LONDON SCHOOL of HYGIENE &TROPICAL MEDICINE

Super Learner

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*based on Prof Karla Diaz-Ordaz's 2021 materials

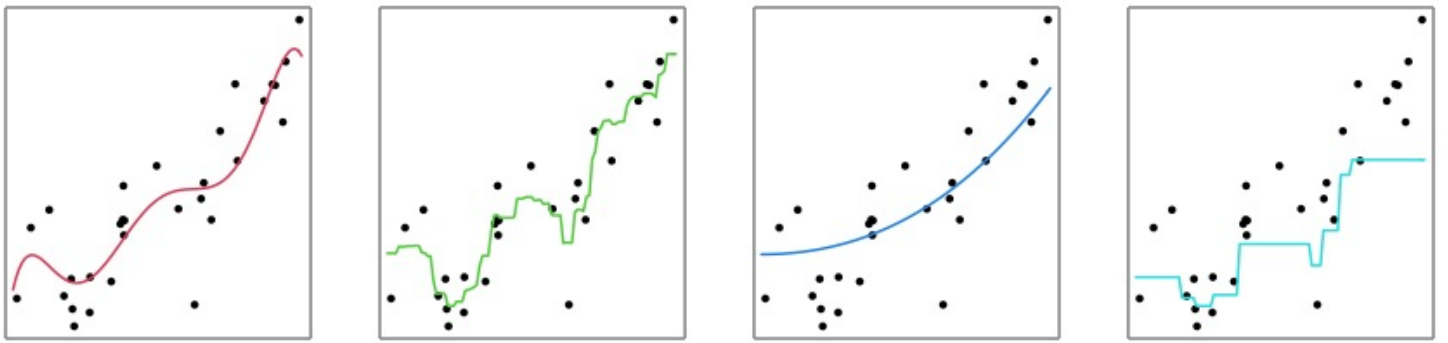
Learning Outcomes

After completing today's session, you will

- understand the basic idea of Super Learner (SL)
- understand the 3 important choices to be made for using SL
- be able to apply SL in a practical example
- know how to use cross-validation to measure the performance of a SL

Motivation

- You have experience with a wide library of prediction models (learners):



- Your collaborators/colleagues may have many more!
- For a given application, there may be several candidate learners
- How might you choose between the candidates?

