

Super Learning (SL) and sl3

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ENAR 2023

Overview of Super Learner

Super Learner (SL)

LIBRARY

Linear model

BART

Random Forest

Neural
Network

Lasso

HAL

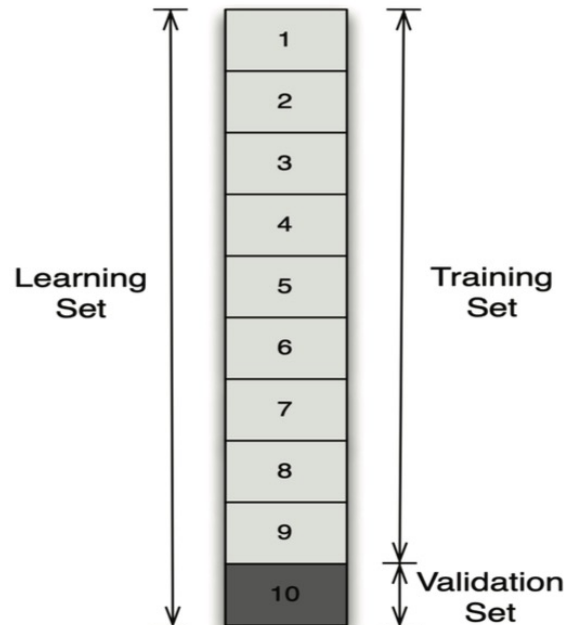
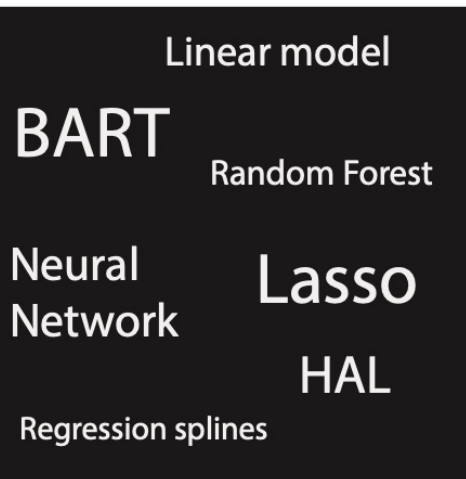
Regression splines

Super Learner (SL)

LIBRARY

COMPETITION

Cross-validated
performance of
learners + ensembles



Super Learner (SL)

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COMPETITION

WINNER

Cross-validated
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Linear model

BART

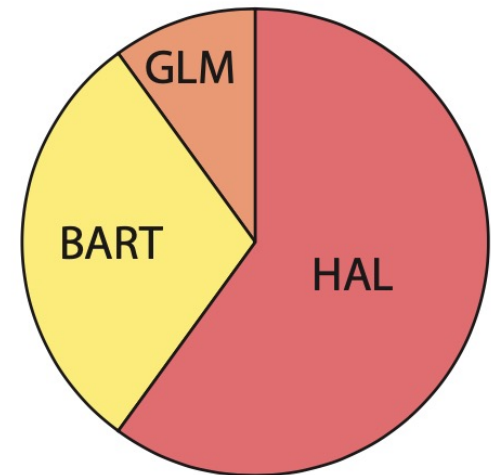
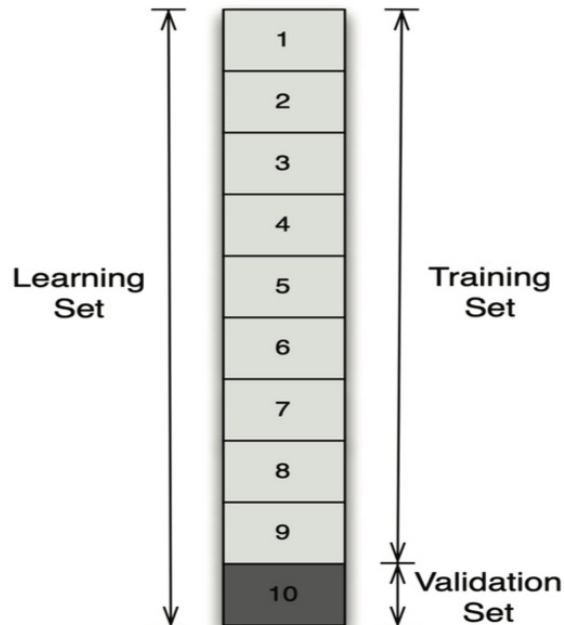
Random Forest

