

Feature Selection – Ten Effective Techniques with Examples

In machine learning, Feature selection is the process of choosing variables that are useful in predicting the response [Y]. It is considered a good practice to identify which features are important when building predictive models. In this post, you will see how to implement 10 powerful feature selection approaches in R.



Feature Selection Methods

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Introduction

In real-world datasets, it is fairly common to have columns that are nothing but noise.

You are better off getting rid of such variables because of the memory space they occupy, the time and the computational resources it is going to cost, especially in large datasets.

Sometimes, you have a variable that makes business sense, but you are not sure if it actually helps in predicting the Y. You also need to consider the fact that, a feature that could be useful in one ML algorithm (say a decision tree) may go underrepresented or unused by another (like a regression model).

Having said that, it is still possible that a variable that shows poor signs of helping to explain the response variable [Y], can turn out to be significantly useful in the presence of [or combination with] other predictors. What I mean by that is, a variable might have a low correlation value of [~ 0.2] with Y. But in the presence of other variables, it can help to explain certain patterns/phenomenon that other variables can't explain.

In such cases, it can be hard to make a call whether to include or exclude such variables.

The strategies we are about to discuss can help fix such problems. Not only that, it will also help understand if a particular variable is important or not and how much it is contributing to the model

An important caveat. It is always best to have variables that have sound business logic backing the inclusion of a variable and rely solely on variable importance metrics.

Alright. Let's load up the 'Glaucoma' dataset where the goal is to predict if a patient has Glaucoma or not based on 63 different physiological measurements. You can directly run the codes or [download the dataset here](https://raw.githubusercontent.com/selva86/datasets/master/GlaucomaM.csv) (<https://raw.githubusercontent.com/selva86/datasets/master/GlaucomaM.csv>).

A lot of interesting examples ahead. Let's get started.

```
# Load Packages and prepare dataset
library(TH.data)
library(caret)
data("GlaucomaM", package = "TH.data")
trainData <- GlaucomaM
head(trainData)
```

	ag	at	as	an	ai	eag	eat	eas	ean	eai	...	tmt	tms	tmn	tmi	mr	rnf	mdic	emd	mv	Class
2	2.220	0.354	0.580	0.686	0.601	1.267	0.336	0.346	0.255	0.331	...	-0.018	-0.230	-0.510	-0.158	0.841	0.410	0.137	0.239	0.035	normal
43	2.681	0.475	0.672	0.868	0.667	2.053	0.440	0.520	0.639	0.454	...	-0.014	-0.165	-0.317	-0.192	0.924	0.256	0.252	0.329	0.022	normal
25	1.979	0.343	0.508	0.624	0.504	1.200	0.299	0.396	0.259	0.246	...	-0.097	-0.235	-0.337	-0.020	0.795	0.378	0.152	0.250	0.029	normal
65	1.747	0.269	0.476	0.525	0.476	0.612	0.147	0.017	0.044	0.405	...	-0.035	-0.449	-0.217	-0.091	0.746	0.200	0.027	0.078	0.023	normal
70	2.990	0.599	0.686	1.039	0.667	2.513	0.543	0.607	0.871	0.492	...	-0.105	0.084	-0.012	-0.054	0.977	0.193	0.297	0.354	0.034	normal
16	2.917	0.483	0.763	0.901	0.770	2.200	0.462	0.637	0.504	0.597	...	0.087	0.018	-0.094	-0.051	0.965	0.339	0.333	0.442	0.028	normal

(https://www.machinelearningplus.com/wp-content/uploads/2018/05/glaucoma_dataset.png)

GLAUCOMA DATASET

1. Boruta

Boruta is a feature ranking and selection algorithm based on random forests algorithm.

The advantage with **Boruta** is that it clearly decides if a variable is important or not and helps to select variables that are statistically significant (<https://www.machinelearningplus.com/statistics/statistical-significance-tests-r/>). Besides, you can adjust the strictness of the algorithm by adjusting the p values that defaults to 0.01 and the `maxRuns`.

`maxRuns` is the number of times the algorithm is run. The higher the `maxRuns` the more selective you get in picking the variables. The default value is 100.

In the process of deciding if a feature is important or not, some features may be marked by Boruta as 'Tentative'. Sometimes increasing the `maxRuns` can help resolve the 'Tentativeness' of the feature.

Lets see an example based on the `Glaucoma` dataset from `TH.data` package that I created earlier.

```
# install.packages('Boruta')  
library(Boruta)
```

The `boruta` function uses a formula interface just like most predictive modeling functions. So the first argument to `boruta()` is the formula with the response variable on the left and all the predictors on the right.

By placing a dot, all the variables in `trainData` other than `Class` will be included in the model.

The `doTrace` argument controls the amount of output printed to the console. Higher the value, more the log details you get. So save space I have set it to 0, but try setting it to 1 and 2 if you are running the code.

Finally the output is stored in `boruta_output`.

```
# Perform Boruta search  
boruta_output <- Boruta(Class ~ ., data=na.omit(trainData), doTrace=0)
```

Let's see what the `boruta_output` contains.

```
names(boruta_output)
```

1. 'finalDecision'
2. 'ImpHistory'
3. 'pValue'
4. 'maxRuns'
5. 'light'
6. 'mcAdj'
7. 'timeTaken'
8. 'roughfixed'

9. 'call'

10. 'impSource'

```
# Get significant variables including tentatives
boruta_signif <- getSelectedAttributes(boruta_output, withTentative = TRUE)
print(boruta_signif)
```

```
[1] "as"  "ean" "abrg" "abrs" "abrn" "abri" "hic" "mhcg" "mhc" "mhci"
[11] "phcg" "phcn" "phci" "hvc" "vbss" "vbsn" "vbsi" "vasg" "vass" "vasi"
[21] "vbrg" "vbrs" "vbrn" "vbri" "varg" "vart" "vars" "varn" "vari" "mdn"
[31] "tmg"  "tmt"  "tms"  "tmn"  "tmi"  "rnf"  "mdic" "emd"
```

If you are not sure about the tentative variables being selected for granted, you can choose a **TentativeRoughFix** ON **boruta_output**.

```
# Do a tentative rough fix
roughFixMod <- TentativeRoughFix(boruta_output)
boruta_signif <- getSelectedAttributes(roughFixMod)
print(boruta_signif)
```

```
[1] "abrg" "abrs" "abrn" "abri" "hic"  "mhcg" "mhc" "mhci" "phcg" "phcn"
[11] "phci" "hvc"  "vbsn" "vbsi" "vasg" "vbrg" "vbrs" "vbrn" "vbri" "varg"
[21] "vart" "vars" "varn" "vari" "tmg"  "tms"  "tmi"  "rnf"  "mdic" "emd"
```

There you go. Boruta has decided on the 'Tentative' variables on our behalf. Let's find out the importance scores of these variables.

```
# Variable Importance Scores
imps <- attStats(roughFixMod)
imps2 = imps[imps$decision != 'Rejected', c('meanImp', 'decision')]
head(imps2[order(-imps2$meanImp), ]) # descending sort
```

	meanImp	decision
varg	10.279747	Confirmed
vari	10.245936	Confirmed
tmi	9.067300	Confirmed

Feedback

The columns in green are 'confirmed' and the ones in red are not. There are couple of blue bars representing **ShadowMax** and **ShadowMin**. They are not actual features, but are used by the boruta algorithm to decide if a variable is important or not.