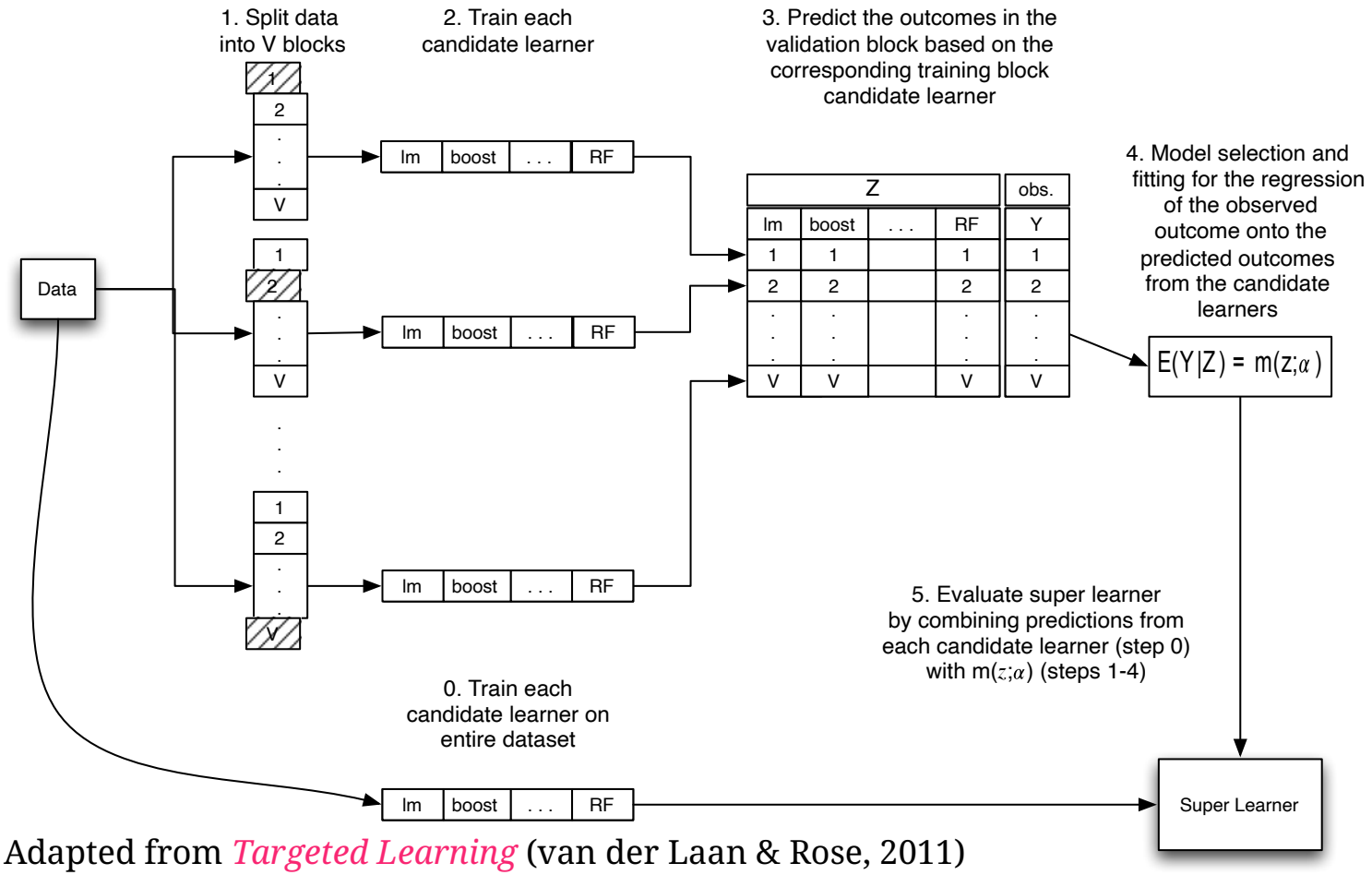
Super Learner: a bird's eye view

The **Super Learner** is a meta-learning algorithm that

- Takes the data and a library $\mathcal{L}$ of L candidate learners as inputs
- Estimates performance of each learner using V-fold cross-validation
- Creates an optimal ensemble $m(Z; \boldsymbol{\alpha})$ of the learners

- The ensemble $m(Z; \boldsymbol{\alpha})$ offers a reproducible way to choose from (or combine) predictions from the candidate learners
- Super Learner ensembles also possess desirable (large sample) guarantees

Super Learner: a bird's eye view



Adapted from *Targeted Learning* (van der Laan & Rose, 2011)

What makes a Super Learner?

Before we can follow the steps from above, we must specify

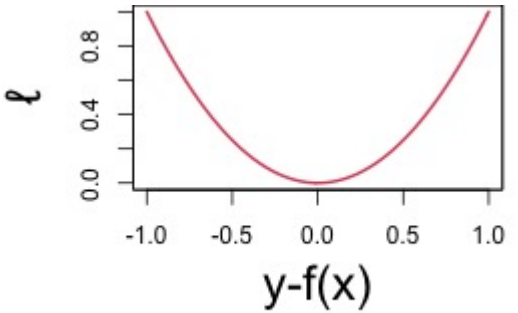
1. The library $\mathcal{L}$ of candidate learners
2. A loss function ℓ to measure performance
3. Form of the meta-learner $m(Z; \alpha)$

Library

- Common algorithms to consider
  - Linear regression
  - Polynomial linear regression
  - Random forest
  - Bagging
  - GAMs
  - Gradient boosting
  - Neural network
  - Polynomial spline regression
- Select the learner algorithms using contextual knowledge of the problem
- If a custom-made algorithm (eg a clinical prediction model) is known to perform well, include it!
- It is recommended to include a parametric model

Loss function

- The loss function is often the squared error loss $\ell = (Y - f(X))^2$



- For binary outcomes where $Y = 0, 1$:
  - Negative binomial log likelihood
  - Rank loss function: maximises the area under the ROC curve (a function of both sensitivity and specificity), thus optimizing the algorithms ability to correctly classify observations.

