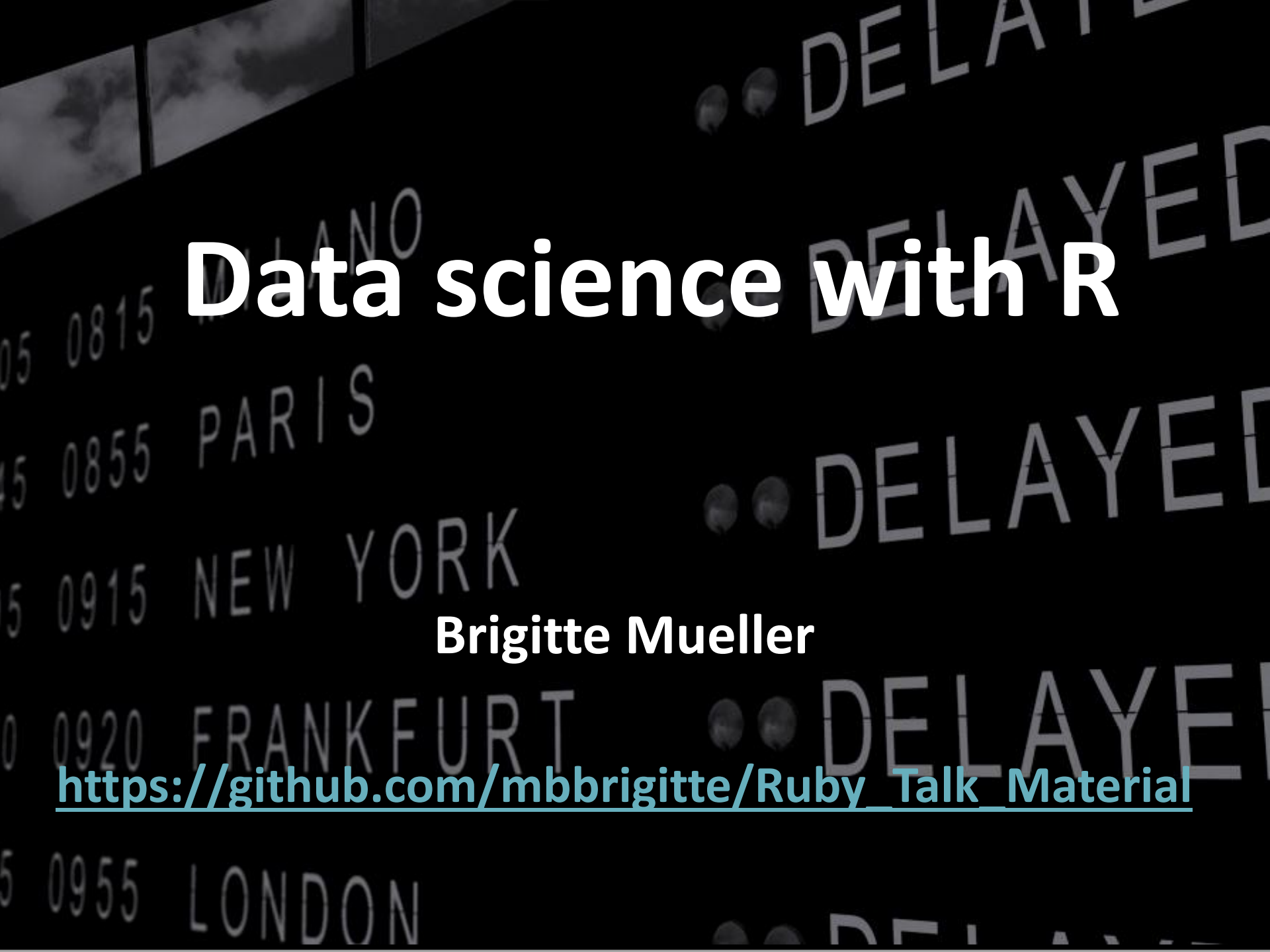


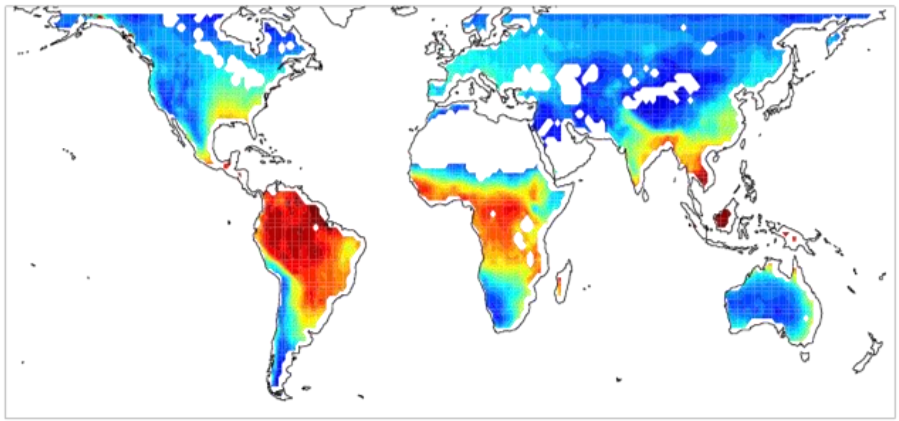
Data science with R

Brigitte Mueller

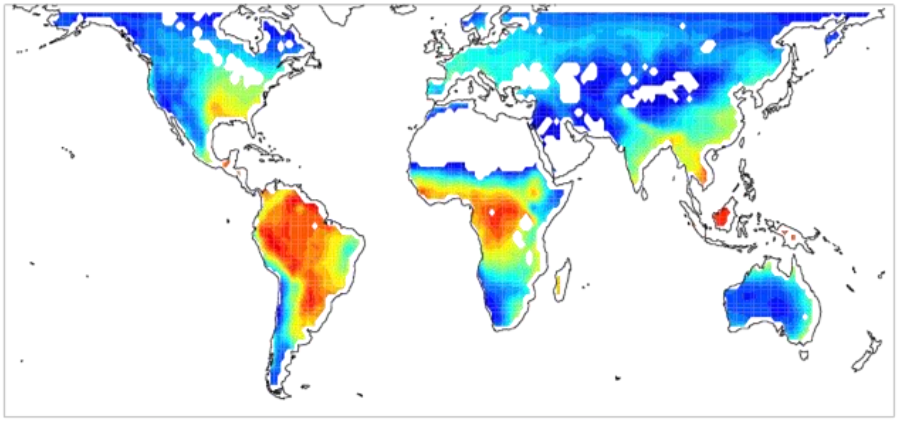
https://github.com/mbbrigitte/Ruby_Talk_Material

How to compare evaporation datasets?

