ML lab – a tutorial related to ligand distances

Regression task using Random Forests

2018-11-14

A. Regression task – the development data and its distribution

Load the development data set D

```
> library(data.table)
> devel.D = fread("plr.dataset.D.development.csv", header=T)
> str(devel.D)
```

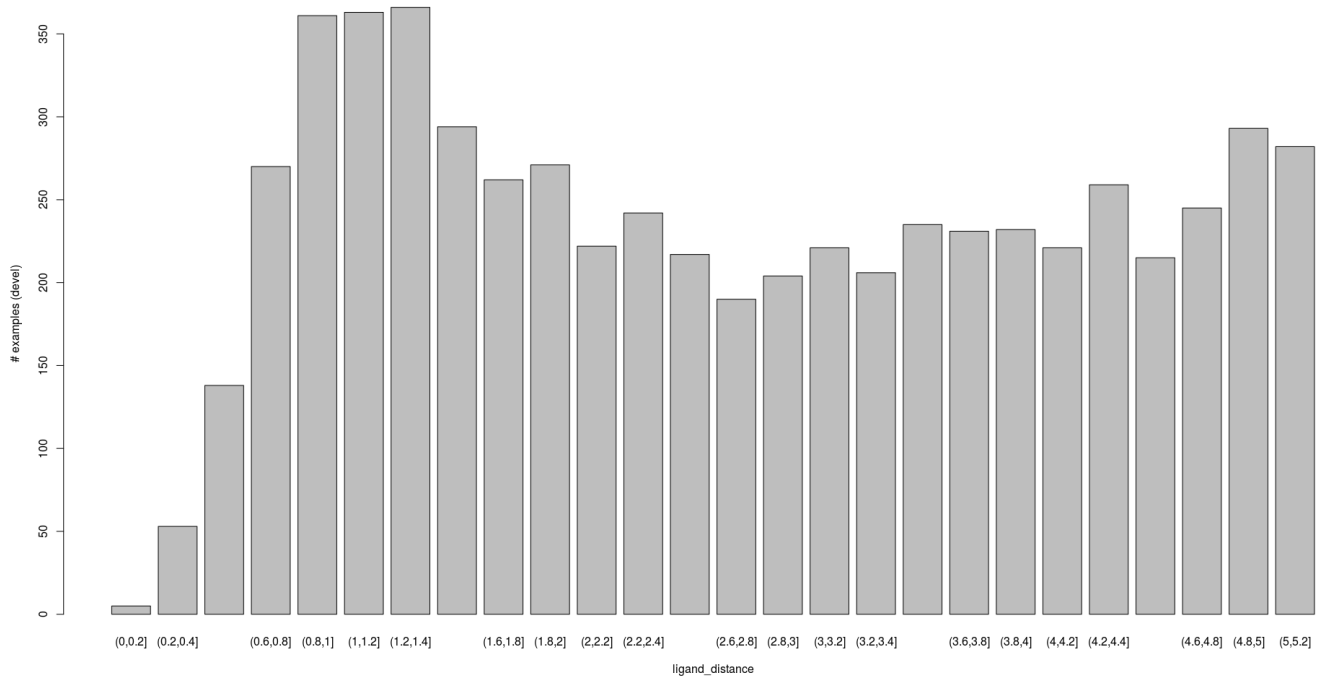
Find the number of different proteins in the data set

Analyze the distribution of ligand_distance

```
> summary(devel.D$ligand_distance)
```

Make a plot of empirical density
Hints

- use `cut(devel.D$ligand_distance)`
- set the intervals into which `ligand_distance` is to be cut by parameter `breaks`



B. Learning a Random Forest regression model

1. Prepare training and test subsets

```
> proteins.devel = unique(devel.D$protein_id)
> length(proteins.devel)

> set.seed(1); test.index = sample(20, 3, rep=F)

> proteins.test = proteins.devel[test.index]
> proteins.test

> proteins.train = proteins.devel[-test.index]
> proteins.train

> data.train = as.data.frame(devel.D[protein_id %in% proteins.train])
> nrow(data.train)
> length(unique(data.train$protein_id))

# remove protein_id
> data.train = data.train[, -1]
> str(data.train)


> data.test = as.data.frame(devel.D[protein_id %in% proteins.test])
> nrow(data.test)
> length(unique(data.test$protein_id))
> data.test = data.test[, -1]
```