Meta-regression model

- We often use non-negative least squares (NNLS)

$$E[Y|X = x] = \alpha_1 \hat{f}_1(x) + \ldots + \alpha_L \hat{f}_L(x)$$

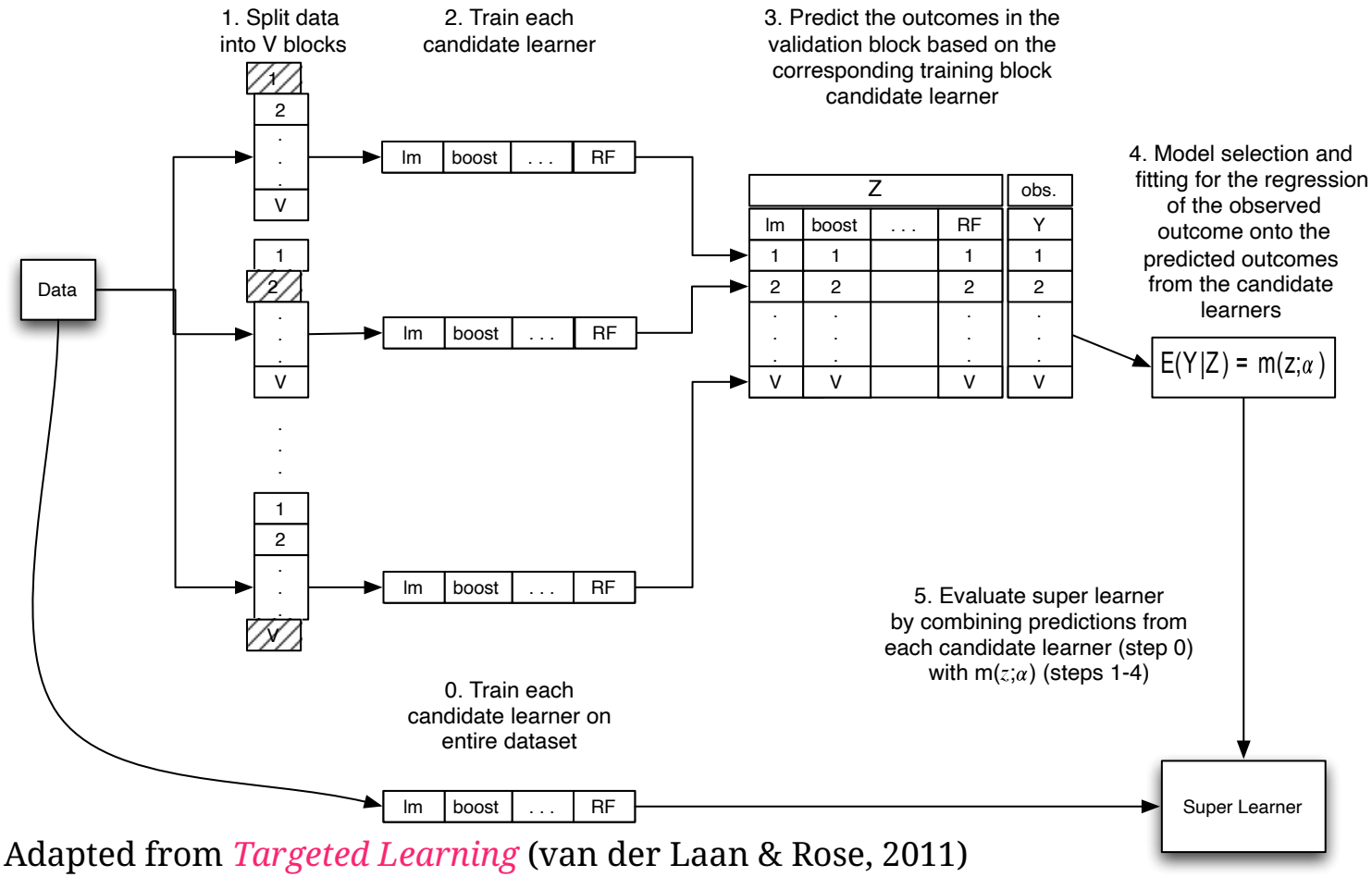
- In NNLS, $\alpha_l \geq 0$ and $\sum_{l=1}^{L} \alpha_l = 1$
- Thus $m(Z_i; \alpha)$ is a convex combination of the learners in $\mathcal{L}$ with weights α chosen to minimise the CV risk of SL:

$$\hat{\alpha} = \arg\min_{\alpha} \sum_i (Y_i - m(Z_i; \alpha))^2$$

- We obtain a **discrete super learner** by instead placing all the weight on the learner $\hat{f}_l$ that performs best using V-fold CV

Super Learner in R

Super Learner: a bird's eye view



Adapted from *Targeted Learning* (van der Laan & Rose, 2011)

Super Learner in R

- You will need the `SuperLearner` package installed for the practical:

```
SL_installed <- require(SuperLearner)

if(!SL_installed) install.packages("SuperLearner")

library(SuperLearner)
```

The SuperLearner function

- The main function in `SuperLearner` is itself called `SuperLearner`:

```
args(SuperLearner)
```

```
## function (Y, X, newX = NULL, family = gaussian(), SL.library,
##     method = "method.NNLS", id = NULL, verbose = FALSE, control = list(),
##     cvControl = list(), obsWeights = NULL, env = parent.frame())
## NULL
```

Key arguments for customising your Super Learner:

- `SL.library`: character vector of learners (this is $\mathcal{L}$)
- `method`: method to estimate meta-learner (based on ℓ and $m(Z|\alpha)$)
- Enter `?SuperLearner` in your console for more details

Note: when coding learners for your $\mathcal{L}$...

- `SuperLearner` uses a standard interface to automate training/prediction
- This is achieved via wrapper functions that follow this template:

```
SuperLearner::SL.template
```

```
## function (Y, X, newX, family, obsWeights, id, ...)
## {
##     if (family$family == "gaussian") {
##     }
##     if (family$family == "binomial") {
##     }
##     pred <- numeric()
##     fit <- vector("list", length = 0)
##     class(fit) <- c("SL.template")
##     out <- list(pred = pred, fit = fit)
##     return(out)
## }
## <bytecode: 0x7fc0bbaece80>
## <environment: namespace:SuperLearner>
```

Built-in wrappers

- You **might** be able to use a built-in wrapper for your learner

```
listWrappers("SL")
```

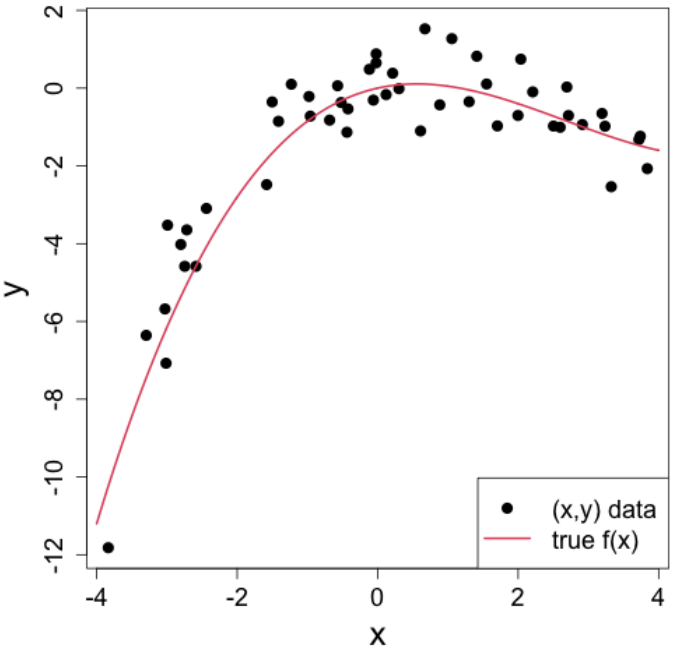
```
## All prediction algorithm wrappers in SuperLearner:

##  [1] "SL.bartMachine"      "SL.bayesglm"         "SL.biglasso"
##  [4] "SL.caret"            "SL.caret.rpart"      "SL.cforest"
##  [7] "SL.earth"            "SL.extraTrees"       "SL.gam"
## [10] "SL.gbm"              "SL.glm"              "SL.glm.interaction"
## [13] "SL.glmnet"           "SL.ipredbagg"        "SL.kernelKnn"
## [16] "SL.knn"              "SL.ksvm"             "SL.lda"
## [19] "SL.leekasso"         "SL.lm"               "SL.loess"
## [22] "SL.logreg"           "SL.mean"             "SL.nnet"
## [25] "SL.nnls"             "SL.polymars"         "SL.qda"
## [28] "SL.randomForest"     "SL.ranger"           "SL.ridge"
## [31] "SL.rpart"            "SL.rpartPrune"       "SL.speedglm"
## [34] "SL.speedlm"          "SL.step"             "SL.step.forward"
## [37] "SL.step.interaction" "SL.stepAIC"          "SL.svm"
## [40] "SL.template"         "SL.xgboost"
```