2. Variable Importance from Machine Learning Algorithms

Another way to look at feature selection is to consider variables most used by various ML algorithms the most to be important.

Depending on how the machine learning algorithm learns the relationship between X's and Y, different machine learning algorithms may possibly end up using different variables (but mostly common vars) to various degrees.

What I mean by that is, the variables that proved useful in a tree-based algorithm like `rpart`, can turn out to be less useful in a regression-based model. So all variables need not be equally useful to all algorithms.

So how do we find the variable importance for a given ML algo?

1. `train()` the desired model using the [caret package](https://www.machinelearningplus.com/machine-learning/caret-package/) (<https://www.machinelearningplus.com/machine-learning/caret-package/>).
2. Then, use `varImp()` to determine the feature importances.

You may want to try out multiple algorithms, to get a feel of the usefulness of the features across algos.

```
# Train an rpart model and compute variable importance.
library(caret)
set.seed(100)
rPartMod <- train(Class ~ ., data=trainData, method="rpart")
rpartImp <- varImp(rPartMod)
print(rpartImp)
```

```
rpart variable importance
```

only 20 most important variables shown (**out** of 62)

Overall

varg	100.00
vari	93.19
vars	85.20
varn	76.86
tmi	72.31
vbss	0.00
eai	0.00
tmg	0.00
tmt	0.00
vbst	0.00
vasg	0.00
at	0.00
abrg	0.00
vbsg	0.00
eag	0.00
phcs	0.00
abrs	0.00
mdic	0.00
abrt	0.00
ean	0.00

Only 5 of the 63 features was used by `rpart` and if you look closely, the 5 variables used here are in the top 6 that `boruta` selected.

Let's do one more: the variable importances from Regularized Random Forest (RRF) algorithm.

```
# Train an RRF model and compute variable importance.
set.seed(100)
rrfMod <- train(Class ~ ., data=trainData, method="RRF")
rrfImp <- varImp(rrfMod, scale=F)
rrfImp
```

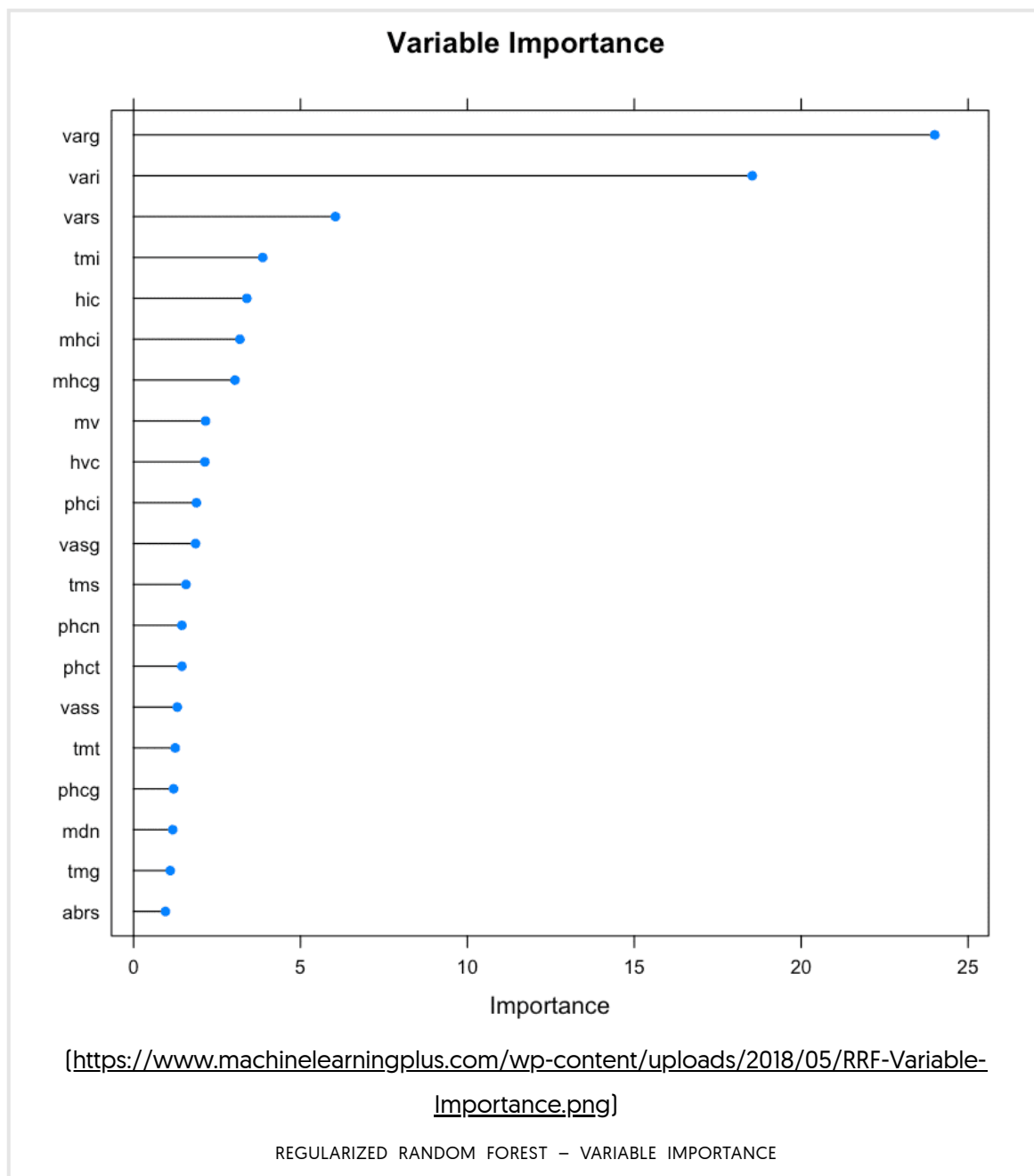

RRF variable importance

only 20 most important variables shown (**out** of 62)

Overall

varg	24.0013
vari	18.5349
vars	6.0483
tmi	3.8699
hic	3.3926
mhci	3.1856
mhcg	3.0383
mv	2.1570
hvc	2.1357
phci	1.8830
vasg	1.8570
tms	1.5705
phcn	1.4475
phct	1.4473
vass	1.3097
tmt	1.2485
phcg	1.1992
mdn	1.1737
tmg	1.0988
abrs	0.9537

```
plot(rrfImp, top = 20, main='Variable Importance')
```



The topmost important variables are pretty much from the top tier of **Boruta**'s selections.