Neural
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Regression splines



Super Learner (SL)

- Uses a library of algorithms for estimating a prediction function
 - Analyst specifies Alg_1, \dots, Alg_K
 - 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 $\hat{Y}_{Alg_1}, \dots, \hat{Y}_{Alg_K}$
 - 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

Defining prediction problem for estimation

Defining prediction problem for estimation

- A performance metric quantifies the success of an estimated prediction function (i.e., a trained algorithm)
 - Expectation of the squared error loss / MSE
 - The area under the ROC curve, AUC

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- The chosen metric needs to be optimized (minimized or maximized) by the true prediction function
 - **This guarantees that the evaluation corresponds to the trained algorithm's success in approximating the true prediction function**

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- The chosen metric should align with the intended real-world use of the 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

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

1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	2
3	3	3	3	3	3	3	3	3	3
4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	6
7	7	7	7	7	7	7	7	7	7
8	8	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9
10	10	10	10	10	10	10	10	10	10
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Fold 6	Fold 7	Fold 8	Fold 9	Fold 10

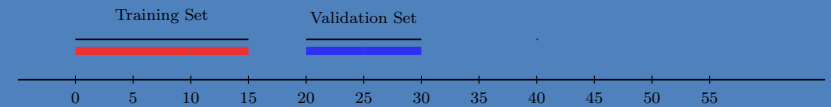
Super learner

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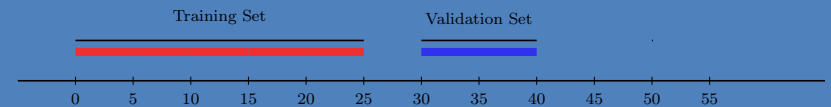
- Measure of performance
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- Diverse library of candidate learners

e.g. rolling origin cross-validation
(cross-validation for time series data)