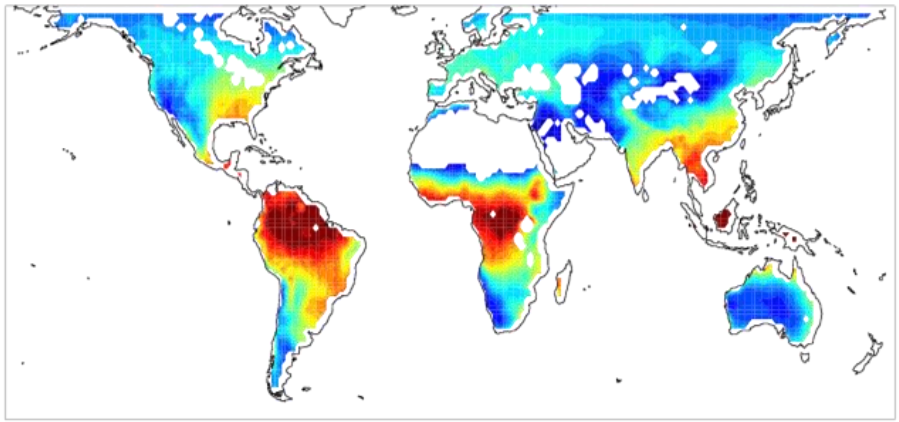
Dataset Number 1



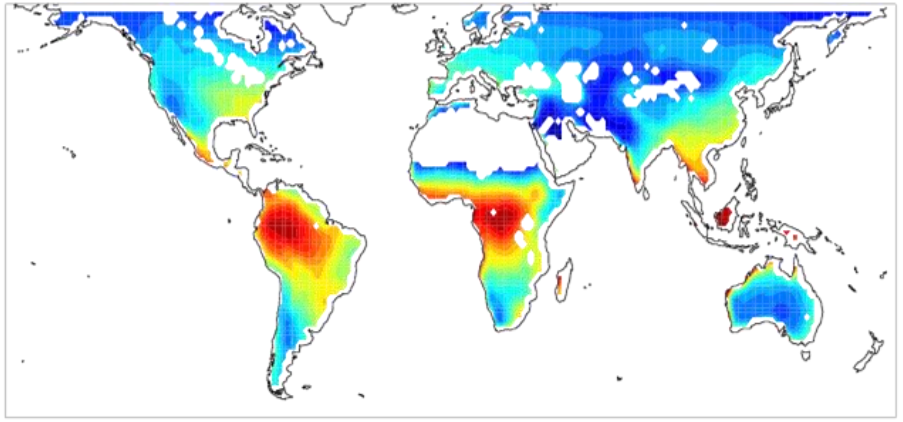
Dataset Number 2

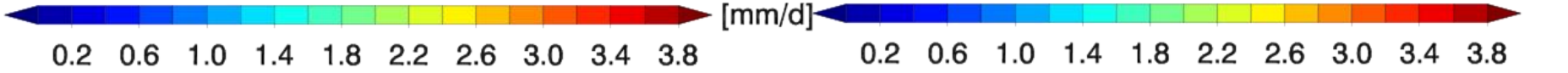


Dataset Number 3



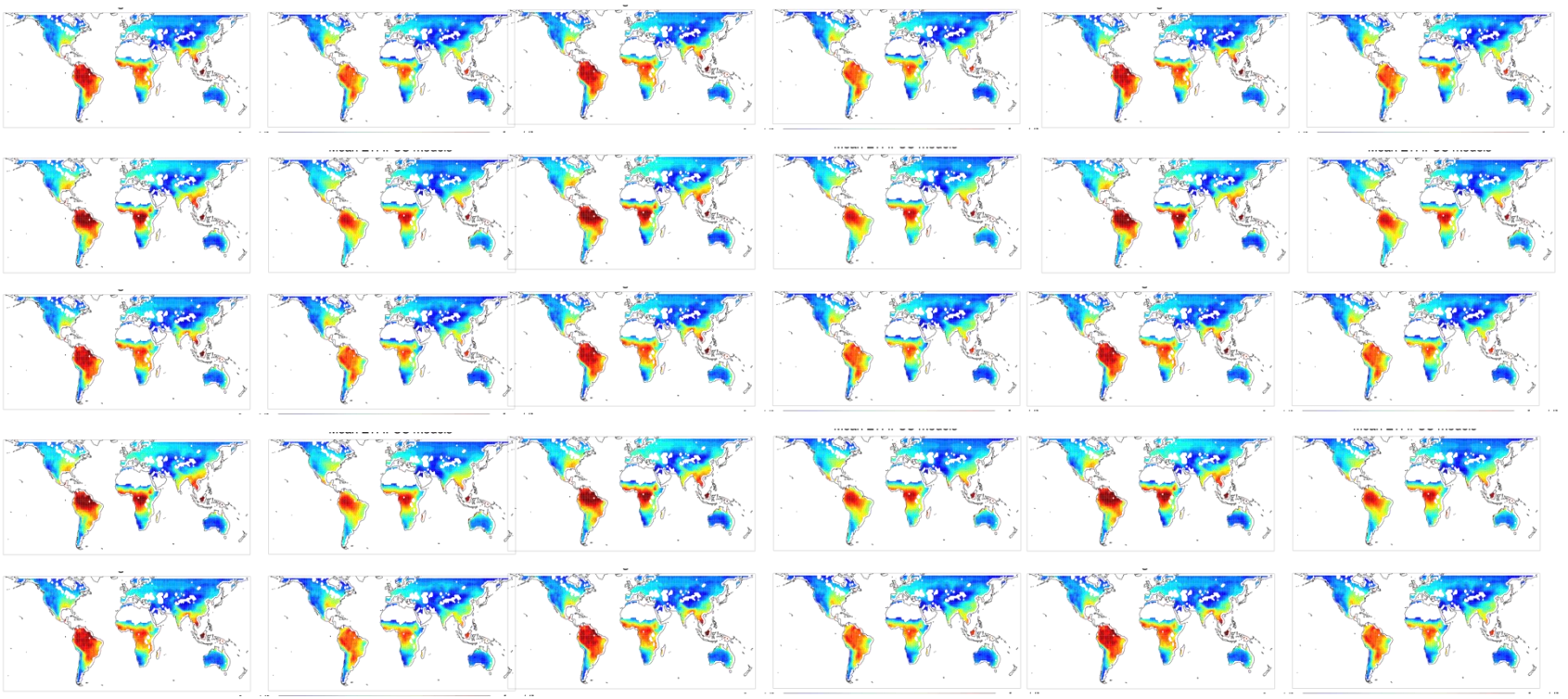
Dataset Number 4





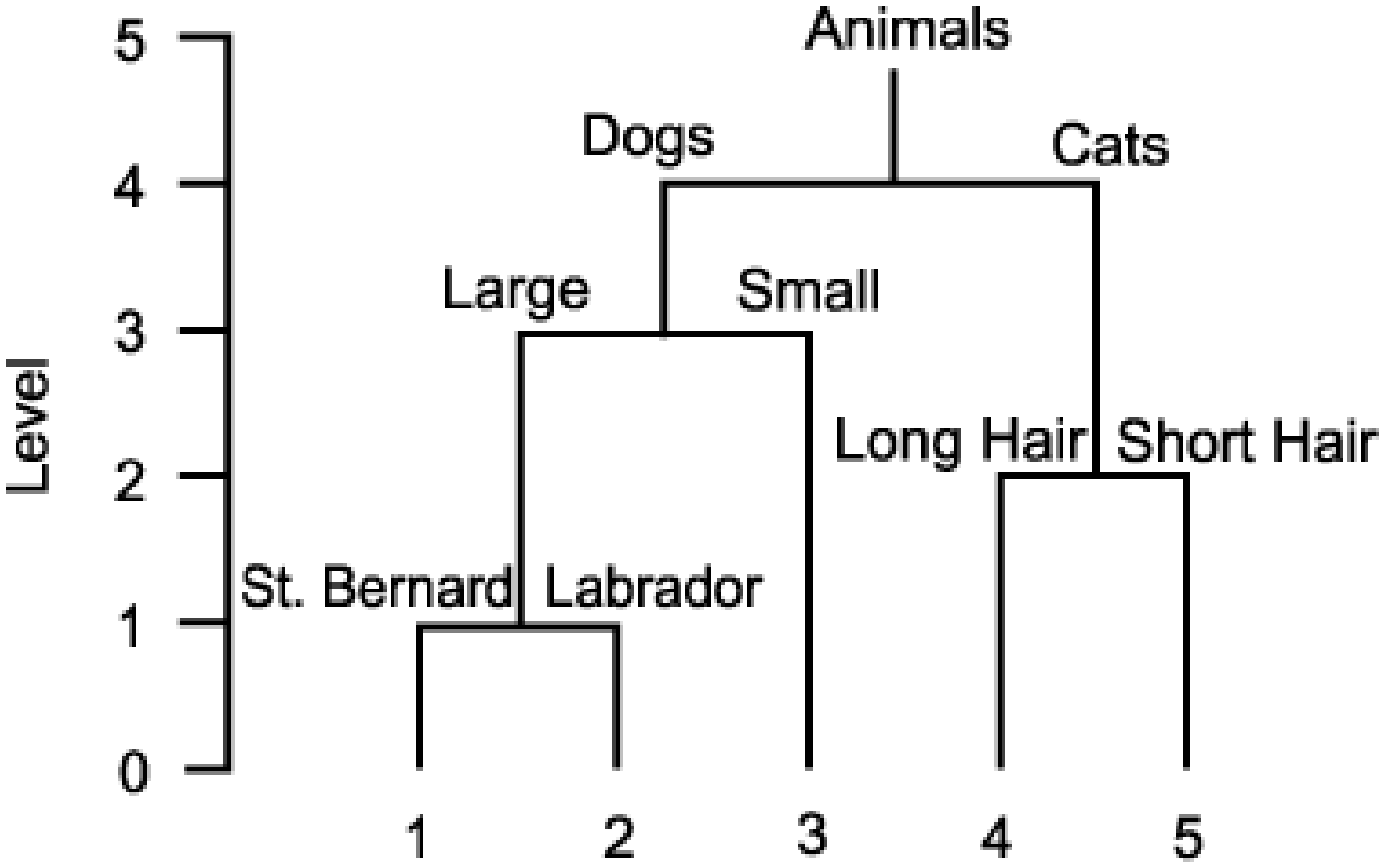
Mueller *et al*. *GRL*, 2011

How to compare 30 datasets?



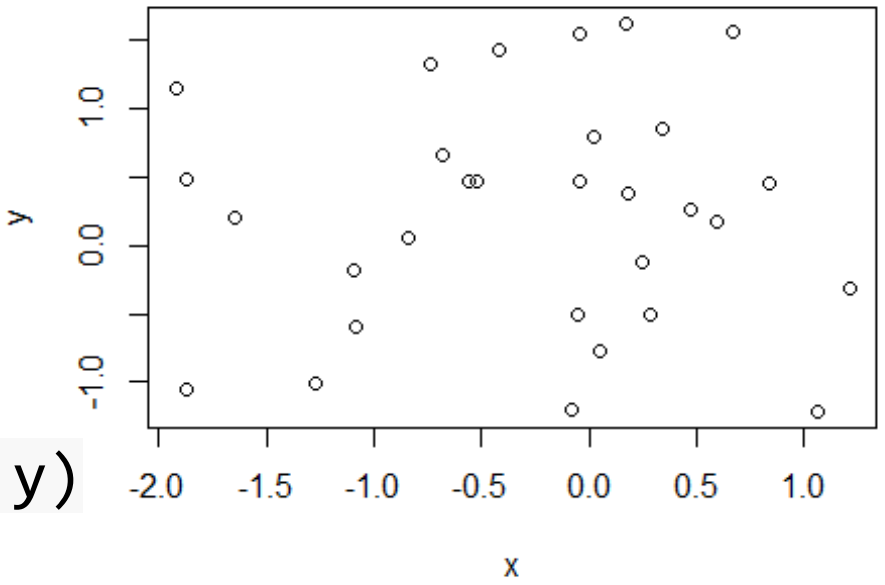
→ Hierarchical clustering

How to compare datasets?



