DublinR - Machine Learning

Machine Learning on Machines

Eoin Brazil - https://github.com/braz/DublinR-ML-machine

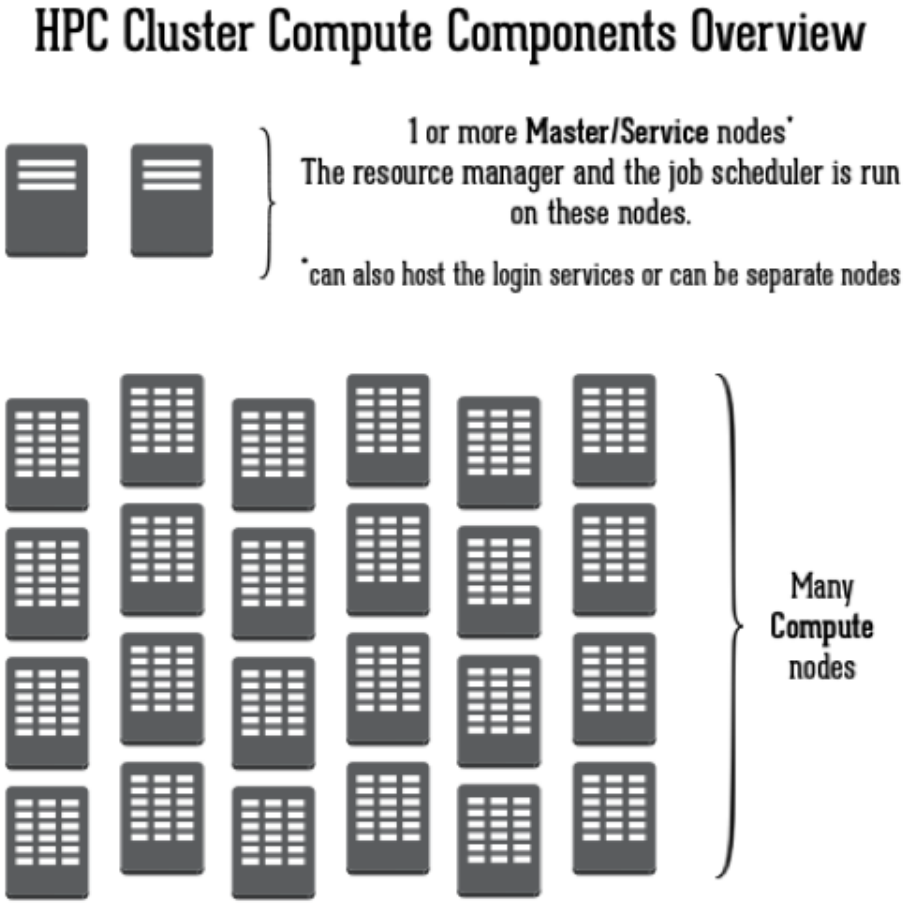
Machine Learning Techniques in R

How can you interpret their results?

A few techniques to improve prediction / reduce over-fitting

Nuts & Bolts - 2 data sets

Large scale computations in clusters



- Large scale clusters have never been more available (e.g Azure, EC2, Bluemix, Compute Engine)
  - Even RStudio has an AMI (http://www.louisaslett.com/RStudio_AMI/). I used RStudio and an EC c4.4xlarge instance with it for many of these examples.
- Monitoring, collecting and interpreting the operational data from these hosts is useful to determine various aspects
  - Type of calculation / job
  - Utilisation of CPU

Type of calculation / job and Utilisation of CPU

Description of the data

Schedule data for computational jobs with domain details

- **Protocol** - 14 types of experimental protocol.
- **Compounds** - number of compounds tested in the job
- **InputFields** - number of input fields applied to the analysis
- **Iterations** - specified number of runs [default is 20]
- **NumPending** - number of other jobs pending when this one was submitted
- **Hour** - Time of day [EST] 0-24 when submitted
- **Day** - Day of week when submitted

Target

- Class - the variable we are trying to predict. VF/very fast <1 min, F/fast 1-5 min, M/moderate 5-30 min, and L/long >30 min

Description of the data

Time and ID

- **sample time** - the date and time the data was sampled.
- **m_id** - the ID of the server the data was sampled at

Process - I/O, Memory, Processes, etc.

- **appxxx_dirio, appxxx_bufio, appxxx_pgflts, appxxx_proccount, appxxx_pagesgbl, appxxx_pagespro** - data about specific application.

Host - Memory, CPU, I/O, Network, etc.