Some of the other algorithms available in `train()` that you can use to compute `varImp` are the following:

ada, AdaBag, AdaBoost.M1, adaboost, bagEarth, bagEarthGCV, bagFDA, bagFDAGCV, bartMachine, blasso, BstLm, bstSm, C5.0, C5.0Cost, C5.0Rules, C5.0Tree, cforest, chaid, ctree, ctree2, cubist, deepboost, earth, enet, evtrees, extraTrees, fda, gamboost, gbm_h2o, gbm, gcvEarth, glmnet_h2o, glmnet, glmStepAIC, J48, JRip, lars, lars2, lasso, LMT, LogitBoost, M5, M5Rules, msaenet, nodeHarvest, OneR, ordinalNet, ORFlog, ORFpls, ORFridge, ORFsvm, pam,

parRF, PART, penalized, PenalizedLDA, qrf, ranger, Rborist, relaxo, rf, rFerns, rfRules, rotationForest, rotationForestCp, rpart, rpart1SE, rpart2, rpartCost, rpartScore, rqlasso, rqnc, RRF, RRFglobal, sdwd, smda, sparseLDA, spikeslab, wsrf, xgbLinear, xgbTree.

3. Lasso Regression

Least Absolute Shrinkage and Selection Operator [LASSO] regression is a type of regularization method that penalizes with L1-norm.

It basically imposes a cost to having large weights (value of coefficients). And its called L1 regularization, because the cost added, is proportional to the absolute value of weight coefficients.

As a result, in the process of shrinking the coefficients, it eventually reduces the coefficients of certain unwanted features all the to zero. That is, it removes the unneeded variables altogether.

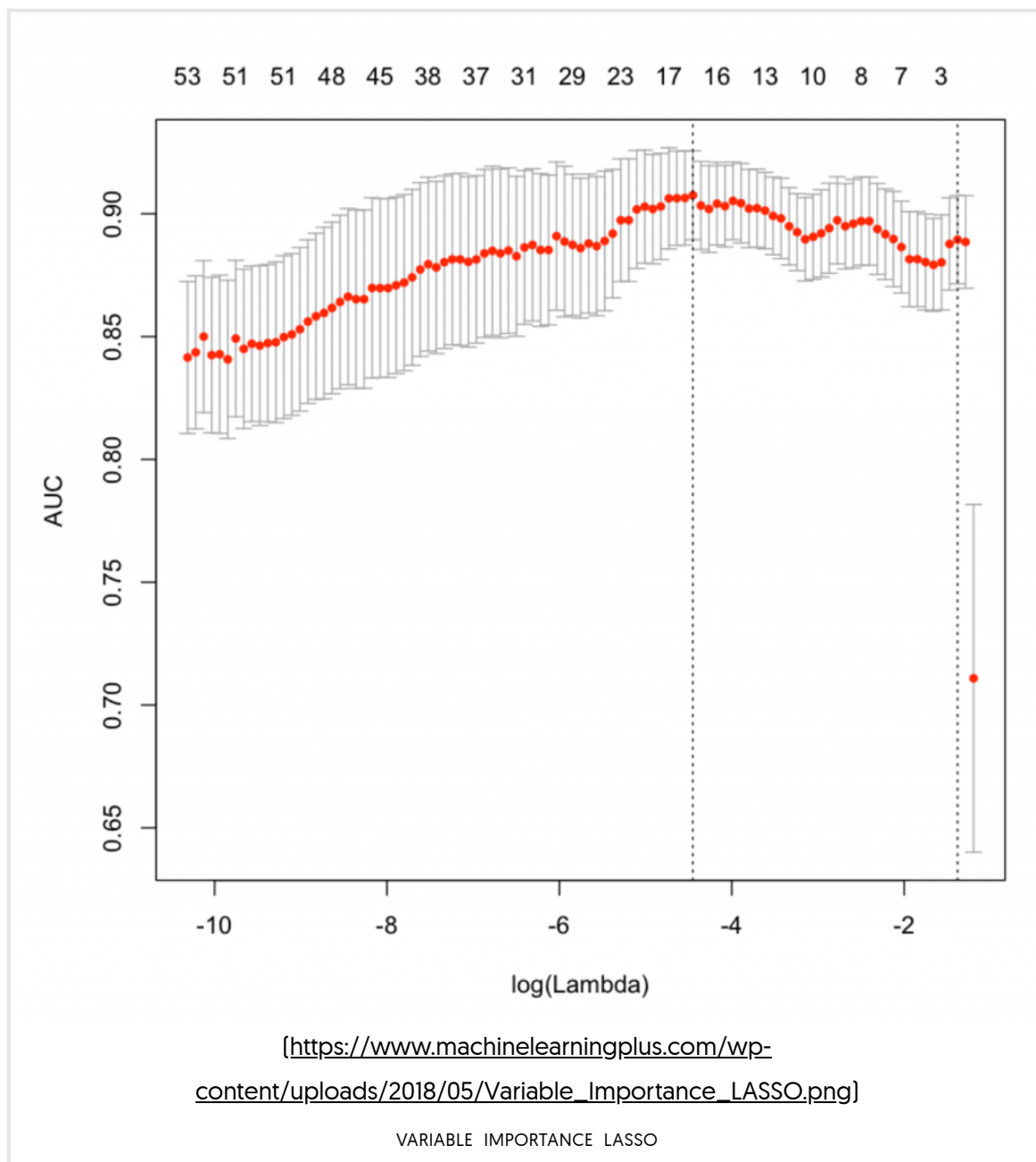
So effectively, LASSO regression can be considered as a variable selection technique as well.

```
library(glmnet)
trainData <- read.csv('https://raw.githubusercontent.com/selva86/datasets/master/GlaucomaM.csv')
# (https://raw.githubusercontent.com/selva86/datasets/master/GlaucomaM.csv)

x <- as.matrix(trainData[, -63]) # all X vars
y <- as.double(as.matrix(ifelse(trainData[, 63] == 'normal', 0, 1))) # Only Class

# Fit the LASSO model (Lasso: Alpha = 1)
set.seed(100)
cv.lasso <- cv.glmnet(x, y, family='binomial', alpha=1, parallel=TRUE, standardize=TRUE,
  type.measure='auc')

# Results
plot(cv.lasso)
```



Let's see how to interpret this plot.

