## Super Learning (SL) and sl3

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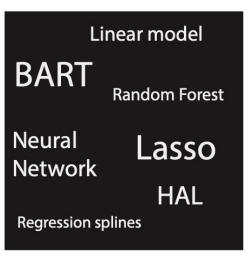
JSM 2023



#### Overview of Super Learner



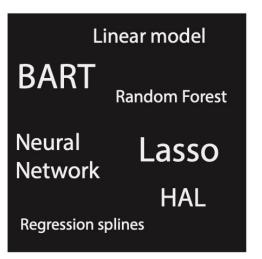
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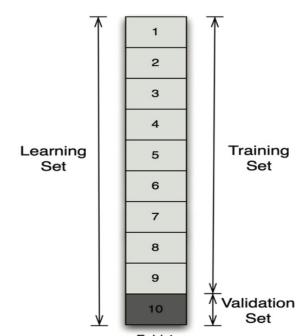


#### LIBRARY

#### COMPETITION

Cross-validated performance of learners + ensembles





LIBRARY

#### COMPETITION

**WINNER** 

Cross-validated performance of learners + ensembles

Linear model

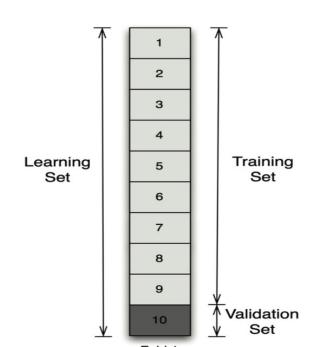
BART

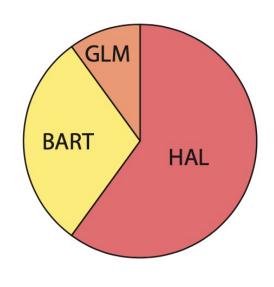
Random Forest

Neural
Network

HAL

Regression splines





- Uses a library of algorithms for estimating a prediction function
  - Analyst specifies Alg<sub>1</sub>, ... Alg<sub>K</sub>
  - Create an optimal combination
    - Optimal with respect to V-fold cross-validated (CV) risk
    - Example risk functions: Negative log likelihood, mean squared error, 1-AUC
- SL predicted values,  $\hat{Y}_{SL}$ , are a combination of  $\hat{Y}_{Alg_1}$ , ...,  $\hat{Y}_{Alg_K}$ 
  - Discrete SL: "winner-take-all", predictions from algorithm with best CV risk
  - Ensemble SL: predictions from multiple algorithms are combined
    - weighted combination
    - some other, possibly complex function of the algorithms' predictions



#### Why super learner (SL)?

- No need to select the one "right" strategy
- Can consider diverse set
- Grounded in statistical optimality theory
- Pre-specified also flexible
- Mitigate statistical model misspecification
- Good initial estimation for estimators common for causal inference (e.g., AIPW, TMLE)



## What does user specify for SL?

- a) Measure of performance
- b) Cross-validation scheme
- c) Diverse library of candidate learners



## Super learner

#### 1. Specify

- a) Measure of performance
- b) Cross-validation scheme
- c) Diverse library of candidate learners

What are you learning from the data? What do you want to optimize for?

Performance measure should be valid (i.e., optimized by underlying target), bounded, corresponds to desired goal

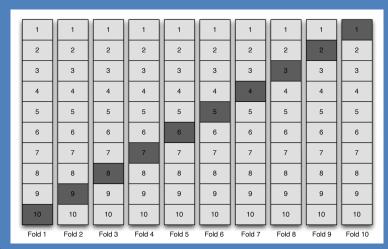


#### Super learner

#### 1. Specify

- a) Measure of performance
- b) Cross-validation scheme -
- c) Diverse library of candidate learners

#### e.g. V-fold cross-validation

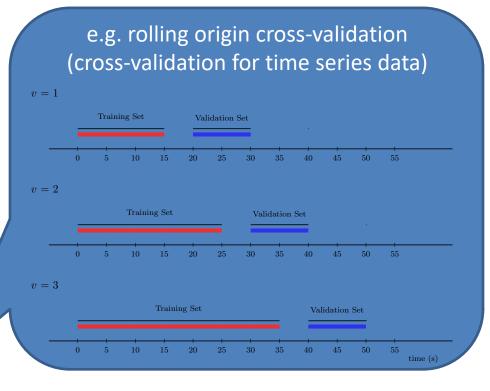




## Super learner

#### 1. Specify

- a) Measure of performand
- b) Cross-validation scheme
- c) Diverse library of candidate learners





### Overview of the algorithm

- 1. Make metalevel dataset with cross-validated candidate predictions and validation set outcomes
- 2. Fit meta-learner to the metalevel dataset
- 3. Full-fit candidates
- 4. Define the SL