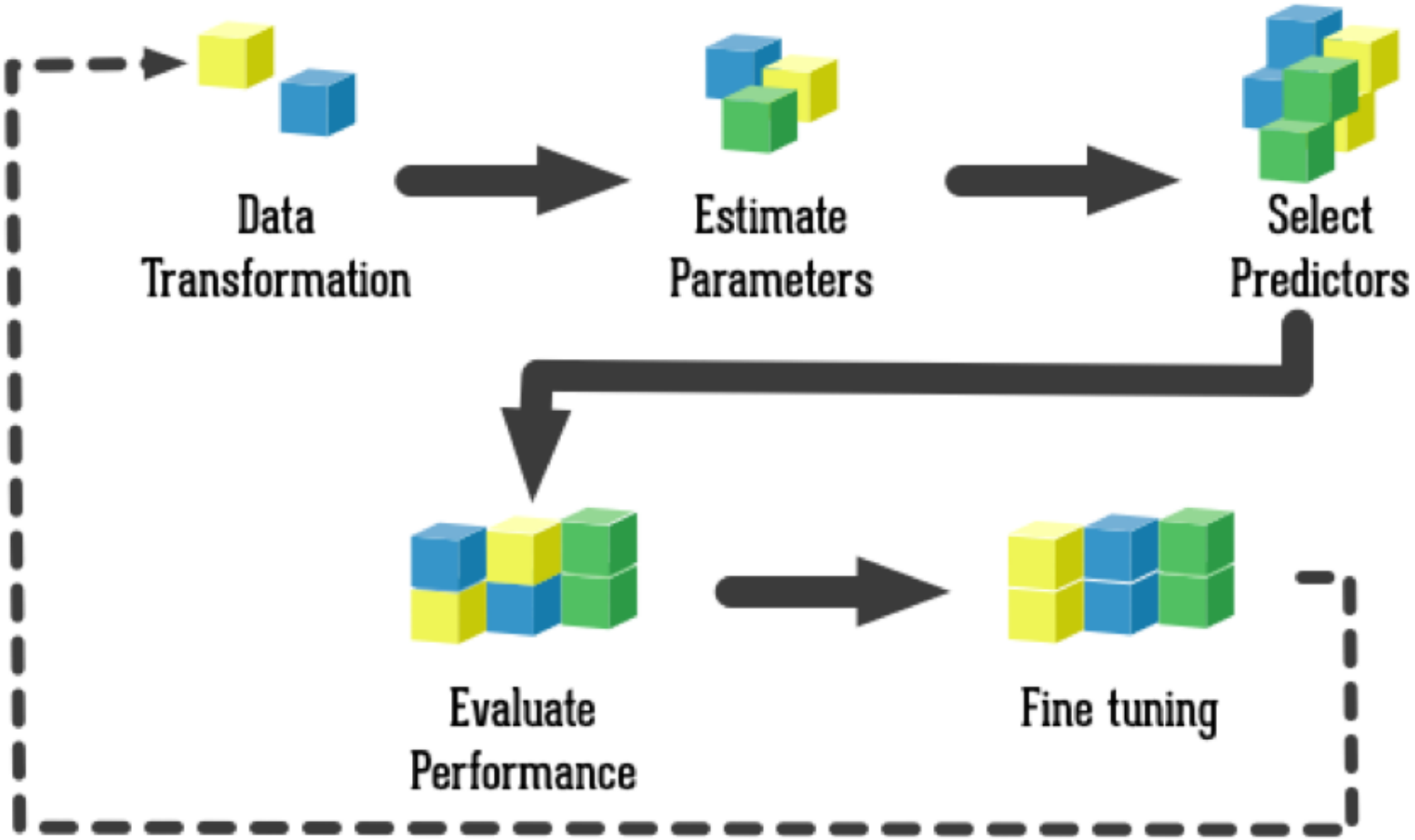
- **page_xxx** - data on memory usage of the server.
- **state_xxx** - data on the state the system is in.
- **syst_xxx** - data on page fault rate, number of processes, etc.
- **io_xxx** - data about general IO usage, [file IO, direct IO].
- **tcp_xxx** - data on incoming and outgoing TCP traffic.
- **lbxxx, ewxxx** - data on incoming and outgoing network traffic

Target

- cpu_01_busy - the variable we are trying to predict.