The X axis of the plot is the log of lambda. That means when it is 2 here, the lambda value is actually 100.

The numbers at the top of the plot show how many predictors were included in the model. The position of red dots along the Y-axis tells what AUC we got when you include as many variables shown on the top x-axis.

You can also see two dashed vertical lines.

The first one on the left points to the lambda with the lowest mean squared error. The one on the right point to the number of variables with the highest deviance within 1 standard deviation.

The best lambda value is stored inside 'cv.lasso\$lambda.min'.

```
# plot(cv.lasso$glmnet.fit, xvar="lambda", label=TRUE)
cat('Min Lambda: ', cv.lasso$lambda.min, '\n 1Sd Lambda: ', cv.lasso$lambda.1se)
df_coef <- round(as.matrix(coef(cv.lasso, s=cv.lasso$lambda.min)), 2)

# See all contributing variables
df_coef[df_coef[, 1] != 0, ]
```

```
Min Lambda: 0.01166507
1Sd Lambda: 0.2513163
```

```
Min Lambda: 0.01166507
1Sd Lambda: 0.2513163
```

```
(Intercept) 3.65
at          -0.17
as          -2.05
eat         -0.53
mhci         6.22
phcs        -0.83
phci         6.03
hvc         -4.15
vass        -23.72
vbrn        -0.26
vars        -25.86
mdt         -2.34
mds          0.5
mdn          0.83
mdi          0.3
tmg          0.01
tms          3.02
tmi          2.65
mv           4.94
```

The above output shows what variables LASSO considered important. A high positive or low negative implies more important is that variable.

4. Step wise Forward and Backward Selection

Stepwise regression can be used to select features if the Y variable is a numeric variable. It is particularly used in selecting best [linear regression models](https://www.machinelearningplus.com/machine-learning/complete-introduction-linear-regression-r/) (<https://www.machinelearningplus.com/machine-learning/complete-introduction-linear-regression-r/>).

It searches for the best possible regression model by iteratively selecting and dropping variables to arrive at a model with the lowest possible AIC.

It can be implemented using the `step()` function and you need to provide it with a lower model, which is the base model from which it won't remove any features and an upper model, which is a full model that has all possible features you want to have.

Our case is not so complicated (< 20 vars), so let's just do a simple stepwise in 'both' directions.

I will use the `ozone` dataset for this where the objective is to predict the `'ozone_reading'` based on other weather related observations.

```
# Load data
trainData <- read.csv("http://rstatistics.net/wp-content/uploads/2015/09/ozone1.csv (http://rstatistics.net/wp-content/uploads/2015/09/ozone1.csv), stringsAsFactors=F)
print(head(trainData))
```

	Month	Day_of_month	Day_of_week	ozone_reading	pressure_height	Wind_speed
1	1	1	4	3	5480	8
2	1	2	5	3	5660	6
3	1	3	6	3	5710	4
4	1	4	7	5	5700	3
5	1	5	1	5	5760	3
6	1	6	2	6	5720	4

	Humidity	Temperature_Sandburg	Temperature_ElMonte	Inversion_base_height
1	20.00000	40.53473	39.77461	5000.000
2	40.96306	38.00000	46.74935	4108.904
3	28.00000	40.00000	49.49278	2693.000
4	37.00000	45.00000	52.29403	590.000
5	51.00000	54.00000	45.32000	1450.000
6	69.00000	35.00000	49.64000	1568.000

	Pressure_gradient	Inversion_temperature	Visibility
1	-15	30.56000	200
2	-14	48.02557	300
3	-25	47.66000	250
4	-24	55.04000	100
5	25	57.02000	60
6	15	53.78000	60

The data is ready. Let's perform the stepwise.

```

# Step 1: Define base intercept only model
base.mod <- lm(ozone_reading ~ 1 , data=trainData)

# Step 2: Full model with all predictors
all.mod <- lm(ozone_reading ~ . , data= trainData)

# Step 3: Perform step-wise algorithm. direction='both' implies both forward and backward stepwise
stepMod <- step(base.mod, scope = list(lower = base.mod, upper = all.mod), direction = "both", trace = 0, steps = 1000)

# Step 4: Get the shortlisted variable.
shortlistedVars <- names(unlist(stepMod[[1]]))
shortlistedVars <- shortlistedVars[!shortlistedVars %in% "(Intercept)"] # remove intercept

# Show
print(shortlistedVars)

```

```

[1] "Temperature_Sandburg" "Humidity" "Temperature_ElMonte"
[4] "Month" "pressure_height" "Inversion_base_height"

```

The selected model has the above 6 features in it.

But if you have too many features (> 100) in training data, then it might be a good idea to split the dataset into chunks of 10 variables each with Y as mandatory in each dataset. Loop through all the chunks and collect the best features.

We are doing it this way because some variables that came as important in a training data with fewer features may not show up in a linear reg model built on lots of features.

Finally, from a pool of shortlisted features [from small chunk models], run a full stepwise model to get the final set of selected features.

You can take this as a learning assignment to be solved within 20 minutes.

5. Relative Importance from Linear Regression

This technique is specific to linear regression models.

Relative importance can be used to assess which variables contributed how much in explaining the linear model's R-squared value. So, if you sum up the produced importances, it will add up to the model's R-sq value.

In essence, it is not directly a feature selection method, because you have already provided the features that go in the model. But after building the model, the `relaimpo` can provide a sense of how important each feature is in contributing to the R-sq, or in other words, in 'explaining the Y variable'.

So, how to calculate relative importance?

