

# Using the **SuperLearner** R Package

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## OUTLINE

- ① SuperLearner
- ② Boston Housing
- ③ ALL data
- ④ van't Veer data

# SUPERLEARNER

The package is available at:

<https://github.com/ecpolley/SuperLearner>

These slides are available in the package and at:

<https://github.com/ecpolley/>

Need to install R packages **nnls** and **quadprog** before installing **SuperLearner**.

# SUPERLEARNER

**Table:** Main functions in the **SuperLearner** package

Function	Description
<code>SuperLearner</code>	fits super learner
<code>CV.SuperLearner</code>	cross-validate in super learner
<code>listWrappers</code>	returns list of wrappers in package
<code>write.SL.template</code>	prediction wrapper template
<code>write.screen.template</code>	screening wrapper template
<code>write.method.template</code>	method wrapper template

# SUPERLEARNER

## SuperLearner

```
fitSL <- SuperLearner(Y = Y,  
                      X = X,  
                      SL.library = c('SL.glm'),  
                      family = gaussian(),  
                      method = 'method.NNLS',  
                      verbose = TRUE,  
                      cvControl = list(V = 10))
```

## SUPERLEARNER

**Table:** Main arguments for SuperLearner

Name	Description	Req.	Default
Y	outcome	Y	–
X	data.frame for fit	Y	–
newX	data.frame for predict	N	x
SL.library	library of algorithms	Y	–
cvControl	list for CV control	N	–
control	optional controls	N	–
verbose	detailed report	N	FALSE
family	error distribution	N	gaussian
method	loss function & model	N	NNLS
id	cluster id	N	–
obsWeights	observations weights	N	–

## SUPERLEARNER

- $Y$  and  $X$  are the data used to fit each algorithm (the learning data)
- $newX$  is not required but can be a helpful shortcut.  
 $newX$  will **not** be used to fit the models.

Example with  $X$  and  $newX$ :

```
fit <- glm(Y ~ ., data = X)
out <- predict(fit, newdata = newX)
```

---

The formula  $Y \sim .$  means an additive linear model using all columns of  $X$

## SUPERLEARNER

`newX` might be a test set, the interesting values of `X` for prediction, a stacked data.frame with exposure levels set to be used with for G-computation, etc

Example setting exposure level for `newX`

```
newData <- rbind(  
  cbind(A = 0, subset(X, select = -A)),  
  cbind(A = 1, subset(X, select = -A))  
)
```



## SUPERLEARNER

- family: currently either `gaussian()` or `binomial()`.
- method: either `'method.NNLS'`, `'method.NNloglik'`, or your own method (see `create.method.template()`).
- verbose: helpful to set this to `TRUE` to see the progress of the estimation.

## SUPERLEARNER

The ensemble model for “NNLS” is:

$$\Psi_{\text{SL}}(W) = \sum_{j=1}^K \alpha_j \Psi_j(W), \quad \alpha_j \geq 0, \quad \sum \alpha_j = 1$$

The ensemble model for “NNloglik” is:

$$\Psi_{\text{SL}}(W) = \frac{1}{1 + \exp \left\{ - \sum_{j=1}^K \alpha_j \text{logit}_{\gamma} (\Psi_j(W)) \right\}}, \quad \alpha_j \geq 0, \quad \sum \alpha_j = 1$$

where  $\text{logit}_{\gamma}$  is the trimmed logit function to control when  $\Psi_j(W)$  is near 0 or 1.

There are two types of algorithms that can be used in `SL.library`:

- 1 **Prediction algorithms.** Algorithms that take as input  $X$  and  $Y$  and return a predicted  $Y$  value.
- 2 **Screening algorithms.** Algorithms designed to reduce the dimension of  $X$ . They take as input  $X$  and  $Y$  and return a logical vector indicating the columns in  $X$  passing the screening. Screening algorithms can be coupled with prediction algorithms to form new prediction algorithms.

listWrappers()

Show in R

```
listWrappers()
```

## SUPERLEARNER

There are two ways to specify the algorithms in `SL.library`:

- 1 A character vector:

```
c('SL.glm', 'SL.glmnet', 'SL.gam')
```

- 2 A list of character vectors:

```
list(c('SL.glm', 'screen.corP'), 'SL.gam')
```

If only using prediction algorithms, easier to use the first method.