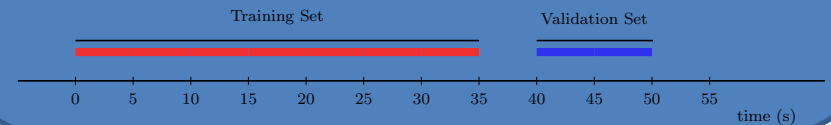
$v = 1$



$v = 2$



$v = 3$

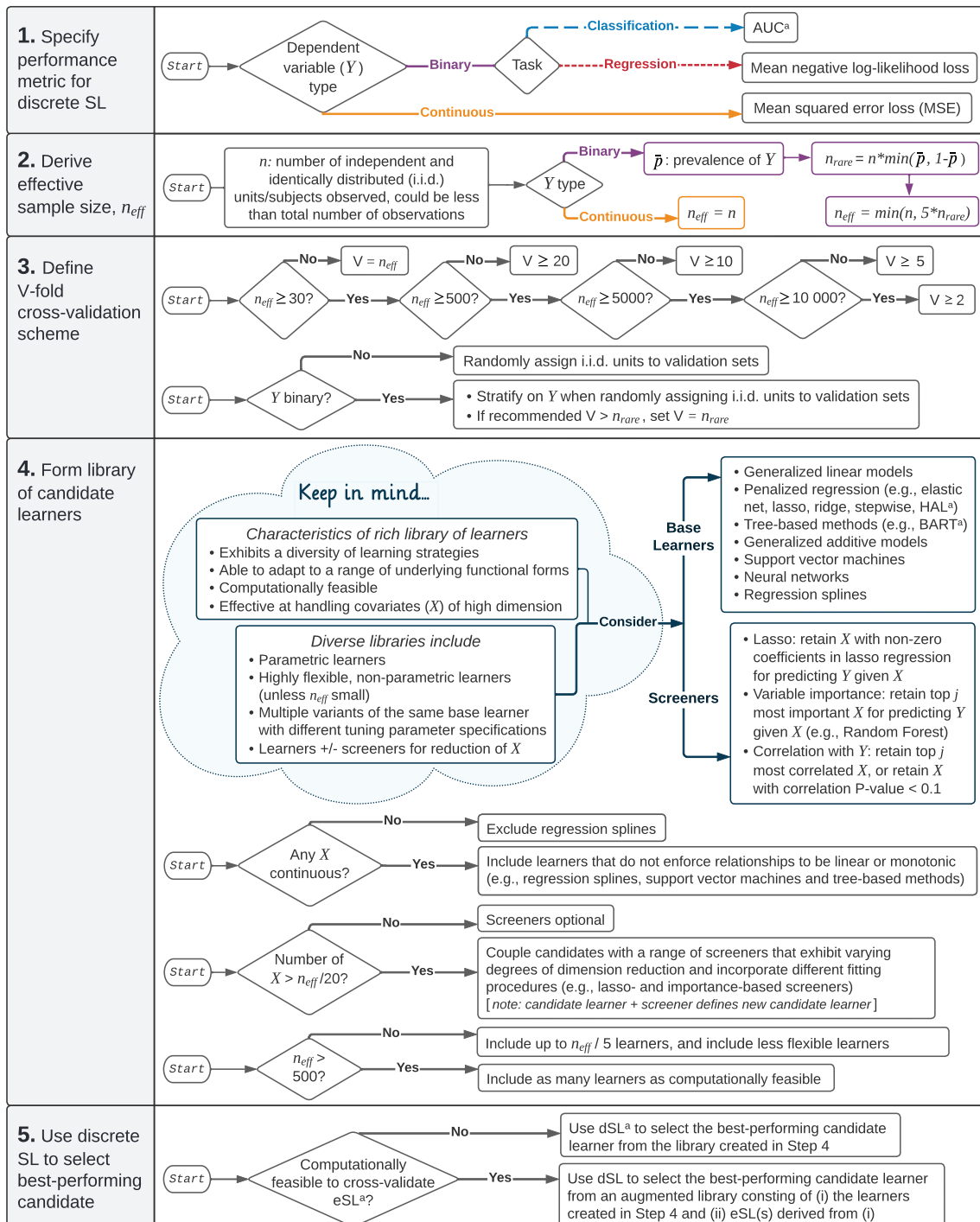


Overview of the algorithm

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>



sl3

SL software package in tlverse

Introductory overview of s13

- Task
- Learners
- Functions

Introductory overview of s13

- Task
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- 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 s13

- Task
- **Learners**
- Functions

Learners in sl3

How to estimate prediction function?

Exercise: Training learner with `s13` wrapper versus package's function

- Prediction tasks in `s13`
- Comparison of R6 methods and S3 methods
 - `s13` R package function, `Lrnr_earth`
 - `earth` R package function, `earth`
- Looking up learners, the `s13` 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.

Learners in sl3

How to estimate prediction function?

Other Learners: `Lrnr_HarmonicReg`, `Lrnr_arima`, `Lrnr_bartMachine`, `Lrnr_base`,
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A diagram with red lines connecting five circled learner names to a box labeled 'Stack'. The circled names are Lrnr_caret, Lrnr_glm, Lrnr_gam, Lrnr_ranger, and Lrnr_ts_weights. The 'Stack' box is highlighted with an orange border.