It is implemented in the `relaimpo` package. Basically, you build a linear regression model and pass that as the main argument to `calc.relimp()`. `relaimpo` has multiple options to compute the relative importance, but the recommended method is to use `type='lmg'`, as I have done below.

```
# install.packages('relaimpo')
library(relaimpo)

# Build linear regression model
model_formula = ozone_reading ~ Temperature_Sandburg + Humidity + Temperature_ElMonte +
  Month + pressure_height + Inversion_base_height
lmMod <- lm(model_formula, data=trainData)

# calculate relative importance
relImportance <- calc.relimp(lmMod, type = "lmg", rela = F)

# Sort
cat('Relative Importances: \n')
sort(round(relImportance$lmg, 3), decreasing=TRUE)
```

```
Relative Importances:
Temperature_ElMonte    0.214
Temperature_Sandburg   0.203
pressure_height        0.104
Inversion_base_height  0.096
Humidity               0.086
Month                 0.012
```

Additionally, you can use bootstrapping (using `boot.relimp`) to compute the confidence intervals of the produced relative importances.

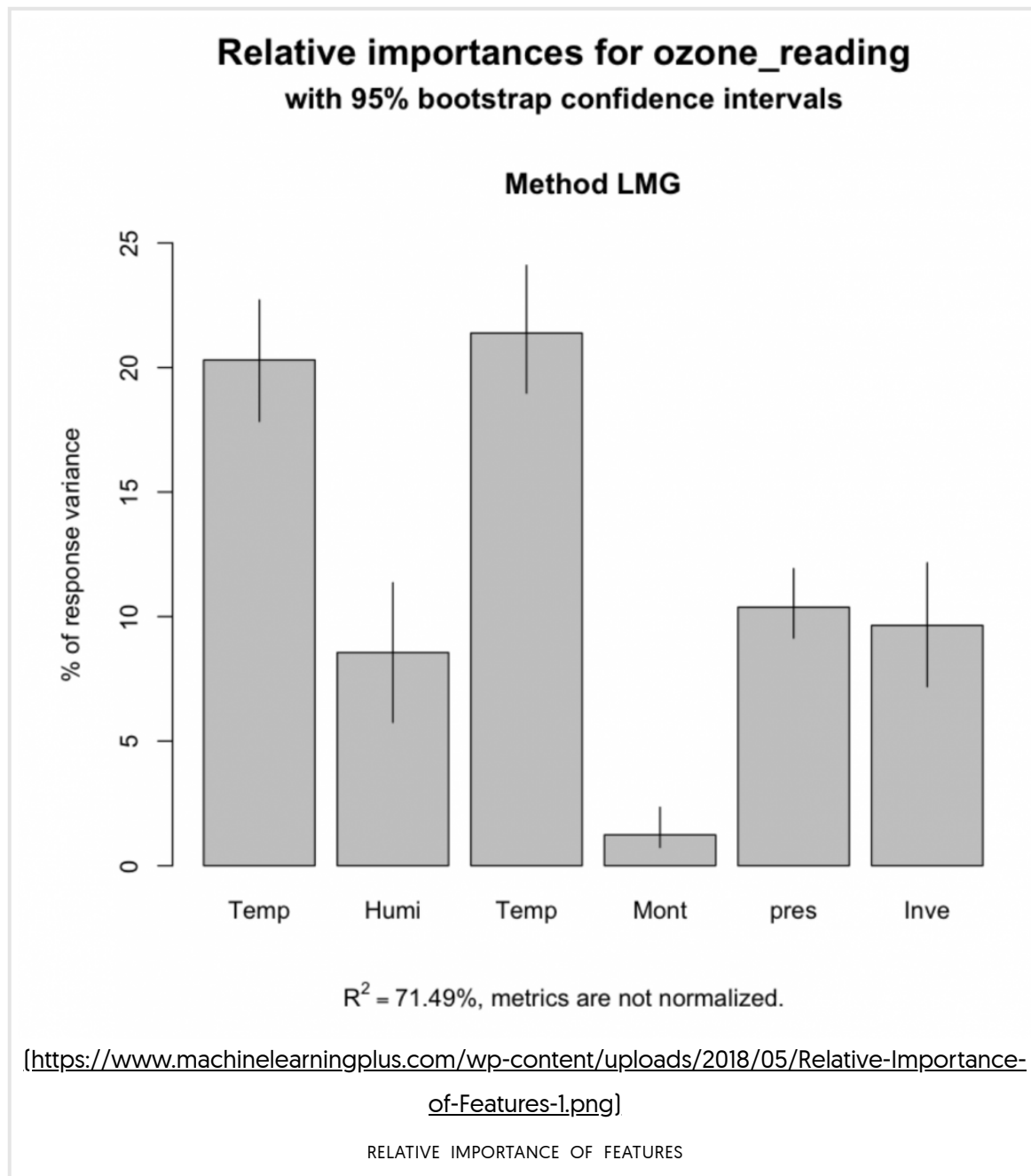
Feedback

```

bootsub <- boot.relimp(ozone_reading ~ Temperature_Sandburg + Humidity + Temperature_El
Monte + Month + pressure_height + Inversion_base_height, data=trainData,
                      b = 1000, type = 'lmg', rank = TRUE, diff = TRUE)

plot(booteval.relimp(bootsub, level=.95))

```



6. Recursive Feature Elimination (RFE)

Recursive feature elimination (rfe) [https://www.machinelearningplus.com/machine-learning/caret-package/#5howtodofeatureselectionusingrecursivefeatureeliminationrfe] offers a rigorous way to determine the important variables before you even feed them into a ML algo.

Feedback

It can be implemented using the `rfe()` from `caret` package.

The `rfe()` also takes two important parameters.

- `sizes`
- `rfeControl`

So, what does `sizes` and `rfeControl` represent?

The `sizes` determines the number of most important features the `rfe` should iterate. Below, I have set the size as 1 to 5, 10, 15 and 18.

Secondly, the `rfeControl` parameter receives the output of the `rfeControl()`. You can set what type of variable evaluation algorithm must be used. Here, I have used random forests based `rfFuncs`. The `method='repeatedCV'` means it will do a repeated k-Fold cross validation with `repeats=5`.