If using screening algorithms, the list is required. The syntax for the elements in the list is the prediction algorithm is first, followed by the screening algorithms. Multiple screening algorithms can be used. If a singleton, the default is to apply to all variables.

## SUPERLEARNER

see the help documents for SuperLearner for more examples of  
SL.library

## CREATING WRAPPERS

Many algorithms are included in the package (use `listWrappers()` for a list of included functions), but these are just enough to get you started.

A few reasons to build your own wrappers:

- Want to use an algorithm not currently included
- Problem suggests different values for the tuning parameters
- Want to include a range of tuning parameters, not just the default
- Want to select tuning parameters in a different way (e.g. `SL.glmnet` selecting  $\lambda$ )
- Force variables to be used in step-wise methods

## CREATING WRAPPERS

The **SuperLearner** vignette contains a table of tuning parameters for the algorithms in the package

Show in R

```
vignette("SuperLearner")
```



## CREATING WRAPPERS

Example: Creating new prediction algorithm wrapper

## CREATING WRAPPERS

Consider the `polymars` algorithm in the **polyspline** package.

- continuous outcome `Y`
- data.frame of covariates `X`
- data.frame of covariates `newX`

```
fit.mars <- polymars(Y, X)
out <- predict.polymars(fit.mars,
  x = as.matrix(newX))
```

Now we know how to fit the model and return predicted values, next we check out `write.SL.template` for integrating the code above into the correct syntax for SuperLearner

## CREATING WRAPPERS

write.SL.template()

```
SL.template <- function(Y, X, newX, family,
  obsWeights, id, ...) {
  # require('pkg')
  if(family$family == 'gaussian') { }
  if(family$family == 'binomial') { }
  # pred is the predicted responses for newX
  pred <- numeric()
  # fit returns all objects needed for predict.SL.*
  fit <- list(object = )
  # declare class of fit for predict.SL.template
  class(fit) <- 'SL.template'
  # return a list with pred and fit
  out <- list(pred = pred, fit = fit)
  return(out)
}
}
```

## CREATING WRAPPERS

**Table:** The arguments passed to a prediction algorithm in SuperLearner

Argument	Description
Y	the outcome variable
X	the training data set (the observations used to fit the model)
newX	the validation data set (the observations to return predictions for)
family	a description of the error distribution
id	a cluster identification
obsWeights	observation weights

You do not need to use all these arguments, but if you use any of them, the name must match exactly.

## CREATING WRAPPERS

### SL.polymars

```
My.SL.polymars <- function(Y, X, newX,
  family, ...) {
  if(family$family=="gaussian") {
    fit.mars <- polymars(Y, X)
    out <- predict.polymars(fit.mars,
      x = as.matrix(newX))
  }
  if(family$family=="binomial") {
    # insert estimation function
  }
  ... # next slide
}
```

## CREATING WRAPPERS

What about `family = binomial()`?

Can leave this blank (or add `stop('only gaussian')`) if only for a specific example with continuous outcome.

To be complete, we could look up the code for a binary outcome and add this case:

```
fit.mars <- polyclass(Y, X, cv = 5)
out <- ppolyclass(cov = newX,
  fit = fit.mars)[, 2]
```

## CREATING WRAPPERS

### SL.polymars

```
My.SL.polymars <- function(Y, X, newX,
  family, ...) {
  if(family$family=="gaussian") {
    fit.mars <- polymars(Y, X)
    out <- predict.polymars(fit.mars,
      x = as.matrix(newX))
  }
  if(family$family=="binomial") {
    fit.mars <- polyclass(Y, X, cv = 5)
    out <- ppolyclass(cov = newX,
      fit = fit.mars)[, 2]
  }
  ... # next slide
}
```

## CREATING WRAPPERS

Wrappers need to return 2 values:

- ① **pred**: predicted  $Y$  values for rows in `newX`
- ② **fit**: a list with everything needed to use predict method

In the `polymars` example: For the gaussian case, `predict()` needs:  
`object = fit.mars`

For the binomial case, `predict()` needs: `fit = fit.mars`

**Note:** `SuperLearner` does not use the `fit` list. If you do not plan to use the function `predict.SuperLearner` you can leave the `fit` object as: `fit <- vector("list", length = 0)`