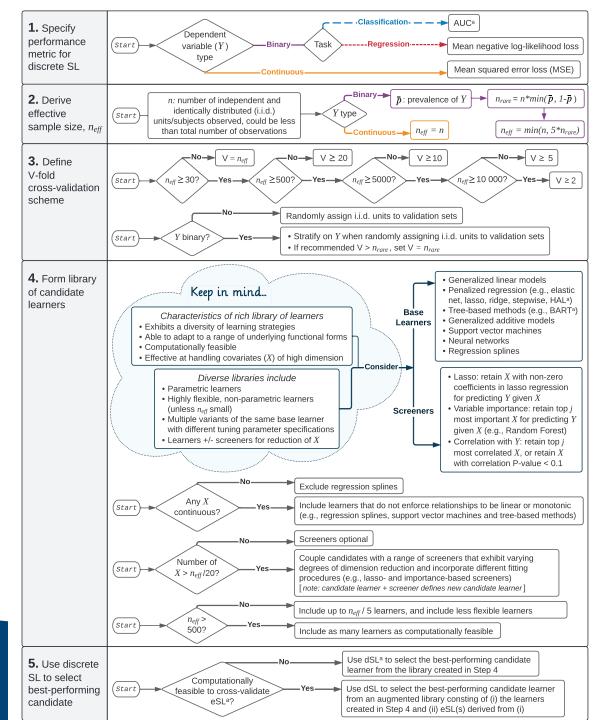


# Practical considerations for specifying SL

Rachael V Phillips, Mark J van der Laan, Hana Lee, Susan Gruber, Practical considerations for specifying a super learner, *International Journal of Epidemiology*, 2023.

https://doi.org/10.1093/ije/dyad023





# Sl software package in tlverse



## Introductory overview of sl3

- Task
- Learners
- Functions



## Introductory overview of sl3

- Task
- Learners
- Functions



#### Tasks in sl3

What is the prediction task? data, covariates, outcome, weights, id, outcome\_type,offset, drop\_missing\_outcome, folds

https://tlverse.org/sl3/reference/sl3\_Task.html



## Introductory overview of sl3

- Task
- Learners
- Functions



## Exercise: Training learner with sl3 wrapper versus package's function

- Prediction tasks in sl3
- Comparison of R6 methods and S3 methods
  - sl3 R package function, Lrnr\_earth
  - earth R package function, earth
- Looking up learners, the sl3 wrapper, and arguments
- Modifying learner parameters
- Data example: Collaborative Perinatal Project (CPP) was a multisite prospective cohort study designed to identify the effects of complications during either pregnancy or the perinatal period on birth and child outcomes.





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Other Learners: Lrnr_HarmonicReg, Lrnr_arima, Lrnr_bartMachine, Lrnr_base,
Lrnr_bayesglm, Lrnr_bilstm, Lrnr_caret, Lrnr_cv_selector, Lrnr_cv, Lrnr_dbarts,
Lrnr_define_interactions, Lrnr_density_discretize, Lrnr_density_hse,
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Lrnr_gbm, Lrnr_glm_fast, Lrnr_glmnet, Lrnr_glm, Lrnr_grf, Lrnr_gru_keras, Lrnr_gts,
Lrnr_h2o_grid, Lrnr_hal9001, Lrnr_haldensify, Lrnr_hts, Lrnr_independent_binomial,
Lrnr_lightgbm, Lrnr_lstm_keras, Lrnr_mean, Lrnr_multiple_ts, Lrnr_multivariate,
Lrnr_nnet, Lrnr_nnls, Lrnr_optim, Lrnr_pca, Lrnr_pkg_SuperLearner, Lrnr_polspline,
Lrnr_pooled_hazards, Lrnr_randomForest, Lrnr_ranger, Lrnr_revere_task, Lrnr_rpart,
Lrnr_rugarch, Lrnr_screener_augment, Lrnr_screener_coefs,
Lrnr_screener_correlation, Lrnr_screener_importance, Lrnr_sl, Lrnr_solnp_density,
Lrnr_solnp, Lrnr_stratified, Lrnr_subset_covariates, Lrnr_svm, Lrnr_tsDyn,
Lrnr_ts_weights, Lrnr_xgboost, Pipeline, Stack, define_h2o_X(),
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```



## Introductory overview of sl3

- Task
- Learners
- Other functions



#### Other sl<sub>3</sub> Functions

- Performance measures:
  - loss functions (e.g., squared error, negative loglikelihood, multinomial log-likelihood)
  - metrics based on ROCR software package, like AUC,
     AUCPR, accuracy, sensitivity, with custom\_ROCR\_risk()
- Variable importance with importance
- Table with each candidate learner's cross-validated predictive performance with cv\_risk
- Cross-validated SL (to see CV risk of SL itself) with cv\_sl



# Live coding exercise with sl3 using WASH Benefits data



#### WASH Benefits Bangladesh

- Study aiming to understand the impact of water quality, sanitation, hand washing, and nutritional (WASH) interventions on child development in rural Bangladesh (WASH Benefits Bangladesh): a cluster randomized controlled trial (Tofail et al. 2018)
- Enrolled pregnant women in first or second trimester from the rural villages of Bangladesh



#### WASH Benefits Bangladesh: Example Dataset for sl<sub>3</sub> Prediction

- We concentrate on child growth (size for age) as the outcome of interest.
- We will use SL (sl3 software) to estimate the prediction function for predicting a child's weightfor-height z-score (whz) given covariate information.
- Next section on TMLE (tmle3 software) focuses on estimation of the (causal) impact of particular intervention on an outcome (e.g., the impact of the WASH intervention on whz)



## Exercise: Training a super learner with sl3

https://tlverse.org/tlverse-handbook/sl3.html

http://tlverse.org/jsm2023-workshop/sl3.html