Source: http://inclass.kaggle.com/c/model-t4 kaggle

Model Building Process



Data Transformations

Data Transformations

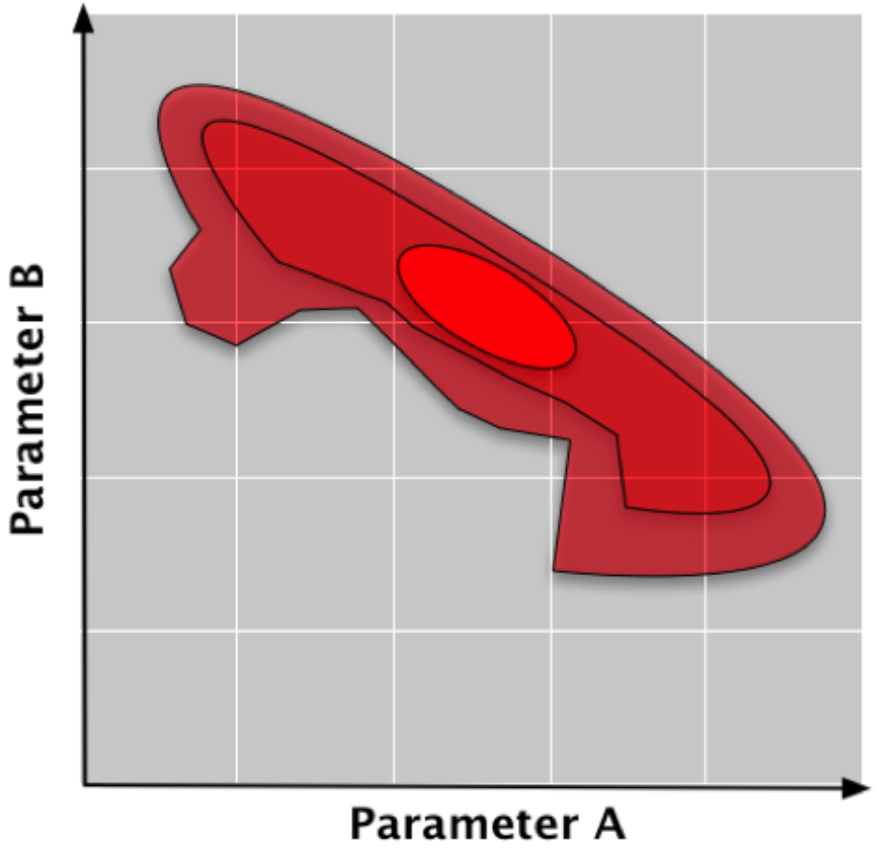
C Zero Mean
S One SD
T √ log INV

} 1 - Predictors - M {

SS M-Dim Sphere
PCA
PLS

Correlation, Dummy Variables, Filtering

Addressing Feature Selection



CARET and Feature Selection

- Recursive Feature Elimination Algorithm

```
> cvCtrl <- trainControl(method = "repeatedcv", repeats = 3,
    summaryFunction = twoClassSummary, classProbs = TRUE)
> rpartTune <- train(hadaffair ~ ., data = affairs.df.train,
    method = "rpart", tuneLength = 10, metric = "ROC", trControl = cvCtrl)
> rpartTune
481 samples
  9 predictors
  2 classes: 'No', 'Yes'

No pre-processing
Resampling: Cross-Validation (10 fold, repeated 3 times)

Summary of sample sizes: 432, 433, 433, 433, 433, 433, ...

Resampling results across tuning parameters:

  cp       ROC    Sens   Spec    ROC SD  Sens SD  Spec SD
  0        0.654  0.911  0.225   0.0793  0.0597   0.11
  0.00417  0.652  0.911  0.222   0.0775  0.0597   0.106
  0.00833  0.594  0.932  0.161   0.121   0.0563   0.105
  0.0125   0.572  0.949  0.156   0.133   0.045    0.0972
  0.0167   0.562  0.958  0.119   0.133   0.0383   0.0839
  0.0208   0.548  0.955  0.119   0.134   0.044    0.092
  0.025    0.554  0.963  0.103   0.124   0.0474   0.092
  0.0292   0.559  0.976  0.0806  0.118   0.0417   0.0861
  0.0333   0.542  0.988  0.0528  0.101   0.037    0.0804
  0.0375   0.516  1      0       0.0692  0        0

ROC was used to select the optimal model using  the largest value.
The final value used for the model was cp = 0.
```

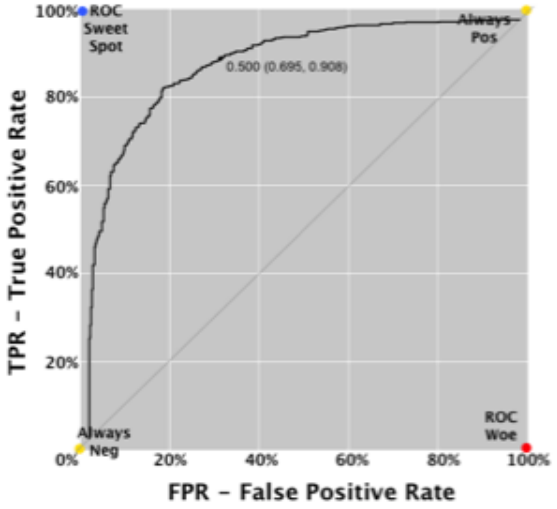
Model Selection and Model Assessment

Assessment [1 & 2]

1

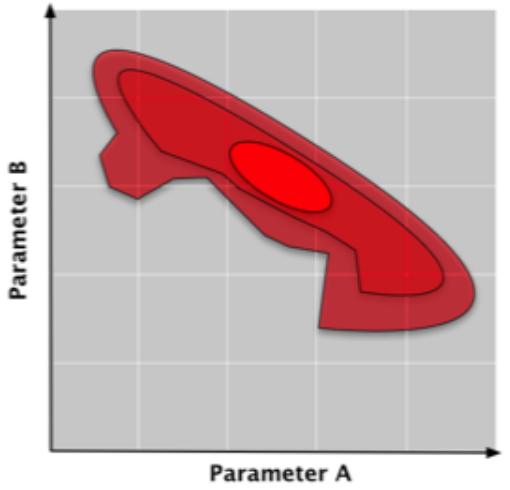
Confusion Matrix	REFERENCE (ACTUAL) HEALTHY (normal)	DISEASED (patient)
PREDICTED HEALTHY (normal)	Actual Healthy Patient and Predicted as Healthy Patient	Actual Diseased Patient but Predicted as Healthy Patient
PREDICTED DISEASED (patient)	Actual Healthy Patient but Predicted as Diseased Patient	Actual Diseased Patient and Predicted as Diseased Patient