## SL.polymars

```
My.SL.polymars <- function(Y, X, newX,
  family, ...) {
  if(family$family=="gaussian") {
    fit.mars <- polymars(Y, X)
    out <- predict.polymars(fit.mars,
      x = as.matrix(newX))
    fit <- list(object = fit.mars)
  }
  if(family$family=="binomial") {
    fit.mars <- polyclass(Y, X, cv = 5)
    out <- ppolyclass(cov = newX,
      fit = fit.mars)[, 2]
    fit <- list(fit = fit.mars)
  }
  ... # next slide
}
```

## CREATING WRAPPERS

Final step is putting everything together into a list object. The list must have 2 elements and the names **must** be `pred` and `fit`

Can also assign a class to the `fit` list. This will be used to look up the correct predict method. I'm using S3 methods here. This is only important if using `predict.SuperLearner` afterwards.

See Chambers (2008) *Software for Data Analysis* for details on S3 and S4 methods.

## CREATING WRAPPERS

### SL.polymars

```
My.SL.polymars <- function(Y, X, newX,  
  family, ...) {  
  ... # previous slides  
  out <- list(pred = pred, fit = fit)  
  class(out$fit) <- c("SL.polymars")  
  return(out)  
}
```

**Note:** out is just a temporary variable name here.

The function should match SL.polymars in the **SuperLearner** package.

## CREATING WRAPPERS

### Important notes for creating wrappers

- Input must follow naming syntax: `Y, X, ...`
- Name of new function must be different than one already in the package
- Must return a list with 2 elements named `pred` and `fit`
- `pred` must be a vector with the predicted `Y` values for the rows in `newX`
- `fit` can be anything if not using predict method, otherwise is a list with elements needed for predict

## CREATING WRAPPERS

predict.SL.template

```
predict.SL.template <- function (object,  
  newdata, family, X = NULL, Y = NULL, ...)  
{  
  pred <- numeric()  
  return(pred)  
}
```

## CREATING WRAPPERS

### predict.SL.polymars

```
predict.SL.polymars <-  
function (object, newdata, family, ...) {  
  if (family$family == "gaussian") {  
    pred <- predict.polymars(object = object$object,  
      x = as.matrix(newdata))  
  }  
  if (family$family == "binomial") {  
    pred <- ppolyclass(cov = newdata,  
      fit = object$fit)[, 2]  
  }  
  return(pred)  
}
```

## CREATING WRAPPERS

Example: creating screening algorithm

## CREATING WRAPPERS

### screening template

```
screen.template <- function (Y, X, family,
  obsWeights, id, ...) {
  # require('pkg')
  if (family$family == "gaussian") {
  }
  if (family$family == "binomial") {
  }
  # whichVariable is a logical vector,
  # TRUE indicates variable will be used
  whichVariable <- rep(TRUE, ncol(X))
  return(whichVariable)
}
```



## CREATING WRAPPERS

**Table:** The arguments passed to a screening algorithm in SuperLearner

Argument	Description
Y	the outcome variable
X	the training data set (the observations used to fit the model)
family	a description of the error distribution
id	a cluster identification
obsWeights	observation weights

You do not need to use all these arguments, but if you use any of them, the name must match exactly.

## screen.randomForest

```
screen.randomForest <- function (Y, X,  
  family, nVar = 10, ntree = 1000, ...) {  
  if (family$family == "gaussian") {  
    rank.rf.fit <- randomForest(Y ~ .,  
      data = X, ntree = ntree)  
  }  
  if (family$family == "binomial") {  
    rank.rf.fit <- randomForest(  
      y = as.factor(Y), x = X,  
      ntree = ntree)  
  }  
  whichVariable <- as.logical(  
    rank(-rank.rf.fit$importance) <= nVar)  
  return(whichVariable)  
}
```

## BOSTON HOUSING EXAMPLE

The outcome variable is the median home value ( $\text{cmedv}$ ) for the 506 census tracts of Boston from the 1970 census.

The covariates are a mix of geographical and socioeconomic variables, like per capita crime rate ( $\text{crim}$ ), average number of rooms per house ( $\text{rm}$ ), distance to Boston employment centres ( $\text{dis}$ ), indicator of tract being on the Charles river ( $\text{chas}$ ), etc.

