

A VISUAL GUIDE TO SUPERLEARNING

Katherine Hoffman, MS
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Superlearning, or stacking, weights the results of many individual statistical learning algorithms to create an optimal overall prediction algorithm. Superlearner predictions are expected to perform at least as well as any of the individual learners in large sample sizes.

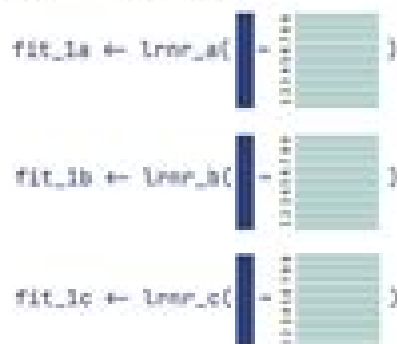
STEP 1

Split data into 10 blocks in preparation for 10-fold cross validation.



STEP 2

Train multiple base learners on 9 of the 10 blocks of data.

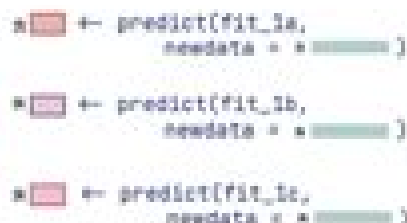


Base learners can include any number of parametric or non-parametric supervised statistical learning algorithms.

An example of three base learners for a binary outcome could be random forest, gradient boosting, and logistic regression.

STEP 3

Obtain predictions from each base learner for the held-out block of data.



STEP 4

Repeat until each of the 10 blocks have served as the hold-out data and you have three sets of cross-validated predictions spanning the full data set.



STEP 5

Using a new learner, a metalearner, predict the outcome using the three sets of cross-validated predictions.



The metalearner can be as simple as a generalized linear model. As with any statistical learning algorithms, the choice reflects a loss function we want to minimize.

STEP 6

Fit the base learners on the entire data set.



STEP 7

Obtain predictions from the full data set for each learner.



STEP 8

Use the coefficients from Step 5 to weight the full data predictions from Step 7. These are the final superlearner predictions.



The final superlearner predictions are a weighted combination, or ensemble, of the base learners' predictions.

STEP 9

To predict on new data, use the base learner fits to obtain base learner predictions (similar to Step 7), then input the base learner predictions into the metalearner fit (similar to Step 8) to obtain the final prediction.

EVALUATION

To test the prediction capability of the superlearner algorithm and prevent overfitting, the entire algorithm (Steps 1-8) could be cross-validated.

APPLICATION

There are several R packages to implement superlearning. This example uses the SuperLearner package to create a superlearner model for a binary outcome with three learners: gradient boosting (xgboost), random forest (ranger), and logistic regression (glm) with a loss function/ metalearning step of negative log-likelihood (method="NNLoglik"):

```
SL_fit <- SuperLearner(
  # outcome variable
  family=binomial(),
  SL.library = c("SL.xgboost",
                 "SL.ranger",
                 "SL.glm"),
  method = "NNLoglik")
```

REFERENCES

Targeted Learning, Chapter 3: Superlearning by Eric Polley, Sherri Rose, and Mark van der Laan.

For a step-by-step tutorial with R code, explanations, and more references: www.khstats.com/blog/10/superlearning.

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