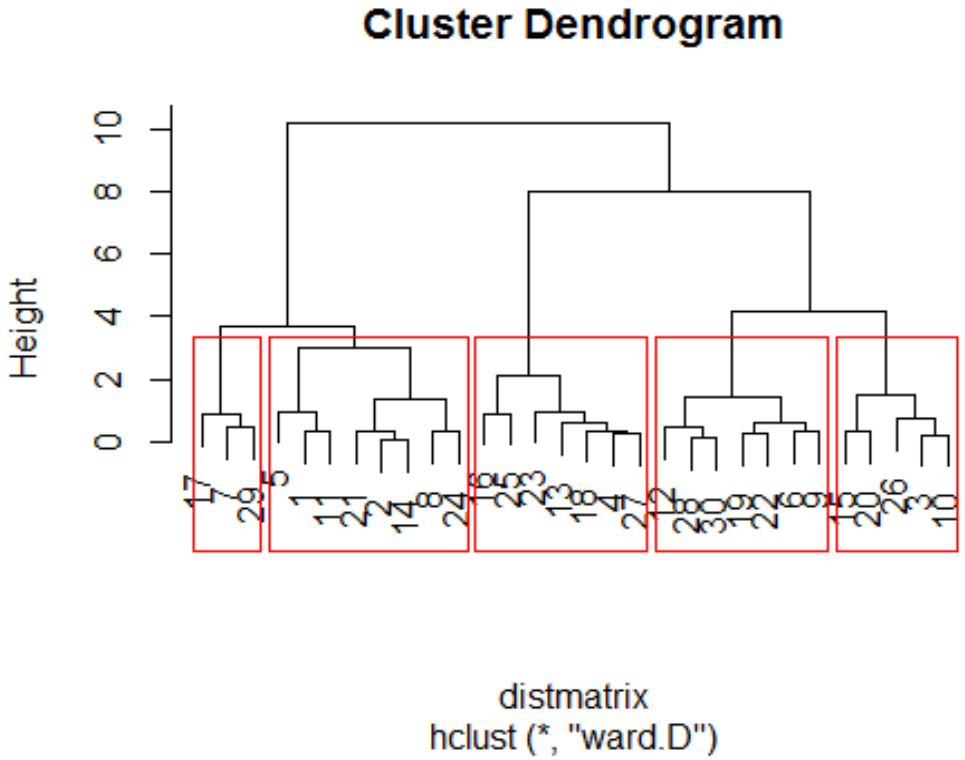
Create some data

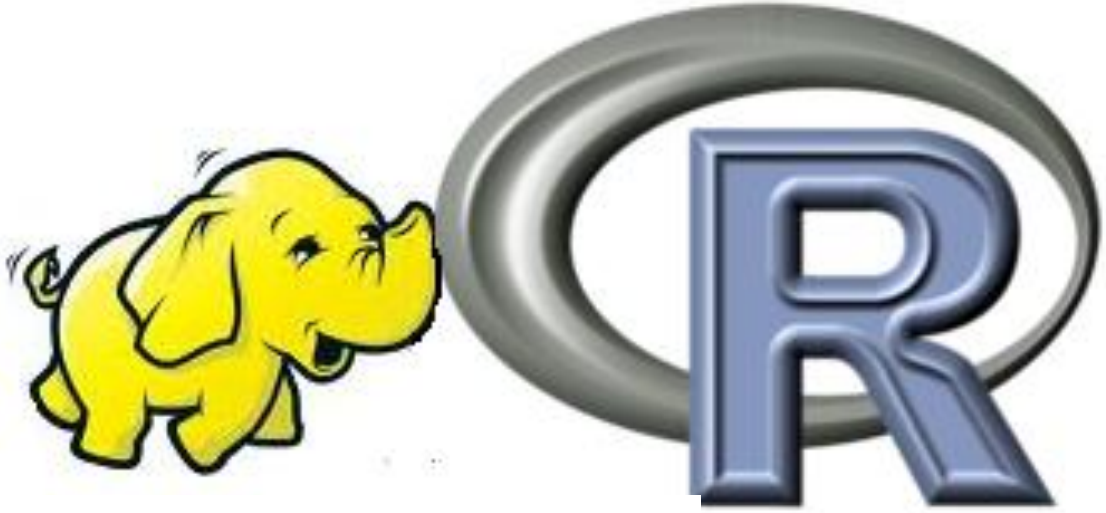
```
x <- rnorm(30)
y <- rnorm(30)
plot(x,y)

datamatrix <- cbind(x,y)
```



Calculate the distances and the clusters

```
distmatrix <- dist(datamatrix)
fit <- hclust(distmatrix, method="ward.D")
plot(fit)
```






Spark


in
Ruby


```
>> require "rinruby"
```

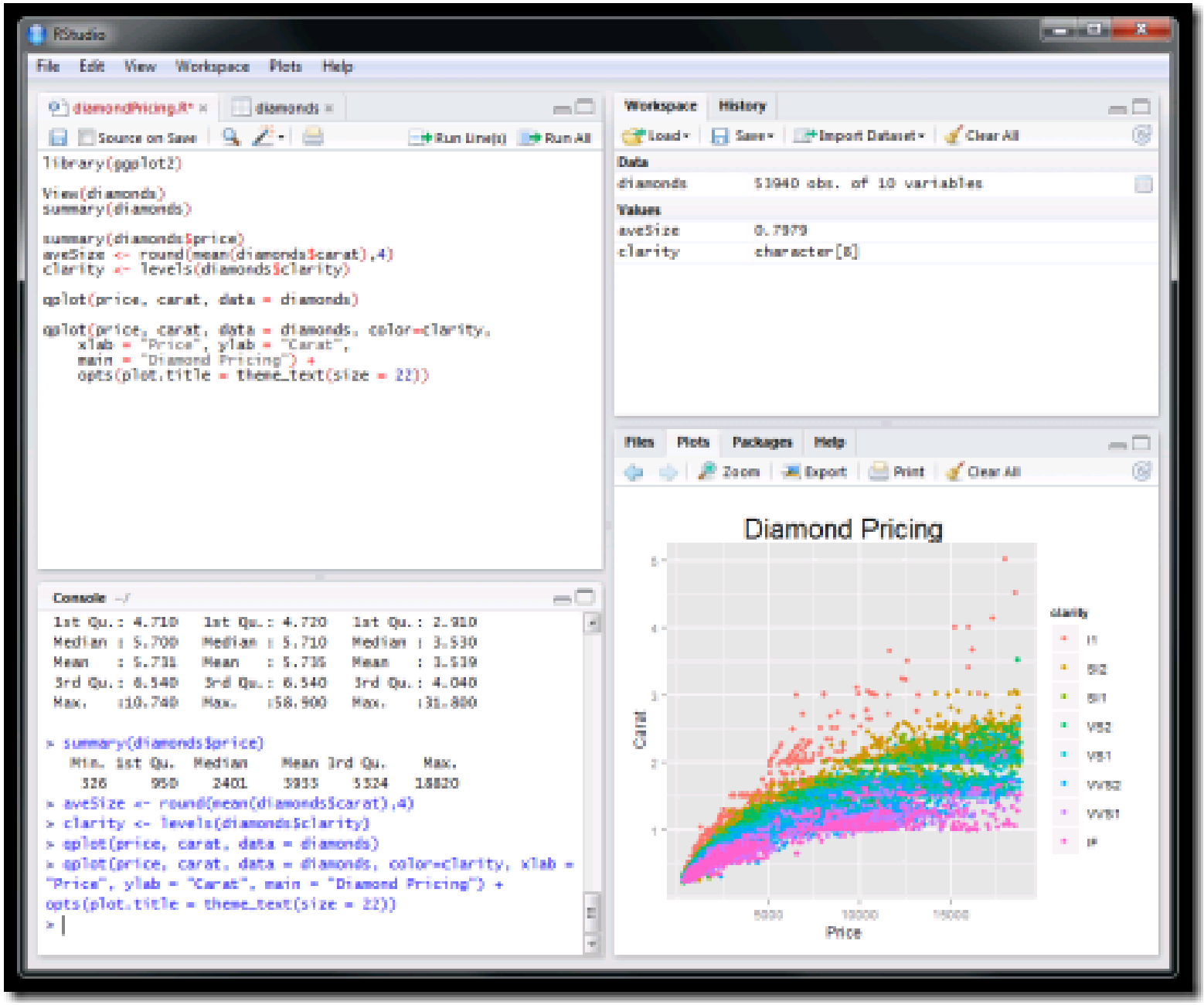
- Reads definition of RinRuby class into Ruby interpreter
- Creates instance of RinRuby class named R
- eval instance method passes R commands contained in the supplied string

```
>>  sample_size = 10
>>  R.eval "x <- rnorm(#{sample_size})"
>>  R.eval "summary(x)"
```

produces the following :

```
   Min.   1st Qu. Median   Mean    3rd Qu.   Max.
-1.88900 -0.84930 -0.45220 -0.49290 -0.06069 0.78160
```