## BOSTON HOUSING

The Boston Housing data can be found in the **mlbench** package.

### Load the data

```
library(mlbench)
data(BostonHousing2)
# convert factors to numeric
BostonHousing2$chas
  <- as.numeric(BostonHousing2$chas=="1")
# select subset of variables
DATA <- BostonHousing2[, c("cmedv", "crim", "zn",
  "indus", "chas", "nox", "rm", "age", "dis",
  "rad", "tax", "ptratio", "b", "lstat")]
```

## BOSTON HOUSING EXAMPLE

First need to decide which prediction algorithms to include in the library

## BOSTON HOUSING

Algorithm	Description	Package
glm	linear model	<b>stats</b>
randomForest	random Forest	<b>randomForest</b>
bagging	bootstrap aggregation of trees	<b>ipred</b>
gam	generalized additive models	<b>gam</b>
gbm	gradient boosting	<b>gbm</b>
nnet	neural network	<b>nnet</b>
polymars	polynomial spline regr.	<b>polspline</b>
bart	Bayesian additive regr. trees	<b>BayesTree</b>
glmnet	elastic net	<b>glmnet</b>
svm	support vector machine	<b>e1071</b>
bayesglm	Bayesian glm	<b>arm</b>
step	stepwise glm	<b>stats</b>

## BOSTON HOUSING

One algorithm to consider is the generalized additive model algorithm. This algorithm has a tuning parameter for the degrees of freedom in the smoother. I have set this to be 2 in `SL.gam` but we might want to consider larger values.

We could create an entirely new wrapper for `gam` and  $df = 3$ , or we can write a wrapper for the wrapper and only change the degrees of freedom value.

## BOSTON HOUSING

look at `SL.gam` to see how the degrees of freedom parameter is specified:



## SL.gam

```
SL.gam <- function(Y, X, newX,  
  family, obsWeights, deg.gam = 2, ...)  
{  
  ... # model: Y ~ s(X, deg.gam)  
      # see full functions for details  
  fit.gam <- gam::gam(gam.model, data = X,  
    family = family,  
    control = gam.control(maxit = 50, bf.maxit = 50),  
    weights = obsWeights)  
  pred <- predict(fit.gam, newdata = newX,  
    type = "response")  
  ... # returns list here  
}
```

## BOSTON HOUSING

The `SL.gam` function contains the argument `deg.gam = 2`.

Wrappers can have additional arguments, but they must have default values.

## BOSTON HOUSING EXAMPLE

For the new wrapper, only need to change the value of `deg.gam`.  
Use `...` to pass everything else between `SL.gam.3` and `SL.gam`.

### Adjusting `deg.gam` in `SL.gam`

```
SL.gam.3 <- function(..., deg.gam = 3) {  
  SL.gam(..., deg.gam = deg.gam)  
}
```

Easy to create new wrappers by changing tuning parameter values. Check the code for the wrappers by typing the name of the function without parentheses to see what tuning parameter values are in the arguments.

## BOSTON HOUSING EXAMPLE

Similar to the `SL.gam` example above, the function `create.SL.glmnet` in the **SuperLearnerExtra** package can be used to create new `SL.glmnet` wrappers:

### Additional wrappers

```
create.SL.glmnet(alpha = c(0.25, 0.50, 0.75))  
# and set gbm to no interactions:  
SL.gbm.1 <- function(...) {  
  SL.gbm(..., interaction.depth = 1)  
}
```

## BOSTON HOUSING EXAMPLE

### SL.library

```
SL.library <- c("SL.gam",  
  "SL.gam.3", "SL.gam.4",  
  "SL.gam.5", "SL.gbm.1",  
  "SL.gbm", "SL.glm",  
  "SL.glmnet", "SL.glmnet.0.25",  
  "SL.glmnet.alpha.0.5", "SL.glmnet.0.75",  
  "SL.polymars", "SL.randomForest",  
  "SL.ridge", "SL.svm",  
  "SL.bayesglm", "SL.step",  
  "SL.step.interaction",  
  "SL.bart")
```

## BOSTON HOUSING EXAMPLE

fitSL

```
fitSL <- SuperLearner(Y = log(DATA$cmedv),  
  X = subset(DATA, select = -c(cmedv)),  
  SL.library = SL.library,  
  family = gaussian()  
)
```