Once complete, you get the accuracy and kappa for each model size you provided. The final selected model subset size is marked with a `*` in the rightmost selected column.

```
str(trainData)
```

```
'data.frame':   366 obs. of  13 variables:
 $ Month          : int  1 1 1 1 1 1 1 1 1 1 ...
 $ Day_of_month   : int  1 2 3 4 5 6 7 8 9 10 ...
 $ Day_of_week    : int  4 5 6 7 1 2 3 4 5 6 ...
 $ ozone_reading  : num  3 3 3 5 5 6 4 4 6 7 ...
 $ pressure_height : num  5480 5660 5710 5700 5760 5720 5790 5790 5700 5700 ...
 $ Wind_speed     : int  8 6 4 3 3 4 6 3 3 3 ...
 $ Humidity       : num  20 41 28 37 51 ...
 $ Temperature_Sandburg : num  40.5 38 40 45 54 ...
 $ Temperature_ElMonte  : num  39.8 46.7 49.5 52.3 45.3 ...
 $ Inversion_base_height: num  5000 4109 2693 590 1450 ...
 $ Pressure_gradient   : num  -15 -14 -25 -24 25 15 -33 -28 23 -2 ...
 $ Inversion_temperature: num  30.6 48 47.7 55 57 ...
 $ Visibility         : int  200 300 250 100 60 60 100 250 120 120 ...
```

```

set.seed(100)
options(warn=-1)

subsets <- c(1:5, 10, 15, 18)

ctrl <- rfeControl(functions = rfFuncs,
                   method = "repeatedcv",
                   repeats = 5,
                   verbose = FALSE)

lmProfile <- rfe(x=trainData[, c(1:3, 5:13)], y=trainData$ozone_reading,
                sizes = subsets,
                rfeControl = ctrl)

lmProfile

```

Recursive feature selection

Outer resampling method: **Cross-Validated** (10 fold, repeated 5 times)

Resampling performance over subset size:

Variables	RMSE	Rsquared	MAE	RMSESD	RsquaredSD	MAESD	Selected
1	5.222	0.5794	4.008	0.9757	0.15034	0.7879	
2	3.971	0.7518	3.067	0.4614	0.07149	0.3276	
3	3.944	0.7553	3.054	0.4675	0.06523	0.3708	
4	3.924	0.7583	3.026	0.5132	0.06640	0.4163	
5	3.880	0.7633	2.950	0.5525	0.07021	0.4334	
10	3.751	0.7796	2.853	0.5550	0.06791	0.4457	*
12	3.767	0.7779	2.869	0.5511	0.06664	0.4424	

The top 5 variables (out of 10):

Temperature_ElMonte, Pressure_gradient, Temperature_Sandburg, Inversion_temperature, Humidity

So, it says, **Temperature_ElMonte**, **Pressure_gradient**, **Temperature_Sandburg**, **Inversion_temperature**, **Humidity** are the top 5 variables in that order.

And the best model size out of the provided models sizes [in `subsets`] is 10.

You can see all of the top 10 variables from '`lmProfile$optVariables`' that was created using '`rfe`' function above.

Feedback

7. Genetic Algorithm

You can perform a supervised feature selection with genetic algorithms using the `gafs()`. This is quite resource expensive so consider that before choosing the number of iterations `[iters]` and the number of repeats in `gafsControl()`.

```
# Define control function
ga_ctrl <- gafsControl(functions = rfGA, # another option is `caretGA`.
                      method = "cv",
                      repeats = 3)

# Genetic Algorithm feature selection
set.seed(100)
ga_obj <- gafs(x=trainData[, c(1:3, 5:13)],
              y=trainData[, 4],
              iters = 3, # normally much higher (100+)
              gafsControl = ga_ctrl)

ga_obj
```

Genetic Algorithm Feature Selection

366 samples

12 predictors

Maximum generations: 3

Population per generation: 50

Crossover probability: 0.8

Mutation probability: 0.1

Elitism: 0

Internal performance values: RMSE, **Rsquared**

Subset selection driven to minimize **internal** RMSE

External performance values: RMSE, **Rsquared**, MAE

Best iteration chose **by** minimizing external RMSE

External resampling method: **Cross-Validated** (10 fold)

During resampling:

- * the top 5 selected variables (out of a possible 12):

- Month** (100%), **Pressure_gradient** (100%), **Temperature_ElMonte** (100%), **Visibility** (90%), **Inversion_temperature** (80%)

- * on average, 7.5 variables were selected (min = 5, max = 10)

In the **final** search **using** the entire training **set**:

- * 6 features selected at iteration 3 including:

- Month**, **Day_of_month**, **Wind_speed**, **Temperature_ElMonte**, **Pressure_gradient** ...

- * external performance at **this** iteration **is**

RMSE	Rsquared	MAE
3.6605	0.7901	2.8010

```
# Optimal variables
```

```
ga_obj$optVariables
```

1. 'Month'
2. 'Day_of_month'
3. 'Wind_speed'
4. 'Temperature_ElMonte'
5. 'Pressure_gradient'

6. 'Visibility'

So the optimal variables according to the genetic algorithms are listed above. But, I wouldn't use it just yet because, the above variant was tuned for only 3 iterations, which is quite low. I had to set it so low to save computing time.

8. Simulated Annealing

Simulated annealing is a global search algorithm that allows a suboptimal solution to be accepted in hope that a better solution will show up eventually.

It works by making small random changes to an initial solution and sees if the performance improved. The change is accepted if it improves, else it can still be accepted if the difference of performances meet an acceptance criteria.

In caret it has been implemented in the `safs()` which accepts a control parameter that can be set using the `safsControl()` function.

`safsControl` is similar to other control functions in caret (like you saw in `rfe` and `ga`), and additionally it accepts an `improve` parameter which is the number of iterations it should wait without improvement until the values are reset to previous iteration.

```
# Define control function
sa_ctrl <- safsControl(functions = rfSA,
                      method = "repeatedcv",
                      repeats = 3,
                      improve = 5) # n iterations without improvement before a reset

# Genetic Algorithm feature selection
set.seed(100)
sa_obj <- safs(x=trainData[, c(1:3, 5:13)],
              y=trainData[, 4],
              safsControl = sa_ctrl)

sa_obj
```

Simulated Annealing Feature Selection

366 samples

12 predictors

Maximum search iterations: 10

Restart after 5 iterations without improvement (0.2 restarts on average)

Internal performance values: RMSE, **Rsquared**

Subset selection driven to minimize **internal** RMSE

External performance values: RMSE, **Rsquared**, MAE

Best iteration chose **by** minimizing external RMSE

External resampling method: **Cross-Validated** (10 fold, repeated 3 times)

During resampling:

- * the top 5 selected variables (**out** of a possible 12):

Temperature_ElMonte (73.3%), **Inversion_temperature** (63.3%), **Month** (60%), **Day_of_week** (50%), **Inversion_base_height** (50%)

- * on average, 6 variables were selected (min = 3, max = 8)

In the final search **using** the entire training **set**:

- * 6 features selected at iteration 10 including:

Month, **Day_of_month**, **Day_of_week**, **Wind_speed**, **Temperature_ElMonte** ...