More info: https://sites.google.com/a/ddahl.org/rinruby-users/documentation


RStudio
File Edit View Workspace Plots Help
diamondPricing.R*
diamonds
Source on Save
Run Line(s)
Run All
library(ggplot2)
View(diamonds)
summary(diamonds)
summary(diamonds$price)
aveSize <- round(mean(diamonds$carat),4)
clarity <- levels(diamonds$clarity)
qplot(price, carat, data = diamonds)
qplot(price, carat, data = diamonds, color=clarity,
xlab = "Price", ylab = "Carat",
main = "Diamond Pricing") +
opts(plot.title = theme_text(size = 22))
Workspace
History
Load
Save
Import Dataset
Clear All
Data
diamonds 53940 obs. of 10 variables
Values
aveSize 0.7979
clarity character[8]
Files
Plots
Packages
Help
Zoom
Export
Print
Clear All
Diamond Pricing
Carat
Price
clarity
I1
SI2
SI1
VS2
VS1
VVS2
VVS1
IF
Console
1st Qu.: 4.710 1st Qu.: 4.720 1st Qu.: 2.910
Median : 5.700 Median : 5.710 Median : 3.530
Mean : 5.731 Mean : 5.735 Mean : 3.539
3rd Qu.: 6.540 3rd Qu.: 6.540 3rd Qu.: 4.040
Max. :10.740 Max. :58.900 Max. :31.800
> summary(diamonds$price)
Min. 1st Qu. Median Mean 3rd Qu. Max.
326 950 2401 3933 5324 18820
> aveSize <- round(mean(diamonds$carat),4)
> clarity <- levels(diamonds$clarity)
> qplot(price, carat, data = diamonds)
> qplot(price, carat, data = diamonds, color=clarity, xlab =
"Price", ylab = "Carat", main = "Diamond Pricing") +
opts(plot.title = theme_text(size = 22))
>

Supervised learning

Delayed or not?

Target

Binary prediction: Delayed 0/1

Arriving late (= 15 minutes)