	Risk	Coef
SL.gam_All	0.03834031	0.0000000
SL.gam.3_All	0.03666449	0.0000000
SL.gam.4_All	0.03589859	0.0000000
SL.gam.5_All	0.03529692	0.0000000
SL.gbm.1_All	0.03040543	0.0000000
SL.gbm.2_All	0.02501729	0.0000000
SL.glm_All	0.03754472	0.0000000
SL.glmnet_All	0.03765112	0.0000000
SL.glmnet.alpha25_All	0.03754278	0.0000000
SL.glmnet.alpha50_All	0.03758802	0.0000000
SL.glmnet.alpha75_All	0.03763085	0.0000000
SL.polymars_All	0.04587432	0.0000000
SL.randomForest_All	0.02105987	0.2956277
SL.ridge_All	0.03753661	0.0000000
SL.svm_All	0.02678290	0.0000000
SL.bayesglm_All	0.03754318	0.0000000
SL.step_All	0.03753337	0.0000000

## BOSTON HOUSING

**Table:** Elements of the output from SuperLearner

Name	Description
SL.predict	super learner predicted values for newX
coef	coefficient for each algorithm
libraryNames	names of algorithms in library
library.predict	matrix of predicted values for newX from each algorithm in the library
cvRisk	V-fold cross-validated risk for each algorithm in the library



## BOSTON HOUSING

The final super learner prediction model is the weighted combination of the library algorithms where the estimates of the weights can be found with `coef(fitSL)`.

To attain predictions on new observations (not in `newX`), the `predict` function will usually work. If you created new wrappers, you also need to create `predict` S3 methods for those new wrappers.

## BOSTON HOUSING

SuperLearner is a model selection algorithm. It does not contain a good estimate for model assessment (you could use the re-substitution method to estimate the risk but this is optimistic).

Our suggestion to assess the performance of the super learner is to run CV.SuperLearner (example in the next case study).

## ALL EXAMPLE

- The outcome variable is an indicator of the molecular biology of the cancer tissue, either **Negative** or **BCR/ABL**.
- The sample consists of 79 individuals (42 Neg, 37 BCR/ABL).
- The data contain 2200 features (X) to be used after the filtering steps.
- Need to select algorithms appropriate for a binary outcome and a large number of covariates.

## ALL

load ALL data

```
# source("http://bioconductor.org/biocLite.R")
# biocLite()
# biocLite("ALL")
library(ALL)
library(genefilter)
data(ALL)
```

The next 2 slides are the processing steps following in Gentleman, Huber and Carey (2008) "Supervised Machine Learning" in *Bioconductor Case Studies*.

```
# restrict to only the NEG and BCR/ABL outcomes
bcell <- grep("^B", as.character(ALL$BT))
moltyp <- which(as.character(ALL$mol.biol)
  %in% c("NEG", "BCR/ABL"))
ALL_bcrneg <- ALL[, intersect(bcell, moltyp)]
#drops unused levels
ALL_bcrneg$mol.biol <- factor(ALL_bcrneg$mol.biol)

# filter features
ALLfilt_bcrneg <- nsFilter(ALL_bcrneg,
  var.cutoff = 0.75)$set
```

```

# standardize the features
rowIQRs <- function(eSet) {
  numSamp <- ncol(eSet)
  lowQ <- rowQ(eSet, floor(0.25 * numSamp))
  upQ <- rowQ(eSet, ceiling(0.75 * numSamp))
  upQ - lowQ
}
standardize <- function(x) {
  (x - rowMedians(x)) / rowIQRs(x)
}
exprs(ALLfilt_bcrneg) <- standardize(
  exprs(ALLfilt_bcrneg))

# convert to numeric matrix for the SuperLearner
Y <- as.numeric(
  ALLfilt_bcrneg$mol.biol == "BCR/ABL")
X <- t(exprs(ALLfilt_bcrneg))

```

Possible prediction algorithms include:

- k-nearest neighbors
- elastic net (penalized regression)
- random forest

These algorithms have tuning parameters:

- knn:  $k$
- glmnet:  $\alpha$
- randomForest: `mtry` and `nodesize`

## randomForest

```
tuneGrid <- expand.grid(mtry = c(500, 1000, 2200),
  nodesize = c(1, 5, 10))

for(mm in seq(nrow(tuneGrid))) {
  eval(parse(file = "", text =
    paste("SL.randomForest.", mm,
      "<- function(..., mtry = ", tuneGrid[mm, 1],
      ", nodesize = ", tuneGrid[mm, 2], ") {
      SL.randomForest(..., mtry = mtry,
      nodesize = nodesize) }", sep = "")))
}
```



## ALL

The code above is hard to follow, but I'm doing the same thing we did with `SL.gam.3` just in a for loop.

```
> SL.randomForest.1
function(..., mtry = 500, nodesize = 1) {
  SL.randomForest(..., mtry = mtry,
    nodesize = nodesize) }

> SL.randomForest.2
function(..., mtry = 1000, nodesize = 1) {
  SL.randomForest(..., mtry = mtry,
    nodesize = nodesize) }

> SL.randomForest.9
function(..., mtry = 2200, nodesize = 10) {
  SL.randomForest(..., mtry = mtry,
    nodesize = nodesize) }
```

Add additional knn wrappers using functions in **SuperLearnerExtra**

```
create.SL.knn
```

```
create.SL.knn(k = c(k = 20, 30, 40, 50))
```

## SL.library

```
SL.library <- c("SL.knn",  
  "SL.knn.20",  
  "SL.knn.30",  
  "SL.knn.40",  
  "SL.knn.50",  
  "SL.randomForest",  
  "SL.glmnet",  
  "SL.glmnet.0.25",  
  "SL.glmnet.0.5",  
  "SL.glmnet.0.75",  
  "SL.mean",  
  paste("SL.randomForest.",  
    seq(nrow(tuneGrid)), sep = ""))
```

## ALL example

```
fitSL <- SuperLearner(Y = Y, X = X,  
  SL.library = SL.library, family = binomial(),  
  method = "NNLS",  
  cvControl = list(stratifyCV = TRUE))  
  
fitSL
```

	Risk	Coef
SL.knn_All	0.20658228	0.00000000
SL.knn20_All	0.22423347	0.00000000
SL.knn30_All	0.22299664	0.00000000
SL.knn40_All	0.23445986	0.00000000
SL.knn50_All	0.23920321	0.00000000
SL.randomForest_All	0.12418009	0.00000000
SL.glmnet_All	0.08430633	0.98039534
SL.glmnet.alpha25_All	0.10487930	0.00000000
SL.glmnet.alpha50_All	0.09331539	0.00000000
SL.glmnet.alpha75_All	0.08681511	0.00000000
SL.randomForest.1_All	0.13103528	0.00000000
SL.randomForest.2_All	0.12269094	0.00000000
SL.randomForest.3_All	0.11918439	0.00000000
SL.randomForest.4_All	0.13024104	0.00000000
SL.randomForest.5_All	0.12351049	0.00000000
SL.randomForest.6_All	0.11752733	0.01960466
SL.randomForest.7_All	0.12871385	0.00000000

## CV.SuperLearner

```
fitSL.CV <- CV.SuperLearner(Y = Y, X = X,  
  SL.library = SL.library,  
  V = 20, family = binomial(),  
  method = "method.NNLS",  
  cvControl = list(stratifyCV = TRUE))
```

```
summary(fitSL.CV)
```

```
# can also print the LaTeX table  
# requires Hmisc package  
# latex(summary(fitSL.CV))
```

Algorithm	subset	Risk	SE	Min	Max
SuperLearner	–	0.101	0.020	0.003	0.382
Discrete SL	–	0.095	0.021	0.004	0.347
SL.knn(10)	All	0.212	0.018	0.070	0.460
SL.knn(20)	All	0.220	0.011	0.152	0.322
SL.knn(30)	All	0.223	0.008	0.192	0.274
SL.knn(40)	All	0.232	0.006	0.187	0.268
SL.knn(50)	All	0.238	0.004	0.218	0.260
SL.randomForest	All	0.120	0.014	0.026	0.256
SL.glmnet( $\alpha = 1.0$ )	All	0.088	0.022	0.002	0.395
SL.glmnet( $\alpha = 0.25$ )	All	0.113	0.022	0.007	0.451
SL.glmnet( $\alpha = 0.50$ )	All	0.106	0.023	0.004	0.447
SL.glmnet( $\alpha = 0.75$ )	All	0.093	0.021	0.004	0.347
SL.mean	All	0.249	0.004	0.242	0.251
SL.randomForest.1	All	0.125	0.014	0.034	0.269
SL.randomForest.2	All	0.114	0.014	0.023	0.250
SL.randomForest.3	All	0.111	0.015	0.016	0.238
SL.randomForest.4	All	0.123	0.014	0.036	0.264
SL.randomForest.5	All	0.117	0.014	0.023	0.262
SL.randomForest.6	All	0.110	0.015	0.015	0.252
SL.randomForest.7	All	0.126	0.014	0.034	0.266
SL.randomForest.8	All	0.117	0.014	0.023	0.259
SL.randomForest.9	All	0.110	0.015	0.013	0.245