- * external performance at **this** iteration **is**

RMSE	Rsquared	MAE
4.0574	0.7382	3.0727

```
# Optimal variables
```

```
print(sa_obj$optVariables)
```

```
[1] "Month"           "Day_of_month"    "Day_of_week"
[4] "Wind_speed"      "Temperature_ElMonte" "Visibility"
```

9. Information Value and Weights of Evidence

The Information Value can be used to judge how important a given categorical variable is in explaining the binary Y variable. It goes well with logistic regression

(<https://www.machinelearningplus.com/machine-learning/logistic-regression-tutorial-examples>) Feedback

r/) and other classification models that can model binary variables.

Let's try to find out how important the categorical variables are in predicting if an individual will earn >50k from the 'adult.csv' dataset. Just run the code below to import the dataset.

```
library(InformationValue)
inputData <- read.csv("http://rstatistics.net/wp-content/uploads/2015/09/adult.csv (http://rstatistics.net/wp-content/uploads/2015/09/adult.csv)")
print(head(inputData))
```

	AGE	WORKCLASS	FNLWGT	EDUCATION	EDUCATIONNUM	MARITALSTATUS
1	39	State-gov	77516	Bachelors	13	Never-married
2	50	Self-emp-not-inc	83311	Bachelors	13	Married-civ-spouse
3	38	Private	215646	HS-grad	9	Divorced
4	53	Private	234721	11th	7	Married-civ-spouse
5	28	Private	338409	Bachelors	13	Married-civ-spouse
6	37	Private	284582	Masters	14	Married-civ-spouse

	OCCUPATION	RELATIONSHIP	RACE	SEX	CAPITALGAIN	CAPITALLOSS
1	Adm-clerical	Not-in-family	White	Male	2174	0
2	Exec-managerial	Husband	White	Male	0	0
3	Handlers-cleaners	Not-in-family	White	Male	0	0
4	Handlers-cleaners	Husband	Black	Male	0	0
5	Prof-specialty	Wife	Black	Female	0	0
6	Exec-managerial	Wife	White	Female	0	0

	HOURSPERWEEK	NATIVECOUNTRY	ABOVE50K
1	40	United-States	0
2	13	United-States	0
3	40	United-States	0
4	40	United-States	0
5	40	Cuba	0
6	40	United-States	0

Alright, let's now find the information value for the categorical variables in the inputData.

```

# Choose Categorical Variables to compute Info Value.
cat_vars <- c ("WORKCLASS", "EDUCATION", "MARITALSTATUS", "OCCUPATION", "RELATIONSHIP",
  "RACE", "SEX", "NATIVECOUNTRY") # get all categorical variables

# Init Output
df_iv <- data.frame(VARS=cat_vars, IV=numeric(length(cat_vars)), STRENGTH=character(len
gth(cat_vars)), stringsAsFactors = F) # init output dataframe

# Get Information Value for each variable
for (factor_var in factor_vars){
  df_iv[df_iv$VARS == factor_var, "IV"] <- InformationValue::IV(X=inputData[, factor_va
r], Y=inputData$ABOVE50K)
  df_iv[df_iv$VARS == factor_var, "STRENGTH"] <- attr(InformationValue::IV(X=inputData
[, factor_var], Y=inputData$ABOVE50K), "howgood")
}

# Sort
df_iv <- df_iv[order(-df_iv$IV), ]

df_iv

```

	VARS	IV	STRENGTH
5	RELATIONSHIP	1.53560810	Highly Predictive
3	MARITALSTATUS	1.33882907	Highly Predictive
4	OCCUPATION	0.77622839	Highly Predictive
2	EDUCATION	0.74105372	Highly Predictive
7	SEX	0.30328938	Highly Predictive
1	WORKCLASS	0.16338802	Highly Predictive
8	NATIVECOUNTRY	0.07939344	Somewhat Predictive
6	RACE	0.06929987	Somewhat Predictive

Here is what the quantum of Information Value means:

- Less than 0.02, then the predictor is not useful for modeling (separating the Goods from the Bads)
- 0.02 to 0.1, then the predictor has only a weak relationship.

Feedback

- 0.1 to 0.3, then the predictor has a medium strength relationship.
- 0.3 or higher, then the predictor has a strong relationship.

That was about IV. Then what is Weight of Evidence?

Weights of evidence can be useful to find out how important a given categorical variable is in explaining the 'events' [called 'Goods' in below table.]

$$WOE = \ln \left(\frac{\text{perc good of all goods}}{\text{perc bad of all bads}} \right)$$

(https://www.machinelearningplus.com/wp-content/uploads/2018/05/WOE_Formula.png)

WEIGHTS OF EVIDENCE

The 'Information Value' of the categorical variable can then be derived from the respective WOE values.

IV = [perc good of all goods–perc bad of all bads] * WOE

The 'WOETable' below given the computation in more detail.

```
WOETable(X=inputData[, 'WORKCLASS'], Y=inputData$ABOVE50K)
```

CAT	GOODS	BADS	TOTAL	PCT_G	PCT_B	WOE	IV
?	191	1645	1836	0.0242940728	0.0665453074	-1.0076506	0.0425744832
Federal-gov	371	589	960	0.0471890104	0.0238268608	0.6833475	0.0159644662
Local-gov	617	1476	2093	0.0784787586	0.0597087379	0.2733496	0.0051307781
Never-worked	7	7	7	0.0008903587	0.0002831715	1.1455716	0.0006955764
Private	4963	17733	22696	0.6312643093	0.7173543689	-0.1278453	0.0110062102
Self-emp-inc	622	494	1116	0.0791147291	0.0199838188	1.3759762	0.0813627242

CAT	GOODS	BADS	TOTAL	PCT_G	PCT_B	WOE	IV
Self-emp-not-inc	724	1817	2541	0.0920885271	0.0735032362	0.2254209	0.0041895135
State-gov	353	945	1298	0.0448995167	0.0382281553	0.1608547	0.0010731201
Without-pay	14	14	14	0.0017807174	0.0005663430	1.1455716	0.0013911528

The total IV of a variable is the sum of IV's of its categories.

10. DALEX Package

The DALEX is a powerful package that explains various things about the variables used in an ML model.

For example, using the `variable_dropout()` function you can find out how important a variable is based on a dropout loss, that is how much loss is incurred by removing a variable from the model.

Apart from this, it also has the `single_variable()` [\[http://smarterpoland.pl/wp-content/uploads/2018/02/DALEX_single_variable.png\]](http://smarterpoland.pl/wp-content/uploads/2018/02/DALEX_single_variable.png) function that gives you an idea of how the model's output will change by changing the values of one of the X's in the model.