2. Fit a Random Forest model

```
library(randomForest)

RF.ntree = 200                          # number of trees in the ensemble
RF.mtry  = 10                           # the default for regression is p/3

model.RF =
     randomForest(ligand_distance ~ ., data.train, ntree=RF.ntree, mtry=RF.mtry)
```

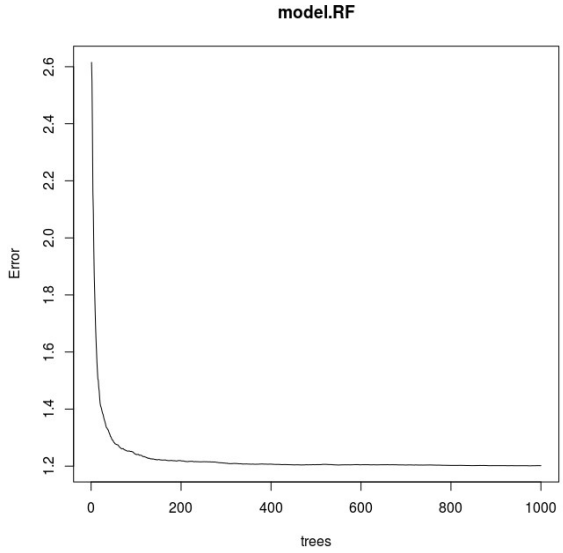
Try different parameter values.

Example of the output

```
> model.RF

Call:
 randomForest(formula = ligand_distance ~ ., data = data.train,
              ntree = RF.ntree, mtry = RF.mtry)

               Type of random forest: regression
                     Number of trees: 100
No. of variables tried at each split: 10

          Mean of squared residuals: 1.20056
                    % Var explained: 42.26
```

3. Evaluate your model

Use `plot(model)` to show the out-of-bag estimate of MSE error



Now compare the plotted error with the training error and test error!
– Why are the values different?

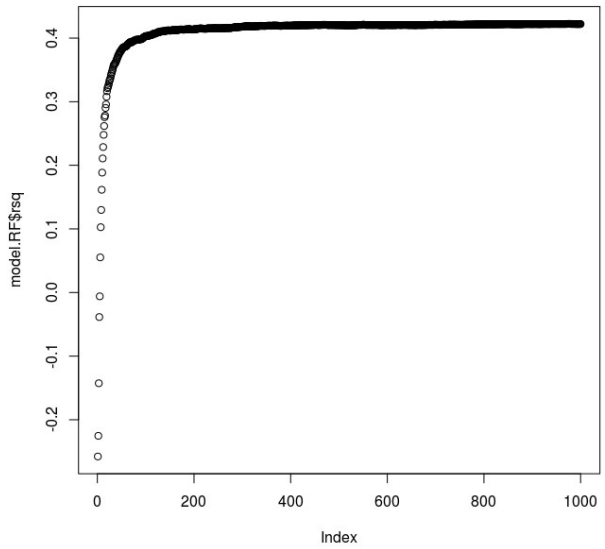
```
# prediction on the test set
> prediction.RF.test = predict(model.RF, data.test, type="response")
> MSE.test = mean( (data.test$ligand_distance - prediction.RF.test)^2 )
```

… and similarly using the training data set

Now do the cross-validation test and observe the variance od the test error. Then repeat whole cross-validation procedure several times (e.g. 10 times) with different random splits. You should always keep whole test proteins separated from the training ones!

Also, look at another plot – "pseudo R-squared": 1 – MSE/Var(y).
Available for regression only.

```
> plot(model.RF$rsq)
```



4. Explore the variable importance

```
> model.RF$importance
> varImpPlot(model.RF)
```