## VAN'T VEER EXAMPLE

- 97 breast cancer patients followed for 5 years.
- Outcome is binary yes/no recur in 5 years (we do not have the date of recurrence)
- 7 clinical variables are available (age, tumor grade, etc.)
- 4348 gene expression values post-filtering



## VAN'T VEER DATA

The original data is available at:

<http://www.rii.com/publications/2002/vantveer.html>

One interesting “screening” is to consider the prediction algorithms on only the clinical variables or on only the gene expression variables.

screening

```
screen.clinical <- function(...){  
  return(c(rep(TRUE, 7), rep(FALSE, 4348)))  
}  
  
screen.array <- function(...){  
  return(c(rep(FALSE, 7), rep(TRUE, 4348)))  
}
```

```
SL.library <- list(  
  c("SL.knn", "All", "screen.clinical",  
    "screen.corP", "screen.corP.01", "screen.glmnet"),  
  c("SL.knn.20", "All", "screen.clinical",  
    "screen.corP", "screen.corP.01", "screen.glmnet"),  
  c("SL.glmnet", "screen.corRank.50",  
    "screen.corRank.20"),  
  c("SL.glmnet.0.75", "screen.corRank.50",  
    "screen.corRank.20"),  
  c("SL.glmnet.0.5", "screen.corRank.50",  
    "screen.corRank.20"),  
  c("SL.glmnet.0.25", "screen.corRank.50",  
    "screen.corRank.20"),  
  c("SL.randomForest", "screen.clinical",  
    "screen.corP.01", "screen.glmnet"),  
  c("SL.bagging", "screen.clinical",  
    "screen.corP.01", "screen.glmnet"),  
  c("SL.bart", "screen.clinical",
```

## SuperLearner

```
fitSL <- SuperLearner(Y = surv.resp, X = X,  
  SL.library = SL.library,  
  family = binomial(),  
  method = "method.NNLS",  
  control = list(saveFitLibrary = FALSE))
```

```
fitSL
```

fitSL

	Risk	Coef
...		
SL.knn_screen.corP.01	0.2129897	0.27517459
...		
SL.glmnet_screen.corRank.20	0.2210815	0.22256164
...		
SL.randomForest_clinical	0.2151708	0.08636558
...		
SL.bart_clinical	0.2084039	0.41589818

Only presenting results for non-zero coefficients. Table does not fit on a slide.

## CV.SuperLearner

```
fitSL.CV <- CV.SuperLearner(Y=surv.resp, X=X,  
  V = 20,  
  SL.library = SL.library,  
  family = binomial(),  
  method = "method.NNLS",  
  cvControl = list(stratifyCV = TRUE))  
  
summary(fitSL.CV)
```