50%
accuracy

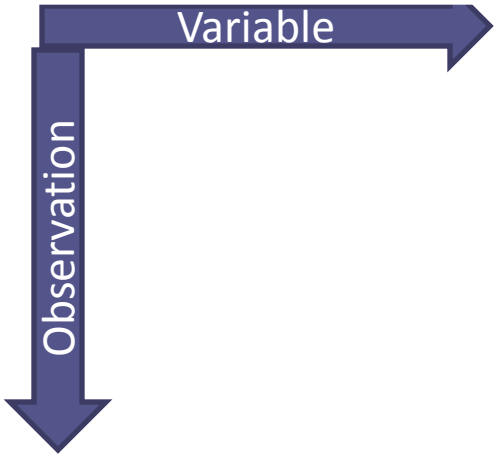
Goal
70% accuracy

Prepare data

Clean, explore, tidy

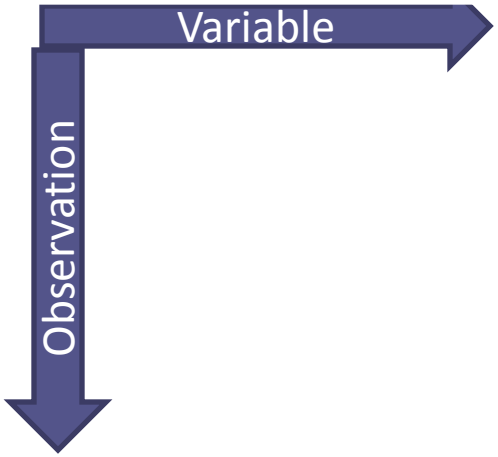
Prepare data

Clean, explore, tidy

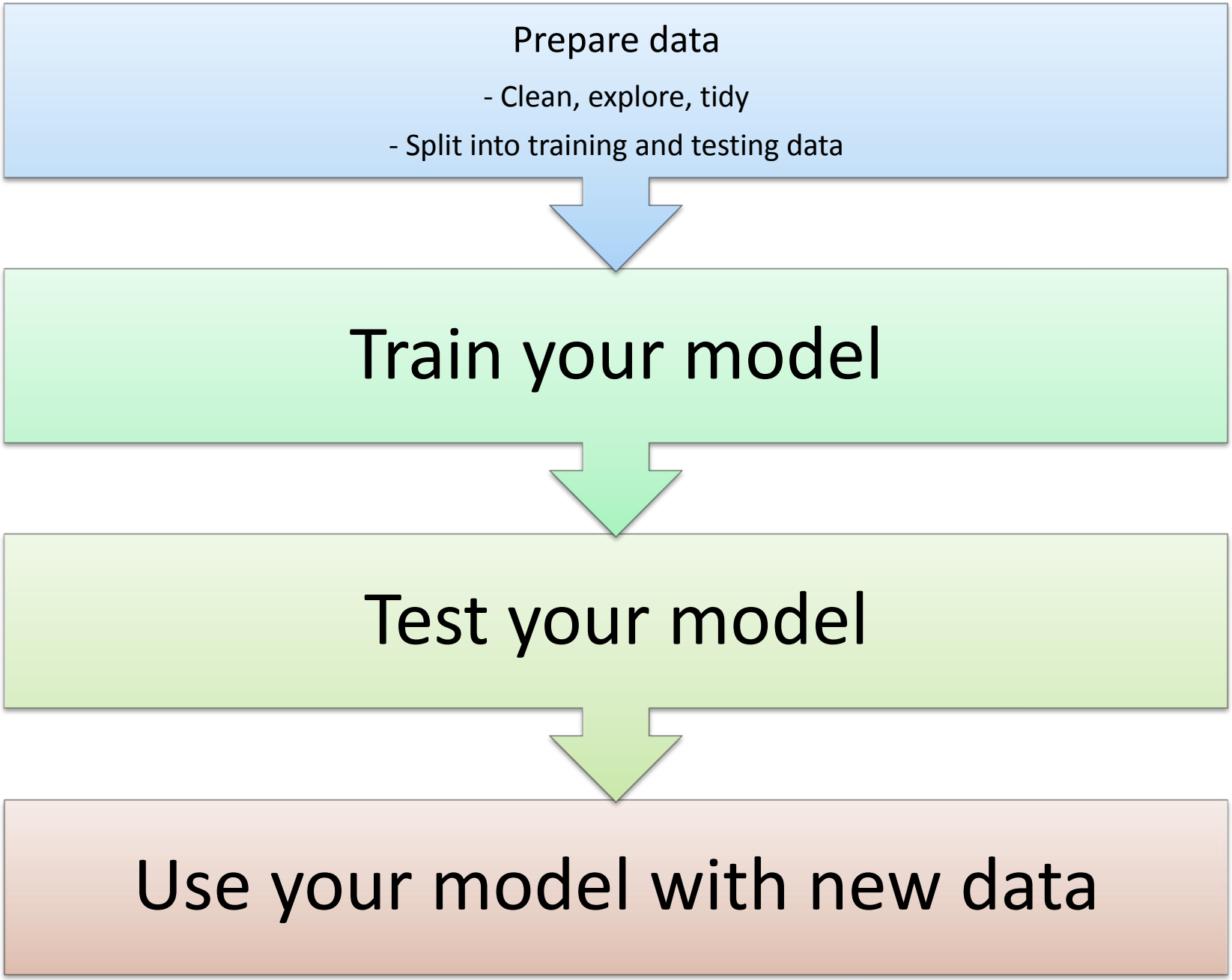


Prepare data

Clean, explore, tidy



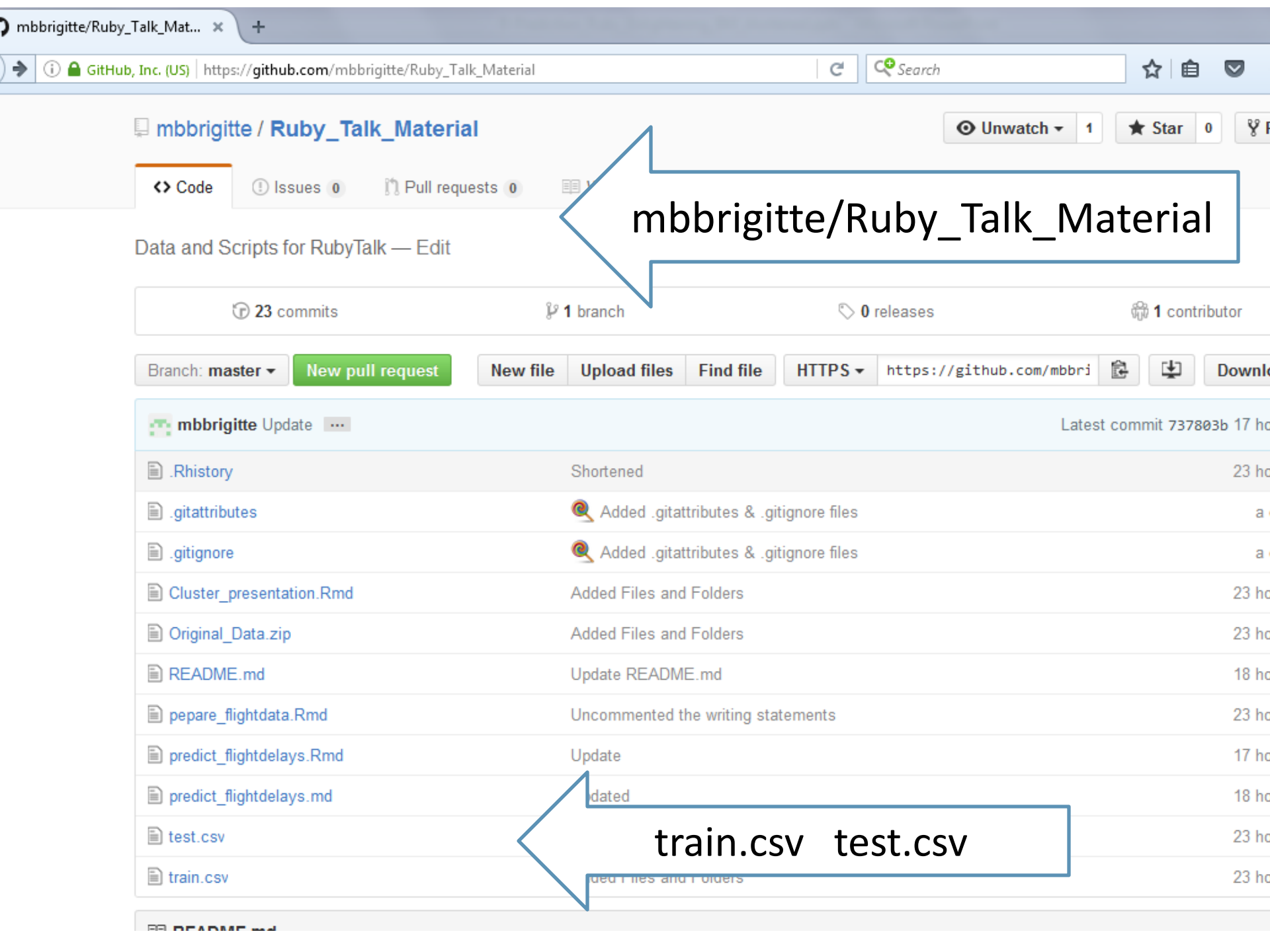
Split into training and testing data

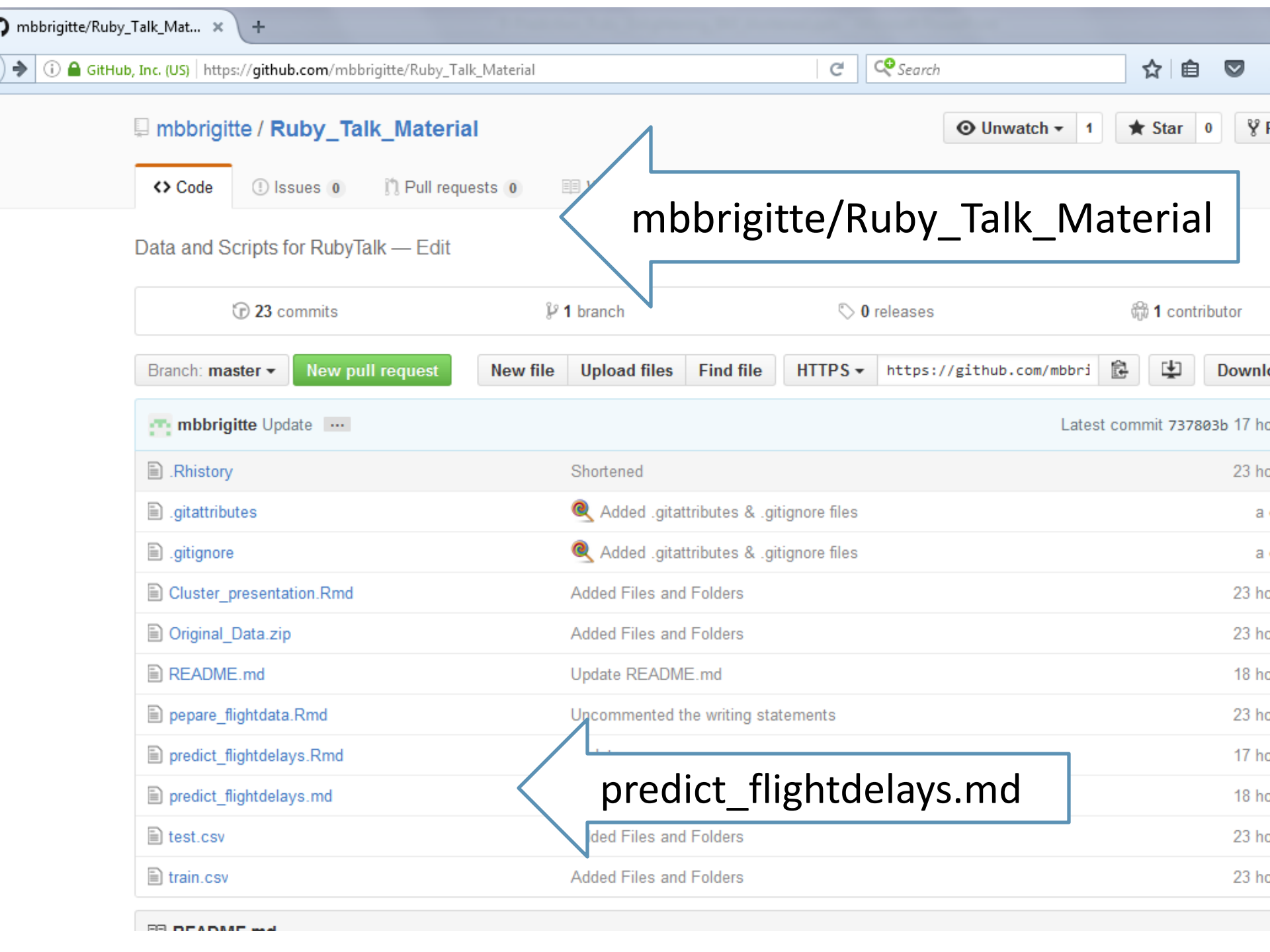

Prepare data
- Clean, explore, tidy
- Split into training and testing data
Train your model
Test your model
Use your model with new data

Data

Prepared for you, tidied and saved as
train.csv test.csv

Download at
https://github.com/mbbrigitte/Ruby_Talk_Material


mbbrigitte/Ruby_Talk_Mat...
GitHub, Inc. (US) https://github.com/mbbrigitte/Ruby_Talk_Material
Search
mbbrigitte / Ruby_Talk_Material
Unwatch 1
Star 0
Code
Issues 0
Pull requests 0
mbbrigitte/Ruby_Talk_Material
Data and Scripts for RubyTalk — Edit
23 commits
1 branch
0 releases
1 contributor
Branch: master
New pull request
New file
Upload files
Find file
HTTPS
https://github.com/mbbri
mbbrigitte Update
Latest commit 737803b 17 ho
.Rhistory Shortened 23 ho
.gitattributes Added .gitattributes & .gitignore files a
.gitignore Added .gitattributes & .gitignore files a
Cluster_presentation.Rmd Added Files and Folders 23 ho
Original_Data.zip Added Files and Folders 23 ho
README.md Update README.md 18 ho
pepare_flightdata.Rmd Uncommented the writing statements 23 ho
predict_flightdelays.Rmd Update 17 ho
predict_flightdelays.md dated 18 ho
test.csv 23 ho
train.csv 23 ho
train.csv test.csv


mbbrigitte/Ruby_Talk_Mat...
GitHub, Inc. (US) https://github.com/mbbrigitte/Ruby_Talk_Material
Search
mbbrigitte / Ruby_Talk_Material
Unwatch 1
Star 0
Code
Issues 0
Pull requests 0
mbbrigitte/Ruby_Talk_Material
Data and Scripts for RubyTalk — Edit
23 commits
1 branch
0 releases
1 contributor
Branch: master
New pull request
New file
Upload files
Find file
HTTPS
https://github.com/mbbri
mbbrigitte Update
Latest commit 737803b 17 ho
.Rhistory Shortened 23 ho
.gitattributes Added .gitattributes & .gitignore files a
.gitignore Added .gitattributes & .gitignore files a
Cluster_presentation.Rmd Added Files and Folders 23 ho
Original_Data.zip Added Files and Folders 23 ho
README.md Update README.md 18 ho
pepare_flightdata.Rmd Uncommented the writing statements 23 ho
predict_flightdelays.Rmd 17 ho
predict_flightdelays.md 18 ho
test.csv ded Files and Folders 23 ho
train.csv Added Files and Folders 23 ho
predict_flightdelays.md

Data

What variables are in the files?
Check with

read.csv(filename)
names(data)