2



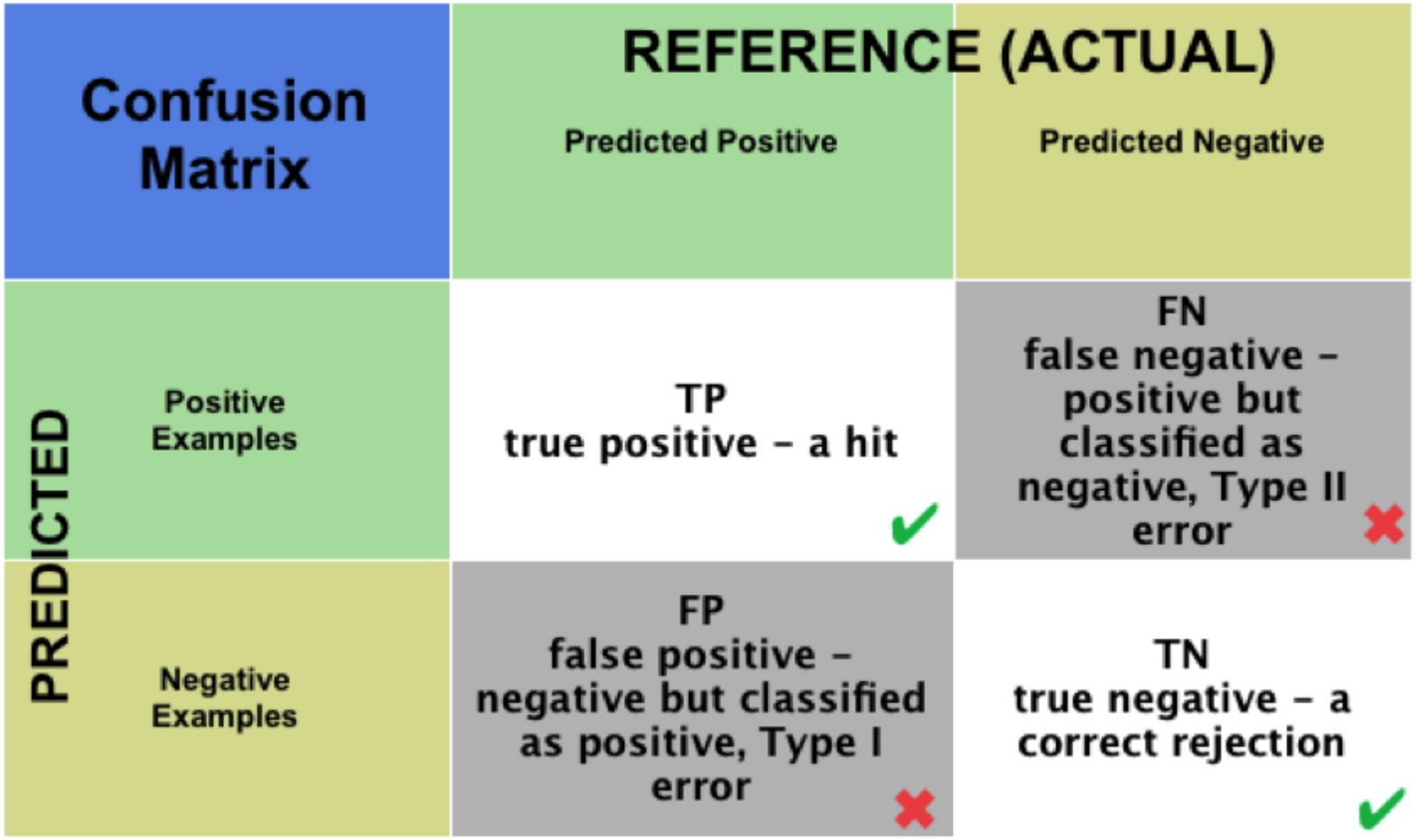
Selection [3 & 4]