Example: a univariate Super Learner

Generating some data:

```
set.seed(2490) #reproducible
n <- 50
x <- runif(n, min=-4, max=4)
f <- function(x)
     {
       .4*x-.4*x^2+.05*x^3
     }
y <- f(x) + rnorm(n)
```

The data and (unknown) regression:



- Let's use GLM and random forest with the NNLS meta-learner

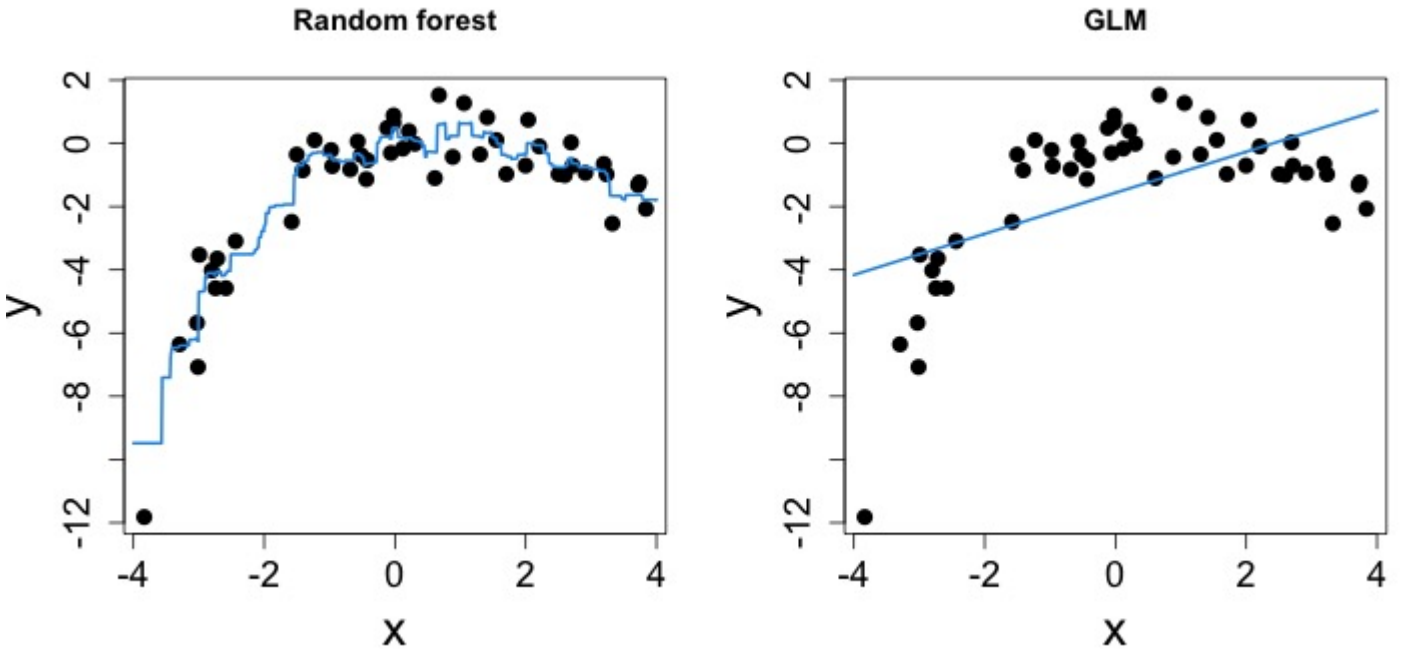
```
my.lib <- c("SL.randomForest", "SL.glm")

fit <- SuperLearner(Y = y, X = data.frame(x),
                    newX = data.frame(x=x0),
                    SL.library = my.lib,
                    method = "method.NNLS",
                    cvControl = list(V=5L),
                    control = list(saveCVFitLibrary=TRUE))
```

```
## Loading required namespace: randomForest
```

```
SL.pred <- fit$SL.predict
```

