

Super Learners

Machine Learning

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Agenda

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Recap

- Queremos predecir y en función de observables (\mathbf{x}_i)

$$y = f(\mathbf{x}_i) + u \quad (1)$$

- donde la estimación de f implica la que mejor generalize (prediga mejor fuera de muestra):

$$\hat{f} = \underset{f}{\operatorname{argmin}} \left\{ \sum_{i=1}^n L(y_i, f(\mathbf{x}_i; \Theta)) \right\} \quad (2)$$

Superlearners: Motivation

- ▶ Superlearning is a technique for prediction that involves combining many individual statistical algorithms to create a new, single prediction algorithm that is expected to perform at least as well as any of the individual algorithms.
- ▶ The innovation?

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- ▶ The innovation?
- ▶ The superlearner algorithm “decides” how to combine, or weight, the individual algorithms based upon how well each one minimizes a specified loss function
- ▶ The motivation for this type of “ensembling” is that a mix of multiple algorithms may be more optimal for a given data set than any single algorithm.
- ▶ For example, a tree based model averaged with a linear model (e.g. random forests and LASSO) could smooth some of the model’s edges to improve predictive performance.

Superlearners: Algorithm

Denote the library \mathcal{L} and its cardinality as $V(n)$.

- 1 Fit each algorithm in \mathcal{L} on the entire data set $X = \{X_i : i = 1, \dots, n\}$ to estimate $f_v(X)$ with $v = 1, \dots, V(n)$

Superlearners: Algorithm

- 2 Split the data set X into a training and validation sample, according to a K-fold cross-validation scheme:

Superlearners: Algorithm

- 3 For the k th fold, fit each algorithm in \mathcal{L} on $T(k)$ and save the predictions on the corresponding test, $\hat{f}_{k,T}(X_i)$ with $X \in Te(k)$

Superlearners: Algorithm

- 4 Bind the predictions from each algorithm together to create a n by V matrix

Superlearners: Algorithm

- 5 Propose a family of weighted combinations of the candidate estimators indexed by weight-vector α :

Superlearners: Algorithm

- 6 Determine the α that minimizes the cross-validated risk of the candidate estimator $\sum_{v=1}^V \alpha_v \hat{f}(X_i)$ over all allowed α -combinations:

Superlearners: Algorithm

- 7 Combine $\hat{\alpha}_v$ with $\hat{f}_v(X_i)$ according to the weights found, and create the final super learner fit

Superlearners: Algorithm

Some considerations:

- ▶ The super learner theory does not place any restrictions on the family of weighted combinations used for ensembling the algorithms in the library.
- ▶ The restriction of the parameter space for α to be the convex combination of the algorithms in the library provides greater stability of the final super learner prediction.

Example: Superlearners



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