Learners in sl3

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Learners in sl3


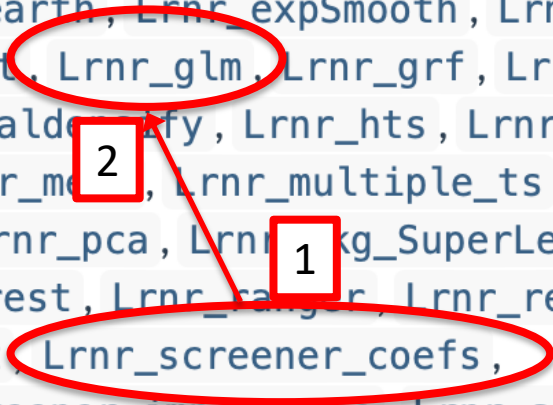
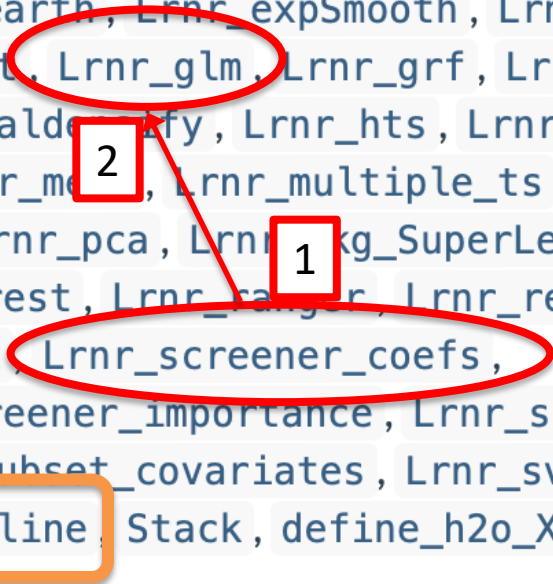
How to estimate prediction function?

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, Lrnr_density_semiparametric, Lrnr_earth, Lrnr_expSmooth, Lrnr_gam, Lrnr_ga, 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(),

Learners in sl3

How to estimate prediction function?

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, Lrnr_density_semiparametric, Lrnr_earth, Lrnr_expSmooth, Lrnr_gam, Lrnr_ga, Lrnr_gbm, Lrnr_glm_fast, Lrnr_glmnet, Lrnr_glm, Lrnr_grf, Lrnr_gru_keras, Lrnr_gts, Lrnr_h2o_grid, Lrnr_hal9001, Lrnr_halder, Lrnr_hf, Lrnr_hsts, Lrnr_independent_binomial, Lrnr_lightgbm, Lrnr_lstm_keras, Lrnr_m, Lrnr_multiple_ts, Lrnr_multivariate, Lrnr_nnet, Lrnr_nnls, Lrnr_optim, Lrnr_pca, Lrnr_pkg_SuperLearner, Lrnr_polspline, Lrnr_pooled_hazards, Lrnr_randomForest, Lrnr_sanger, 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(),



Introductory overview of s13

- Task
- Learners
- **Other functions**

Other `sl3` Functions

- Performance measures:
 - loss functions (e.g., squared error, negative log-likelihood, 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 with `cv_sl`

Live coding exercise with sl3 using WASH Benefits data

WASH Benefits Bangladesh

Example Dataset

- Study aiming to understand the effect of water quality, sanitation, hand washing, and nutritional interventions on child development in rural Bangladesh (WASH Benefits Bangladesh): a cluster randomized controlled trial (Tofail et al. [2018](#)).
- Enrolled pregnant women in their first or second trimester from the rural villages of Gazipur, Kishoreganj, Mymensingh, and Tangail districts of central Bangladesh, with an average of 8 women per cluster.

WASH Benefits Bangladesh

Example Dataset

- Six intervention groups:
 - chlorinated drinking water;
 - improved sanitation;
 - hand-washing with soap;
 - combined water, sanitation, and hand washing;
 - improved nutrition through counseling and provision of lipid-based nutrient supplements; and
 - combined water, sanitation, handwashing, and nutrition.
- We concentrate on child growth (size for age) as the outcome of interest.

Exercise: Training a super learner with sl3

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

<http://tlverse.org/enar2023-workshop/sl3.html>