Step 0. fit each learner in $\mathcal{L}$ on all data

The $L \times n$ matrix of full-data predictions is stored as `fit$library.predict`



Step 1. Split the data into $V = 5$ blocks

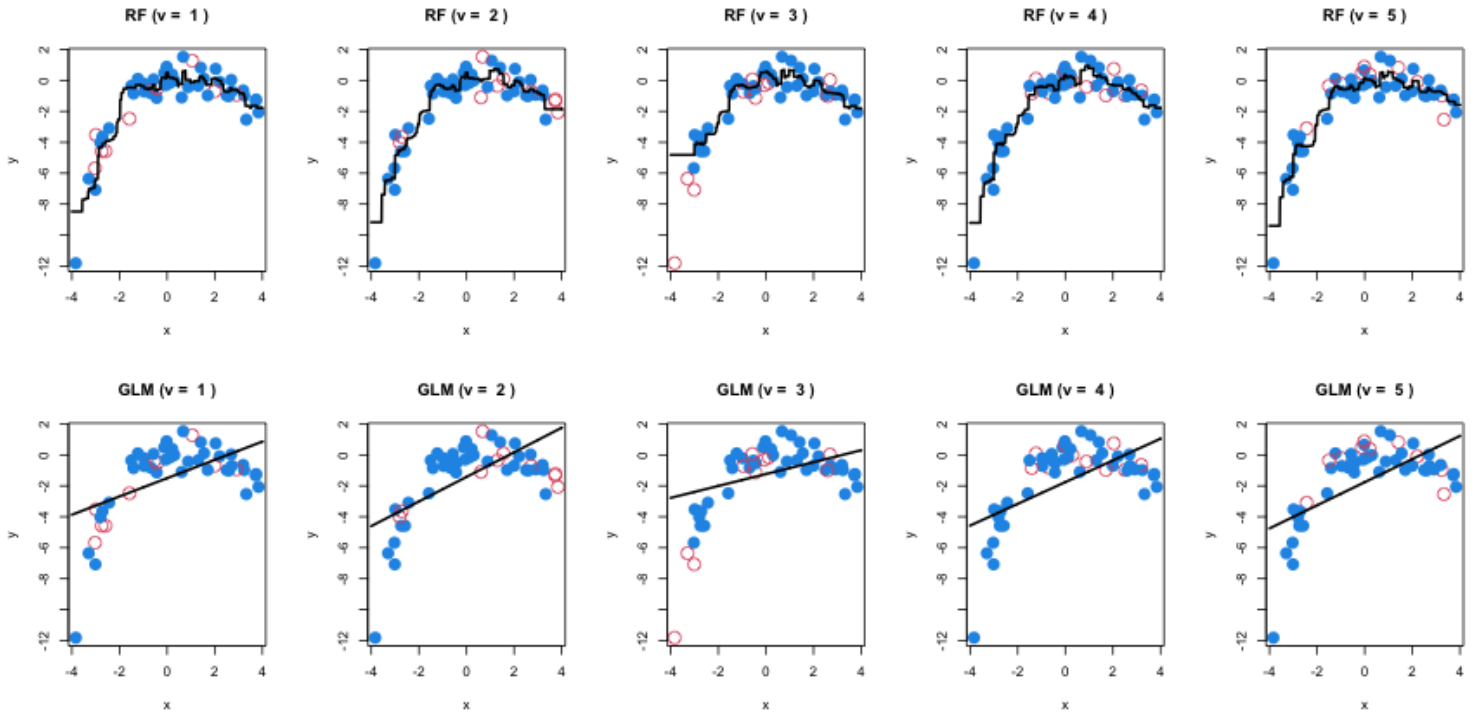
The row numbers for the V-fold cross-validation are stored as a list

```
fit$validRows #think "valid-ation sets 1-5"
```

```
## $`1`
##  [1] 31 35 44 20 22 13 42 25 11 18
##
## $`2`
##  [1] 39 28 40 15 24  4 45 49 37  6
##
## $`3`
##  [1] 21 26 47  7 36 43  9 27 14 29
##
## $`4`
##  [1] 19 30 48  1 50  3 34 12 10 32
##
## $`5`
##  [1]  8 46 17  2  5 38 33 23 41 16
```