3

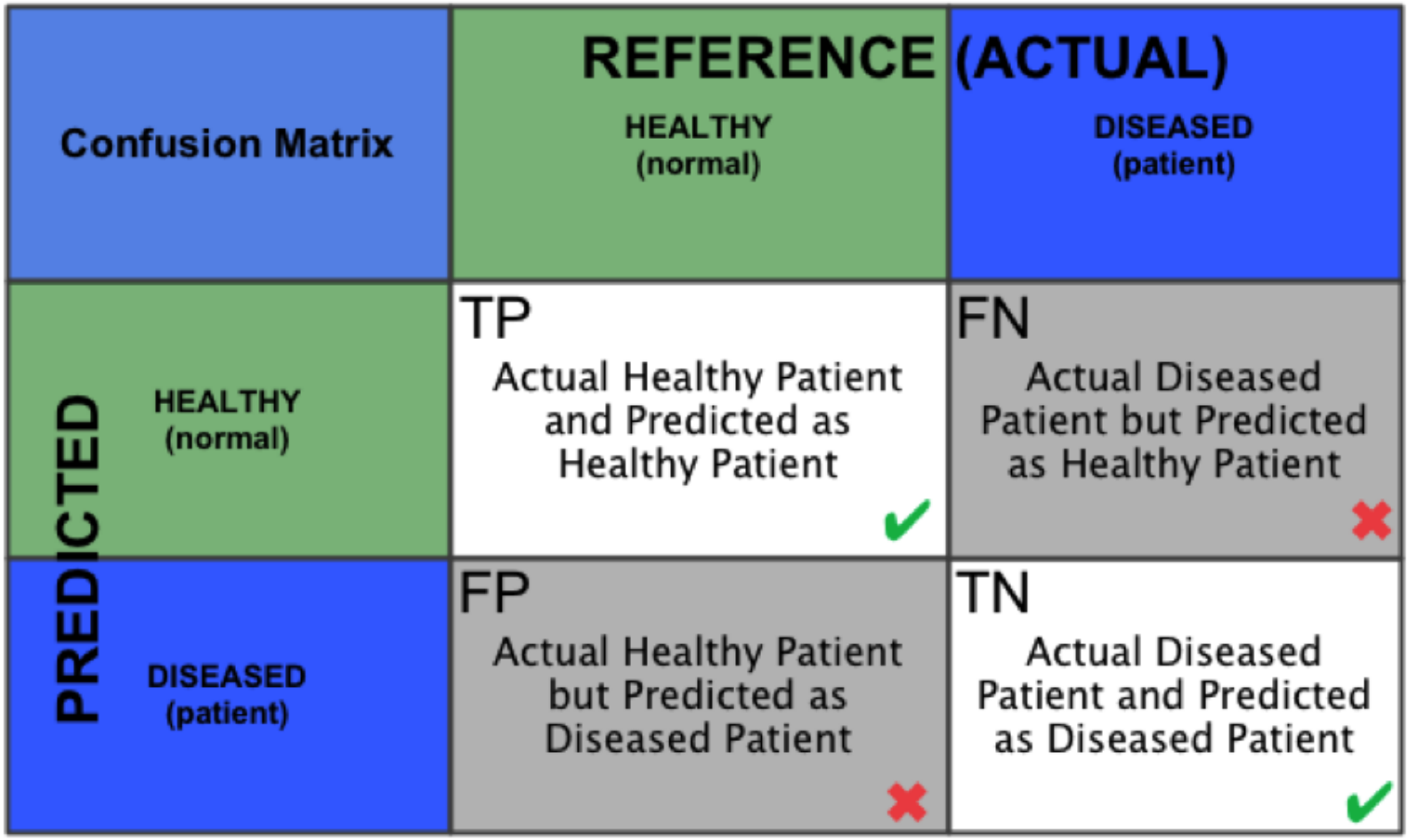


4

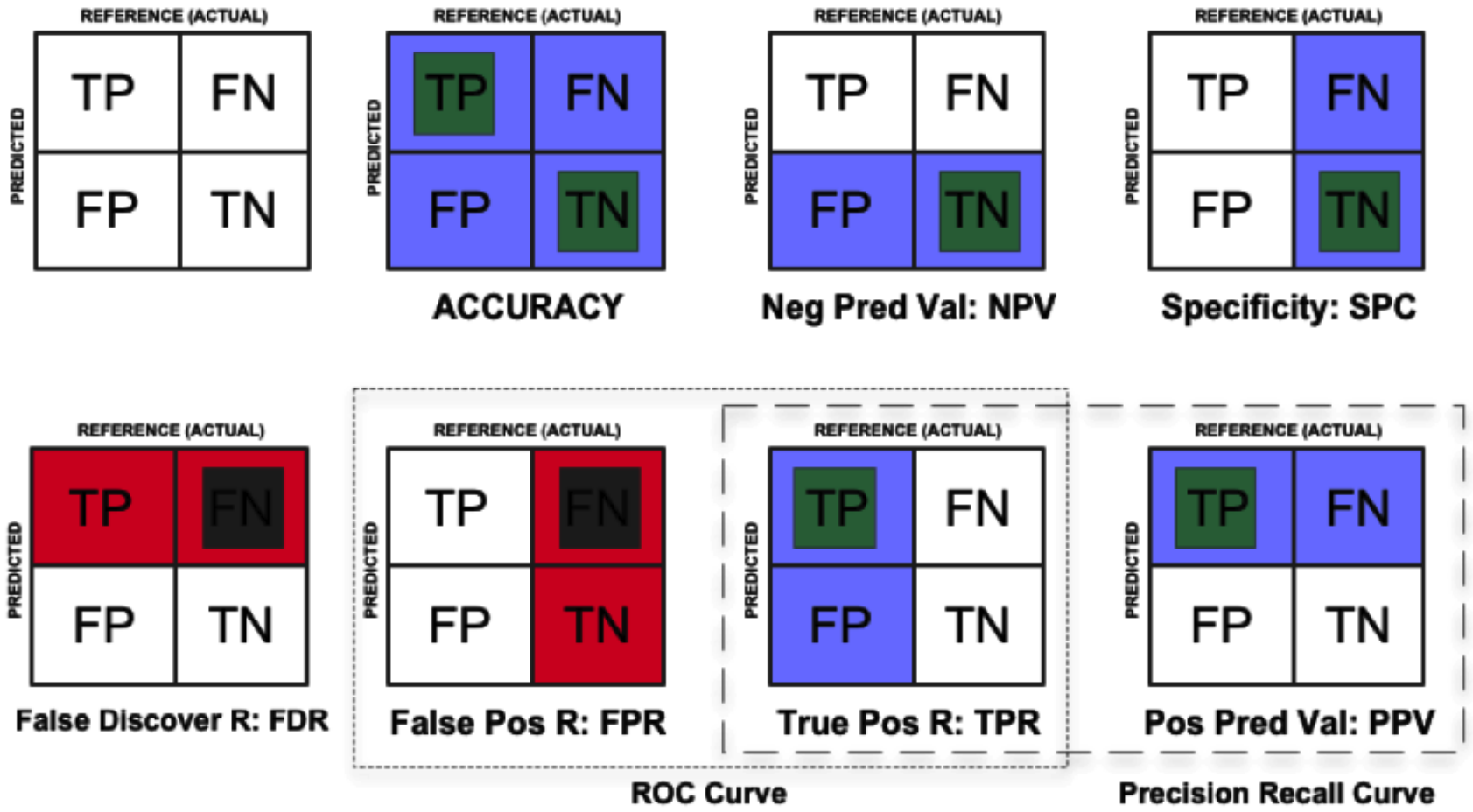
Interpreting A Confusion Matrix



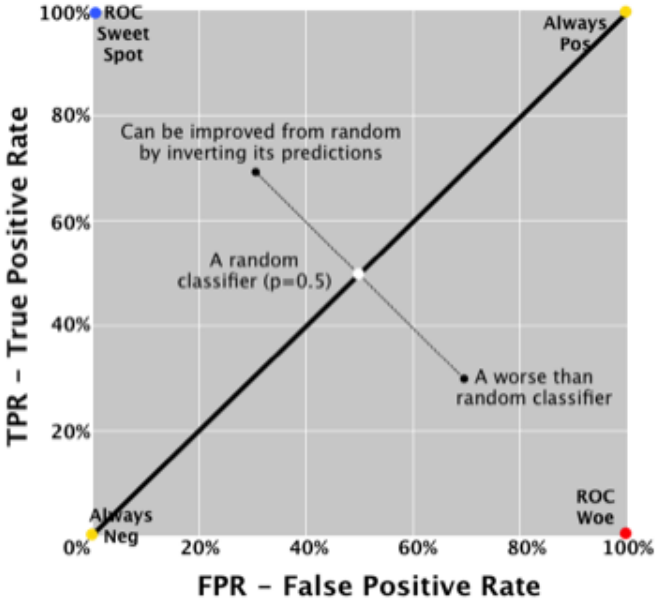
Interpreting A Confusion Matrix Example



Confusion Matrix - Calculations

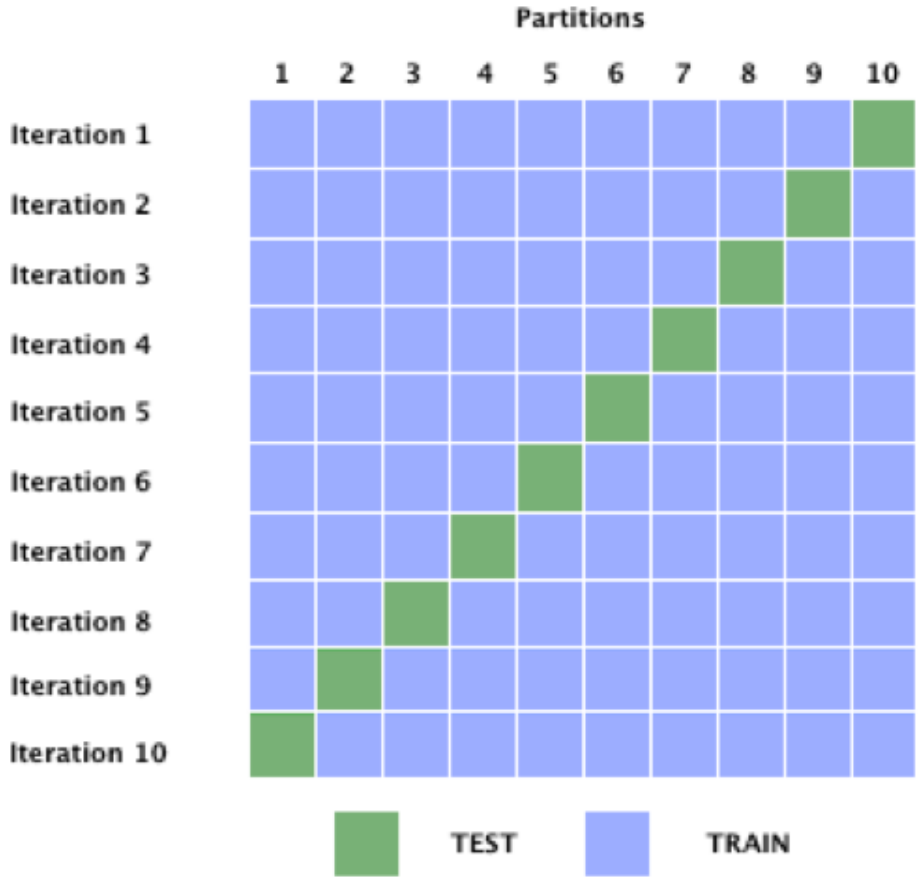


Interpreting A ROC Plot



- A point in this plot is better than another if it is to the northwest (TPR higher / FPR lower / or both)
- ``Conservatives'' - on LHS and near the X-axis - only make positive classification with strong evidence and making few FP errors but low TP rates