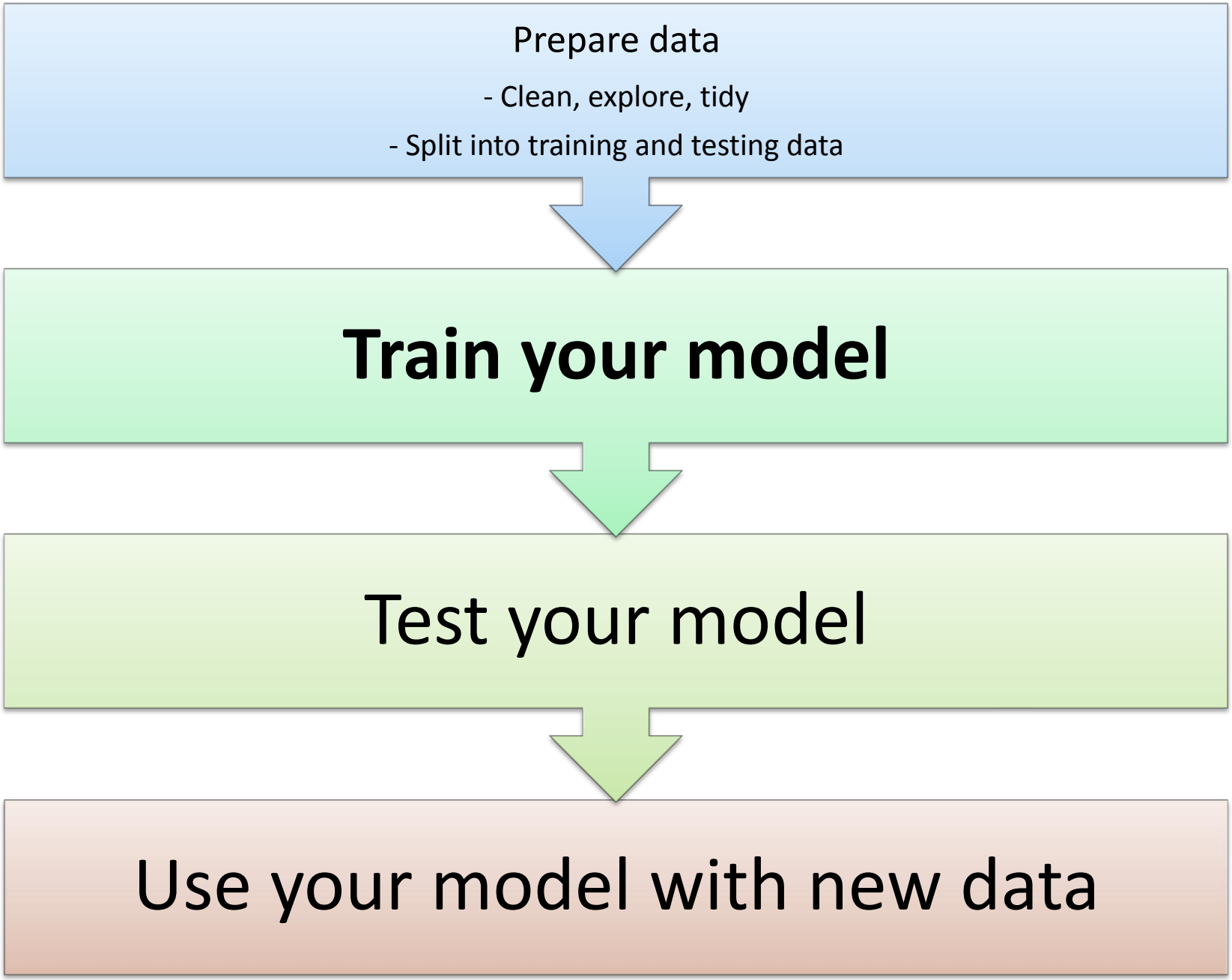
ARR_DEL15, DAY_OF_WEEK, CARRIER, DEST, ORIGIN, DEP_TIME_BLK

Code: Set-up

```
set.seed(100)


install.packages('caret')
library(caret)
```

Code: Read data

```
trainData <- read.csv('train.csv',sep=',', header=TRUE)
testData <- read.csv('test.csv',sep=',', header=TRUE)
```

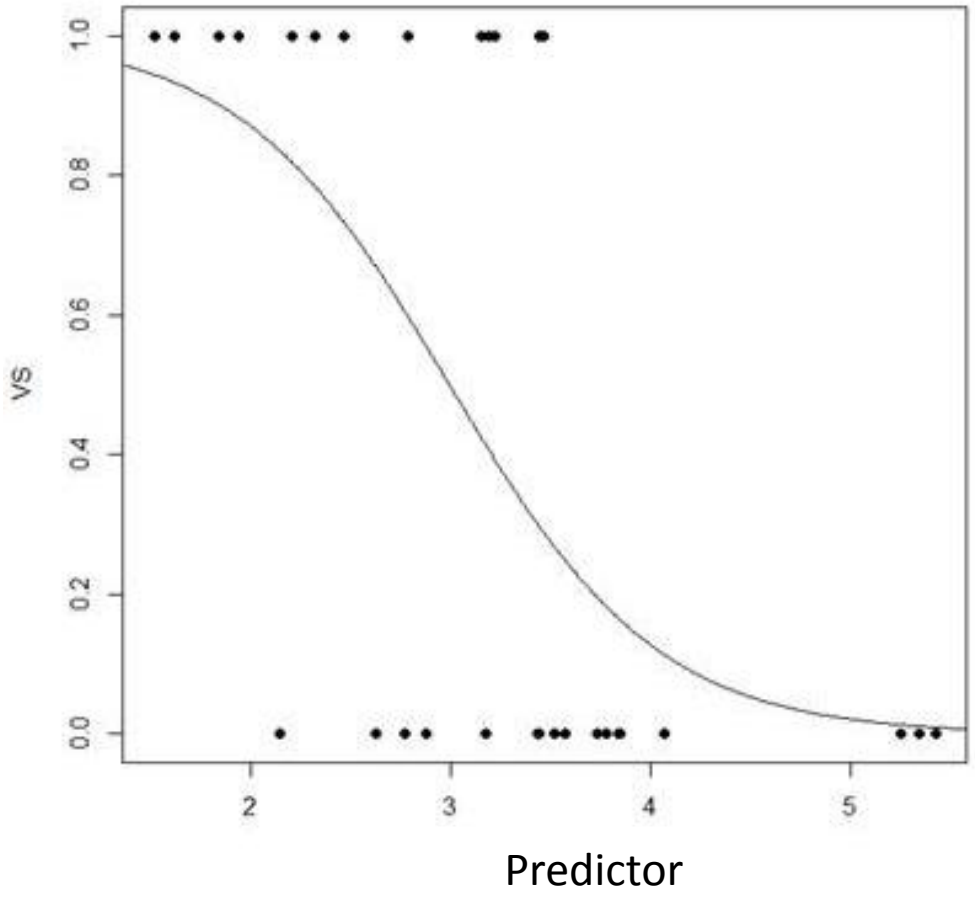

Prepare data
- Clean, explore, tidy
- Split into training and testing data
Train your model
Test your model
Use your model with new data

Select algorithm

- Classification algorithm
- Start simple
- If performance not that good, improve
  - Ensemble algorithms
  - Select more important variables from the data
  - Include additional predictor variables
  - Feature-engineering

Logistic regression

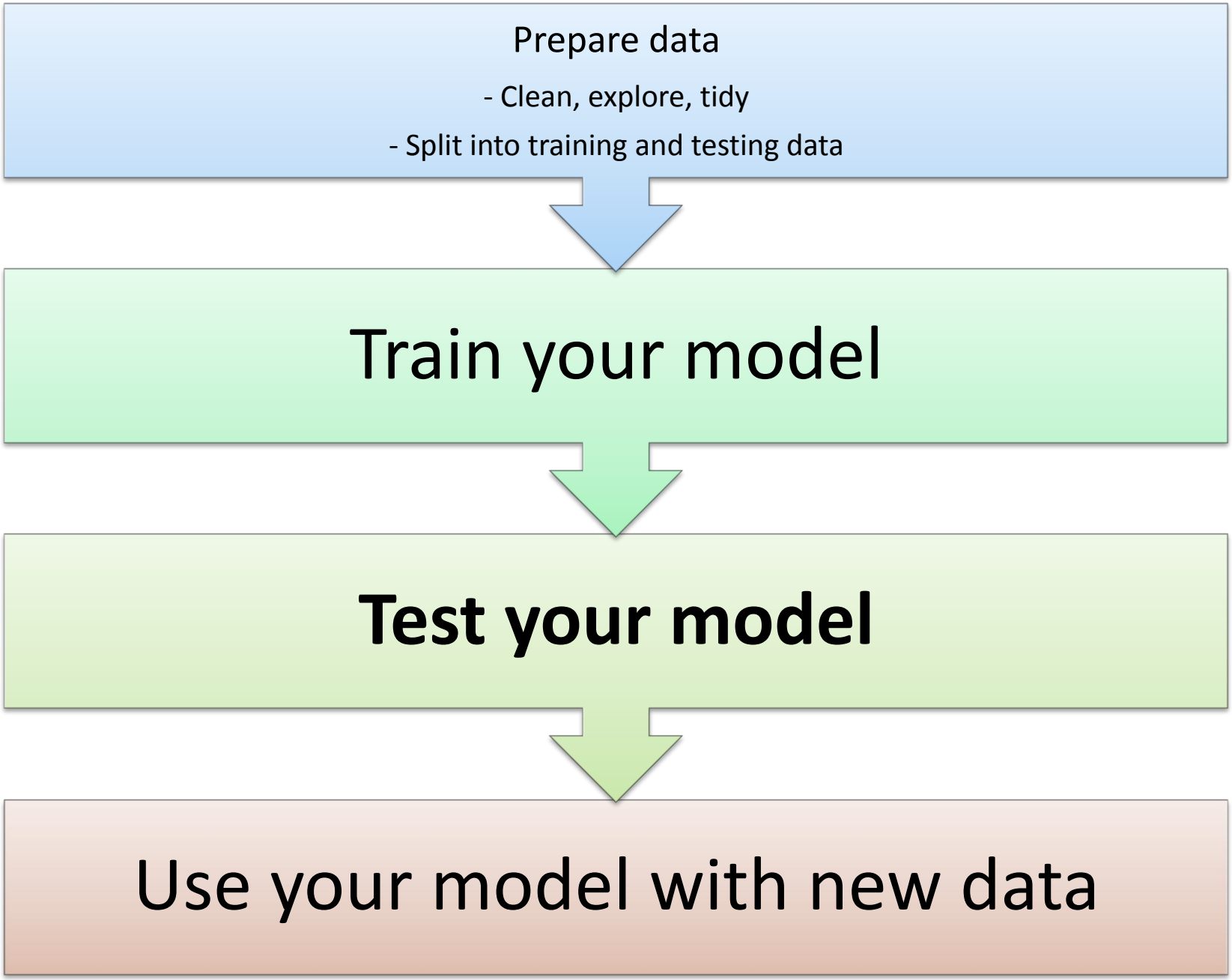
- Regression that predicts a categorical value



Train

```
library(caret)


logisticRegModel <- train(ARR_DEL15 ~ .,
data=trainData, method = 'glm', family =
'binomial')
```

Dot: 'all available variables, i.e. all columns', glm gene ralized linear regression. Family binomial for logistic regression.