It also has the `single_prediction()` [\[http://smarterpoland.pl/index.php/2018/02/dalex-which-variables-influence-this-single-prediction/\]](http://smarterpoland.pl/index.php/2018/02/dalex-which-variables-influence-this-single-prediction/) that can decompose a single model prediction so as to understand which variable caused what effect in predicting the value of Y.

```
library(randomForest)
library(DALEX)

# Load data
inputData <- read.csv("http://rstatistics.net/wp-content/uploads/2015/09/adult.csv (http://rstatistics.net/wp-content/uploads/2015/09/adult.csv)")

# Train random forest model
rf_mod <- randomForest(factor(ABOVE50K) ~ ., data=inputData, ntree=100)
rf_mod

# Variable importance with DALEX
explained_rf <- explain(rf_mod, data=inputData, y=inputData$ABOVE50K)

# Get the variable importances
varimps = variable_dropout(explained_rf, type='raw')

print(varimps)
```

Call:

```
randomForest(formula = factor(ABOVE50K) ~ ., data = inputData, ntree = 100)
```

Type of random forest: classification

Number of trees: 100

No. of variables tried at each split: 3

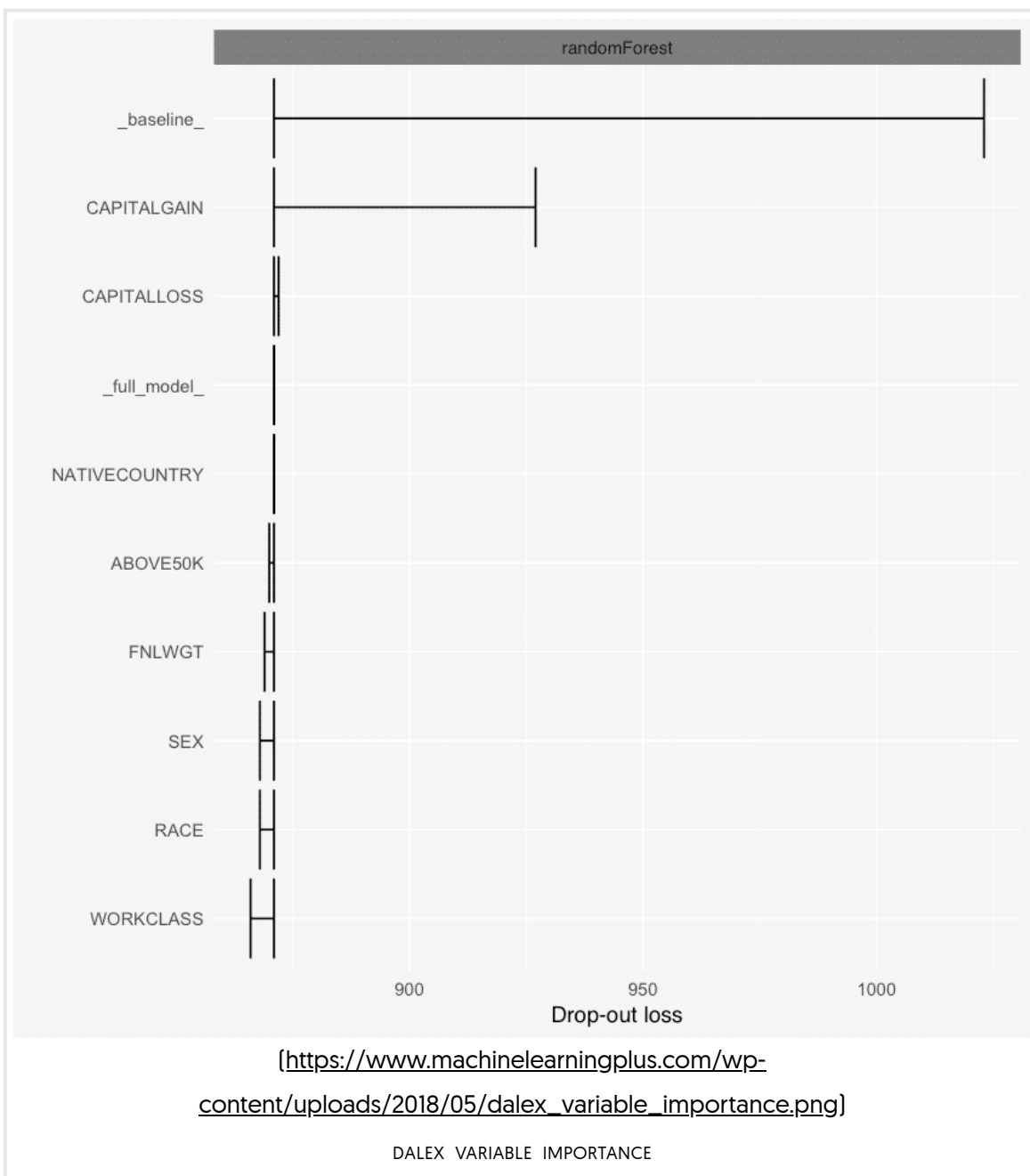
OOB estimate of error rate: 17.4%

Confusion matrix:

```
      0      1 class.error
0 24600  120 0.004854369
1  5547 2294 0.707435276
```

	variable	dropout_loss	label
1	_full_model_	852	randomForest
2	EDUCATIONNUM	842	randomForest
3	EDUCATION	843	randomForest
4	MARITALSTATUS	844	randomForest
5	FNLWGT	845	randomForest
6	OCCUPATION	847	randomForest
7	SEX	847	randomForest
8	CAPITALLOSS	847	randomForest
9	HOURSPERWEEK	847	randomForest
10	AGE	848	randomForest
11	RACE	848	randomForest
12	WORKCLASS	849	randomForest
13	RELATIONSHIP	850	randomForest
14	NATIVECOUNTRY	853	randomForest
15	ABOVE50K	853	randomForest
16	CAPITALGAIN	893	randomForest
17	_baseline_	975	randomForest

```
plot(varimps)
```



Conclusion

Hope you find these methods useful. As it turns out different methods showed different variables as important, or at least the degree of importance changed. This need not be a conflict, because each method gives a different perspective of how the variable can be useful depending on how the algorithms learn $Y \sim x$. So its cool.

If you find any code breaks or bugs, [report the issue here](https://docs.google.com/forms/d/e/1FAIpQLSeIjmlvwe562R7JVpi5J2ydLyhk5-7OrGRMFGYrMJvjPal8eA/viewform) (<https://docs.google.com/forms/d/e/1FAIpQLSeIjmlvwe562R7JVpi5J2ydLyhk5-7OrGRMFGYrMJvjPal8eA/viewform>) or just write it below.

You may also like:

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