- ``Liberals'' - on upper RHS - make positive classifications with weak evidence so nearly all positives identified however high FP rates

Addressing Prediction Error



- K-fold Cross-Validation (e.g. 10-fold)
  - Allows for averaging the error across the models
- Bootstrapping, draw B random samples with replacement from data set to create B bootstrapped data sets with same size as original. These are used as training sets with the original used as the test set.
- Other variations on above:
  - Repeated cross validation
  - The '.632' bootstrap

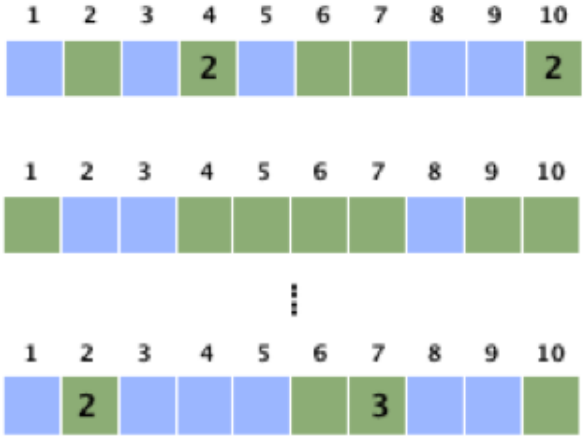
Boosting / Bootstrap aggregation

NumVar	OrdVar	CatVar
1	R2	Good
1.5	R4	Bad
2	R1	Bad
2.5	R5	Good
3	R3	Good
3.5	R3	Bad
⋮	⋮	⋮

Adds weak learners, so new learners pick up the slack. Incrementally increase the accuracy of model as weak learners focus more on misclassified examples from the previous weak learners.

Bagging

Samples the original training set uniformly with replacement to generate new bootstrapped training sets. This reduces variance and helps to avoid overfitting.