Algorithm	subset	Risk	SE	Min	Max
SuperLearner	-	0.194	0.017	0.103	0.309
Discrete SL	-	0.238	0.024	0.127	0.415
SL.knn(10)	All	0.249	0.020	0.144	0.532
SL.knn(10)	clinical	0.239	0.019	0.138	0.496
SL.knn(10)	cor (p < 0.1)	0.262	0.023	0.095	0.443
SL.knn(10)	cor (p < 0.01)	0.224	0.020	0.088	0.365
SL.knn(10)	glmnet	0.219	0.028	0.007	0.465
SL.knn(20)	All	0.242	0.013	0.171	0.397
SL.knn(20)	clinical	0.236	0.012	0.154	0.382
SL.knn(20)	cor (p < 0.1)	0.233	0.017	0.108	0.342
SL.knn(20)	cor (p < 0.01)	0.206	0.018	0.121	0.321
SL.knn(20)	glmnet	0.217	0.026	0.018	0.405
SL.knn(30)	All	0.239	0.013	0.171	0.396
SL.knn(30)	clinical	0.236	0.012	0.169	0.386
SL.knn(30)	cor (p < 0.1)	0.232	0.014	0.143	0.319
SL.knn(30)	cor (p < 0.01)	0.215	0.017	0.136	0.346
SL.knn(30)	glmnet	0.210	0.023	0.039	0.402
SL.knn(40)	All	0.240	0.011	0.182	0.331
SL.knn(40)	clinical	0.238	0.010	0.179	0.319
SL.knn(40)	cor (p < 0.1)	0.236	0.012	0.166	0.316
SL.knn(40)	cor (p < 0.01)	0.219	0.015	0.154	0.309
SL.knn(40)	glmnet	0.211	0.021	0.060	0.346
SL.glmnet( $\alpha = 1.0$ )	corRank.50	0.229	0.029	0.078	0.445
SL.glmnet( $\alpha = 1.0$ )	corRank.20	0.208	0.026	0.048	0.424
SL.glmnet( $\alpha = 0.75$ )	corRank.50	0.221	0.027	0.077	0.420
SL.glmnet( $\alpha = 0.75$ )	corRank.20	0.209	0.026	0.046	0.421
SL.glmnet( $\alpha = 0.50$ )	corRank.50	0.226	0.027	0.077	0.426
SL.glmnet( $\alpha = 0.50$ )	corRank.20	0.211	0.026	0.059	0.419
SL.glmnet( $\alpha = 0.25$ )	corRank.50	0.229	0.027	0.084	0.424
SL.glmnet( $\alpha = 0.25$ )	corRank.20	0.216	0.025	0.072	0.406
SL.randomForest	clinical	0.198	0.019	0.098	0.391
SL.randomForest	cor (p < 0.01)	0.204	0.018	0.101	0.341
SL.randomForest	glmnet	0.220	0.025	0.072	0.378
SL.bagging	clinical	0.207	0.016	0.108	0.408
SL.bagging	cor (p < 0.01)	0.205	0.018	0.107	0.353
SL.bagging	glmnet	0.206	0.022	0.077	0.388
SL.bart	clinical	0.202	0.018	0.109	0.365
SL.bart	cor (p < 0.01)	0.210	0.021	0.092	0.376
SL.bart	glmnet	0.220	0.028	0.043	0.423
SL.mean	All	0.250	0.003	0.246	0.251

### Installing suggested packages

```
install.packages(c("glmnet", "randomForest",  
  "class", "gam", "gbm", "nnet", "polspline",  
  "MASS", "e1071", "stepAIC", "arm", "party",  
  "spls", "LogicReg", "nnls", "multicore",  
  "SIS", "BayesTree", "quadprog", "ipred",  
  "mlbench", "rpart", "caret", "mda", "earth"),  
  type="source",  
  repos="http://cran.cnr.Berkeley.edu",  
  dependencies=c("Depends", "Imports"))  
# missing DSA, not available on CRAN
```

Can remove type = 'source' if system not setup to install packages from source.



## COLOPHON

- Slides created with  $\text{\LaTeX}$  package **Beamer**
- Code blocks adapted from the **tikzDevice** R package
- $\text{\LaTeX}$  package **tikz** and **sweave** for code styles
- R version 2.13.0 and **SuperLearner** version 2.0-1
- Other packages: arm 1.4-10, BayesTree 0.3-1, caret 4.88, class 7.3-3, DSA 3.1.4, e1071 1.5-25, earth 2.6-2, gam 1.04, gbm 1.6-3, glmnet 1.6, Hmisc 3.8-3, ipred 0.8-11, leaps 2.9, lme4 0.999375-39, LogicReg 1.4.10, MASS 7.3-13, mda 0.4-2, mlbench 2.1-0, modelUtils 3.1.4, nnet 7.3-1, nnls 1.3, party 0.9-9994, polspline 1.1.5, quadprog 1.5-4, randomForest 4.6-2, rpart 3.1-50, SIS 0.6,