Prepare data
- Clean, explore, tidy
- Split into training and testing data
Train your model
Test your model
Use your model with new data

Predict and test

Use your model and the test data to check how well we predict flight arrival delays.

```
logRegPrediction <- predict(logisticRegModel, testData)

logRegConfMat <- confusionMatrix(logRegPrediction,
                 testData[,"ARR_DEL15"])

logRegConfMat
```

```
## Confusion Matrix and Statistics
##           Reference
## Prediction    0    1
##          0 7465 2273
##          1   65   94
##
##               Accuracy : 0.7638
##                 95% CI : (0.7553, 0.7721)
##    No Information Rate : 0.7608
##    P-Value [Acc > NIR] : 0.2513
##
##                  Kappa : 0.0457
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.99137
##             Specificity : 0.03971
##          Pos Pred Value : 0.76658
##          Neg Pred Value : 0.59119
##              Prevalence : 0.76084
##          Detection Rate : 0.75427
##    Detection Prevalence : 0.98393
##       Balanced Accuracy : 0.51554
##
##        'Positive' Class : 0
```

```
## Confusion Matrix and Statistics
##                Reference
## Prediction    0    1
##         0       7465 2273
##         1         65   94
##
##               Accuracy : 0.7638
##                 95% CI : (0.7553, 0.7721)
##    No Information Rate : 0.7608
##    P-Value [Acc > NIR] : 0.2513
##
##                  Kappa : 0.0457
##  Mcnemar's Test P-Value : <2e-16
##
##          Sensitivity : 0.99137
##          Specificity : 0.03971
##       Pos Pred Value : 0.76658
##       Neg Pred Value : 0.59119
##           Prevalence : 0.76084
##       Detection Rate : 0.75427
##    Detection Prevalence : 0.98393
##      Balanced Accuracy : 0.51554
##
##       'Positive' Class : 0
```

```
## Confusion Matrix and Statistics
##                Reference
## Prediction    0    1
##         0       7465 2273
##         1         65   94
##
##               Accuracy : 0.7638
##                 95% CI : (0.7553, 0.7
##    No Information Rate : 0.7608
##    P-Value [Acc > NIR] : 0.2513
##
##                  Kappa : 0.0457
##  Mcnemar's Test P-Value : <2e-16
##
##             Sensitivity : 0.99137
##             Specificity : 0.03971
##          Pos Pred Value : 0.76658
##          Neg Pred Value : 0.59119
##              Prevalence : 0.76084
##          Detection Rate : 0.75427
##    Detection Prevalence : 0.98393
##       Balanced Accuracy : 0.51554
##
##        'Positive' Class : 0
```

		Reference	
		0 not delayed	1 delayed
Prediction	0 not delayed	7465	2273
	1 delayed	64	94

Specificity = 94/(2273+94)

Specificity
proportion of negatives that are correctly identified as such

Specificity is low - Improve model

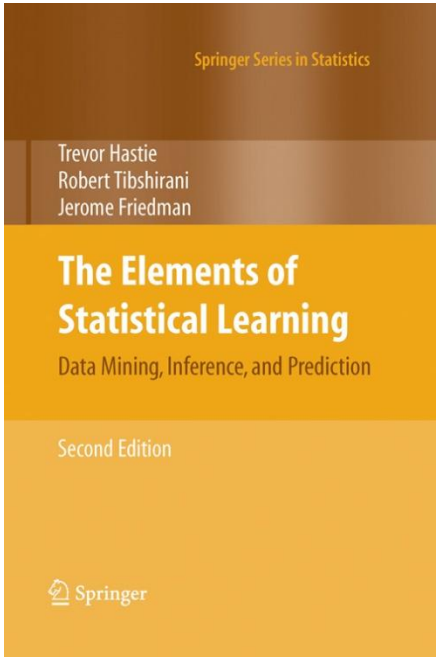
```
names(getModelInfo())

logisticRegModel <- train(ARR_DEL15 ~ .,
data=trainData, method = 'glm', family =
'binomial')
```

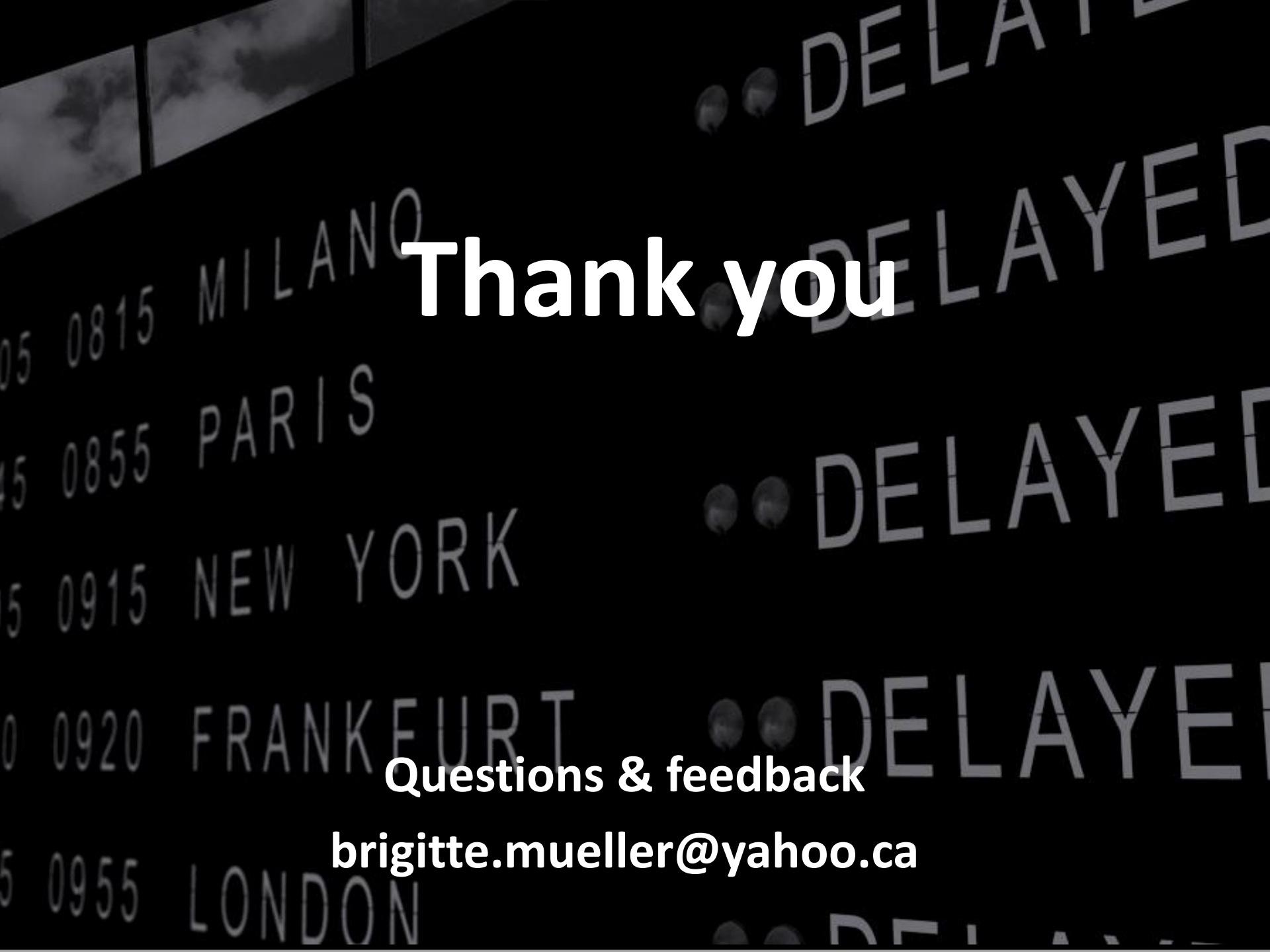
Next steps

- Try basics yourself
  - Improve model used with data in this talk
  - Titanic dataset: http://amunategui.github.io/binary-outcome-modeling/
  - https://www.datacamp.com/courses/kaggle-tutorial-on-machine-learing-the-sinking-of-the-titanic
- Try advanced methods
  - Kaggle
- Find your own dataset
- Learn more about machine learning and R:

Further reading

Elements of Statistical Learning, Hastie et al. 2009, Springer:
Available for fee
http://statweb.stanford.edu/~tibs/ElemStatLearn/





Thank you

Questions & feedback

brigitte.mueller@yahoo.ca

Picture sources

- http://www.tronviggroup.com/open-source-evolution/ (world with people)
- http://twit88.com/blog/2011/03/01/open-source-ide-for-r/ (R IDE)
- http://www.dailymail.co.uk (Coin toss)
- http://www.theanalysisfactor.com/r-glm-plotting/ (log. Regression figure)