Steps 2-3. Train each learner, then predict

Recall that we do this $L \times V$ times (train on $V - 1$ folds, predict on last fold)



(We plot training sets as solid blue, test sets as empty red)

Step 3. Fit the meta-learner

- The $n \times L$ matrix of fitted values on the training data are stored in `fit$Z`
  - Remember each data point is belongs to **exactly one** validation set!

```
head(fit$Z)
```

```
##              [,1]       [,2]
## [1,] -0.31717312 -2.2417058
## [2,] -0.80226697  0.6553930
## [3,] -1.24058623  0.4831672
## [4,] -1.86230006  1.5361682
## [5,] -0.03448410 -0.1135900
## [6,] -0.06711427 -0.9365990
```

- The coefficient vector from NNLS is available as `fit$coef`

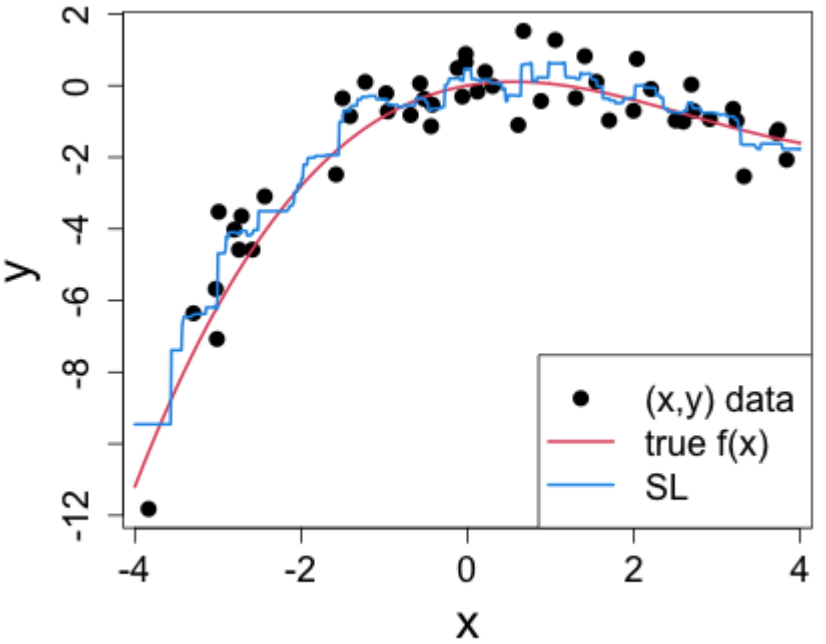
```
fit$coef
```

```
## SL.randomForest_All          SL.glm_All
##         0.994654219        0.005345781
```

- Here, most of the weight is placed on random forest

Step 4. Predict on new data

- Predictions for `newX` are at `fit$SL.predict`



Your turn to practice!

... Super Learner will return in part 2