosa
                              .2 Setosa Setosa
        5.5 4.2
                      1.4
4 Setosa
5 Setosa
         4.9
                3.6
                      1.4
                              .1 Setosa
                                           Setosa
[5 rows x 7 columns]
```

4

Regression prediction

Example 4

In this example, we show how to obtain predictions for regression.

We again use auto.dta.

```
. use https://www.stata-press.com/data/r18/auto
(1978 automobile data)
. h2o init
 (output omitted)
. _h2oframe put, into(auto)
Progress (%): 0 100
. _h2oframe change auto
```

We perform gradient boosting regression to predict prices.

```
. h2oml gbregress price mpg weight length, ntrees(100) h2orseed(19)
Progress (%): 0 100
Gradient boosting regression using H2O
Response: price
Loss:
         Gaussian
Frame:
                                     Number of observations:
 Training: auto
                                                Training =
                                                               74
Model parameters
Number of trees
                 = 100
                                                        =
                                     Learning rate
                                                               .1
             actual = 100
                                     Learning rate decay =
                                                               1
                                     Pred. sampling rate =
Tree depth:
                                                               1
          Input max =
                      5
                                    Sampling rate
                                                      =
                                                               1
                min = 3
                                    No. of bins cat. = 1,024
                avg = 4.1
                                    No. of bins root = 1,024
                                    No. of bins cont. =
                max =
                      5
                                                               20
Min. obs. leaf split = 10
                                    Min. split thresh. = .00001
Metric summary
   Metric
              Training
  Deviance
               1612524
      MSE
               1612524
     RMSE
              1269.852
    RMSLE
              .1750365
```

Then we use h2omlpredict to obtain predictions.

853.3532 .8121031

. h2omlpredict pricehat

Progress (%): 0 100

MAE

R-squared

The new variable (H2O column) pricehat now contains the predicted prices based on our model.

References

Anderson, E. 1935. The irises of the Gaspé Peninsula. Bulletin of the American Iris Society 59: 2-5.

Fisher, R. A. 1936. The use of multiple measurements in taxonomic problems. Annals of Eugenics 7: 179–188. https://doi.org/10.1111/j.1469-1809.1936.tb02137.x.

Also see

[H2OML] h2oml — Introduction to commands for Stata integration with H2O machine learning⁺

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