Do it yourself

- Download and install R https://www.r-project.org/ and RStudio https://www.rstudio.com/ if you want to (it is convenient)
- Download the train.csv and test.csv files from Github https://github.com/mbbrigitte/Ruby_Talk_Material
- Use the ….Rmd files in R or just browse the code with the ….md file in your explorer

R: Packages and functions

- Lots of statistical packages (libraries)

```
install.packages('caret')
```

```
library(caret)
```

- Run line by line or write programms with ending .R

```
source("foo.R")
```

- Function

```
myfun<- function(arg1, arg2, …)
    w=arg1^2
    return(arg2 + w)
    }
```

```
myfun(arg=3,arg2=5)
```

R: Subsetting

- Matrix

  mat <- matrix(data=c(9,2,3,4,5,6),ncol=3)

  mat[1,2] #output is 3

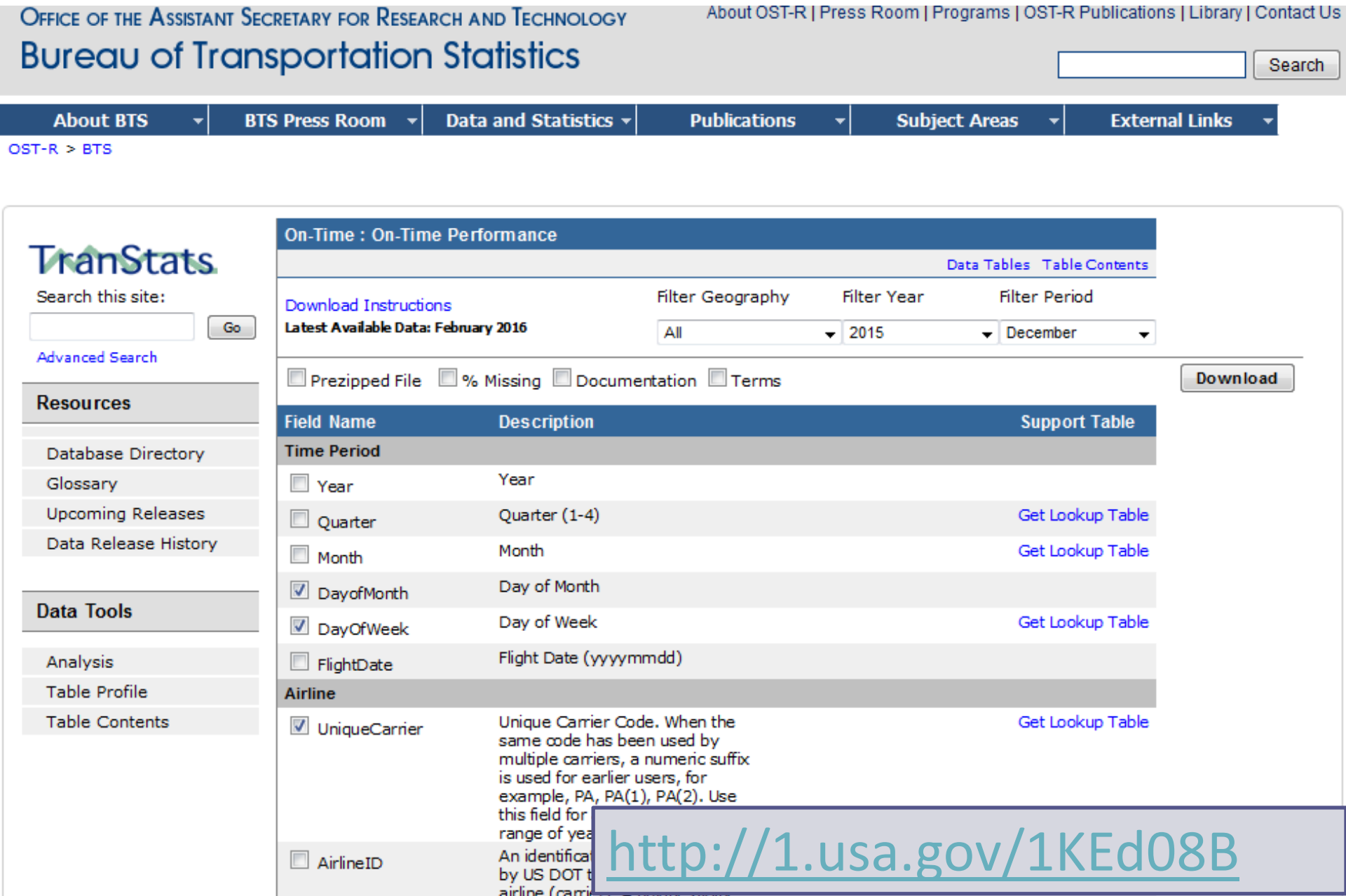
  mat[2,] #output is 2,4,6

- Lists:

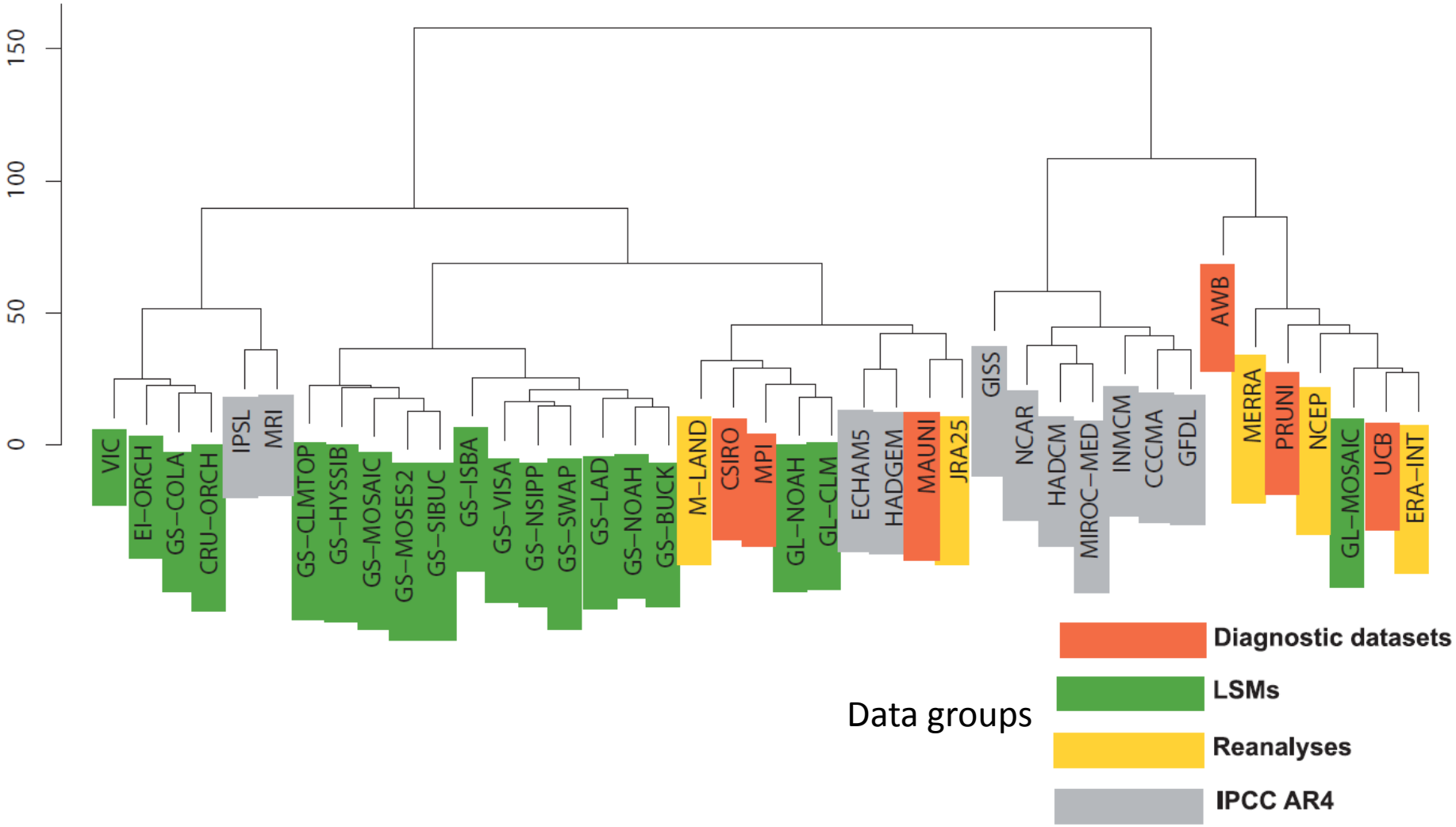
  L = list(one=1, two=c(1,2), five=seq(0, 1,length=5))

  L$five #output 0.00 0.25 0.50 0.75 1.00

Original data source



Results from evaporation dataset clustering



Mueller *et al*. *GRL*, 2011

Example with gbm instead of glm method, i.e. boosted tree model: see http://topepo.github.io/caret/training.html

```
fitControl <- trainControl(method = 'repeatedcv', number = 10, repeats = 10)


gbmFit1 <- train(ARR_DEL15 ~ ., data=trainData, method = 'gbm',trControl = fitControl,verbose = FALSE)
```