Training set 1 – Bootstrap samples 7

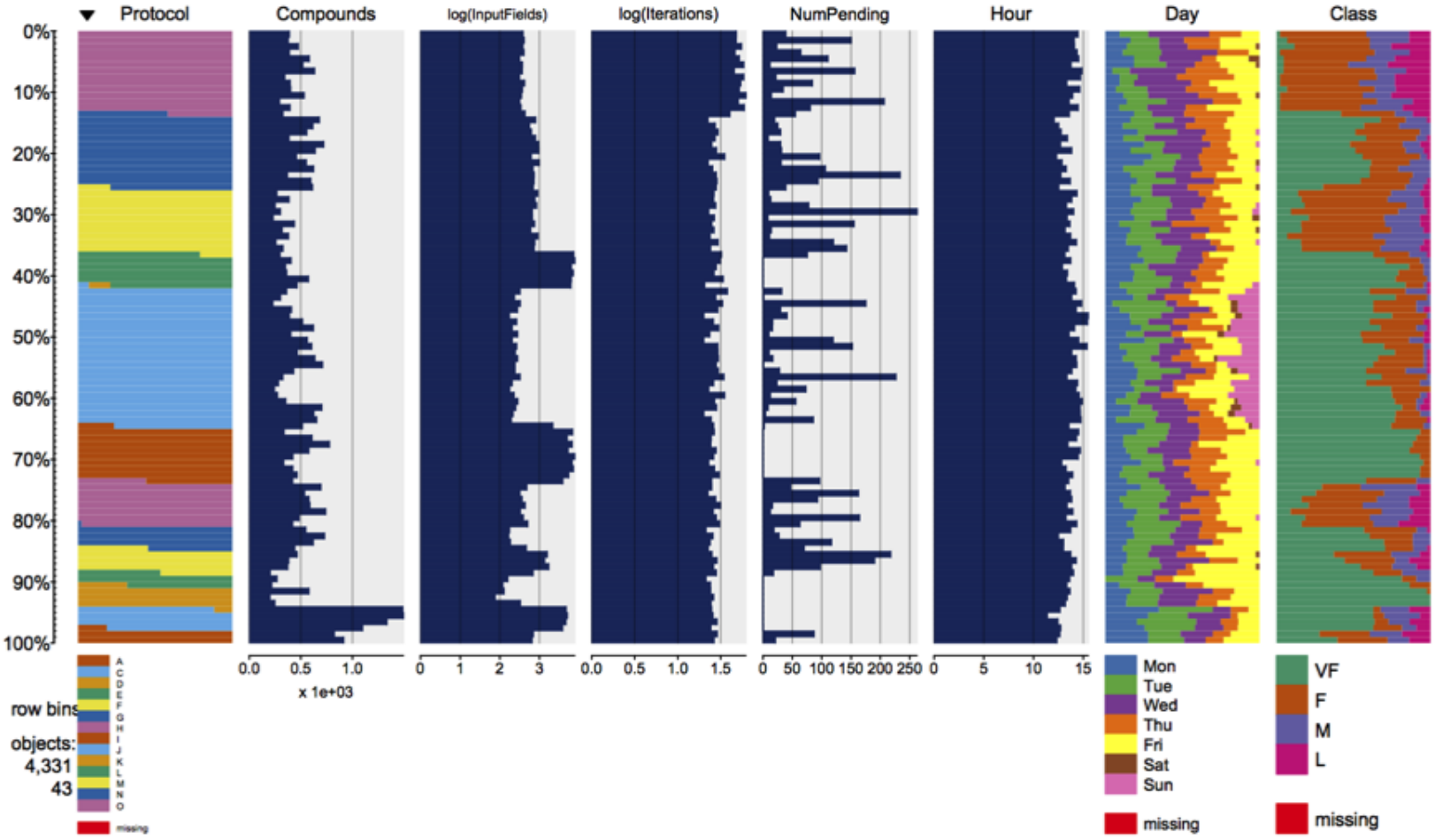
Training set 2 – Bootstrap samples 7

Training set N – Bootstrap samples 7

Dataset 1 - Job Scheduling Data

```
##     Protocol      Compounds        InputFields      Iterations
##  J      : 989   Min.   :   20.0   Min.   :   10   Min.   : 10.00
##  O      : 581   1st Qu.:   98.0   1st Qu.:  134   1st Qu.: 20.00
##  N      : 536   Median :  226.0   Median :  426   Median : 20.00
##  M      : 451   Mean   :  497.7   Mean   : 1537   Mean   : 29.24
##  I      : 381   3rd Qu.:  448.0   3rd Qu.:  991   3rd Qu.: 20.00
##  H      : 321   Max.   :14103.0   Max.   :56671   Max.   :200.00
##  (Other):1072
##    NumPending           Hour            Day      Class
##  Min.   :   0.00   Min.   : 0.01667   Mon:692   VF:2211
##  1st Qu.:   0.00   1st Qu.:10.90000   Tue:900   F :1347
##  Median :   0.00   Median :14.01667   Wed:903   M : 514
##  Mean   :  53.39   Mean   :13.73376   Thu:720   L : 259
##  3rd Qu.:   0.00   3rd Qu.:16.60000   Fri:923
##  Max.   :5605.00   Max.   :23.98333   Sat: 32
##                                       Sun:161
```

Dataset 1 - Job Scheduling Data



Dataset 1 - Job Scheduling Data - Partitioning and Cost Matrix

```
## 'data.frame':    3467 obs. of  8 variables:
##  $ Protocol   : Factor w/ 14 levels "A","C","D","E",..: 4 4 4 4 4 4 4 4 4 4 ...
##  $ Compounds  : num  97 93 100 100 105 98 101 95 102 108 ...
##  $ InputFields: num  103 76 82 82 88 95 91 92 96 104 ...
##  $ Iterations : num  20 20 20 20 20 20 20 20 20 10 ...
##  $ NumPending : num  3 3 3 3 3 3 3 3 3 3 ...
##  $ Hour       : num  13.8 10.1 10.4 16.5 16.4 ...
##  $ Day        : Factor w/ 7 levels "Mon","Tue","Wed",..: 2 5 5 3 5 5 5 3 5 3 ...
##  $ Class      : Factor w/ 4 levels "VF","F","M","L": 1 1 1 1 1 1 1 1 1 1 ...
```

```
##    VF F M  L
## VF  0 1 5 10
## F   1 0 5  5
## M   1 1 0  1
## L   1 1 1  0
```

Dataset 1 - Job Scheduling Data - C50 Single Tree

```
##
## Call:
## C5.0.formula(formula = Class ~ ., data = trainData)
##
## Classification Tree
## Number of samples: 3467
## Number of predictors: 7
##
## Tree size: 199
##
## Non-standard options: attempt to group attributes
```

```
##  Accuracy     Kappa
## 0.8310185 0.7257584
```

Dataset 1 - Job Scheduling Data - C50 Cross-Validated (10 fold, repeated 5 times) - Part 1

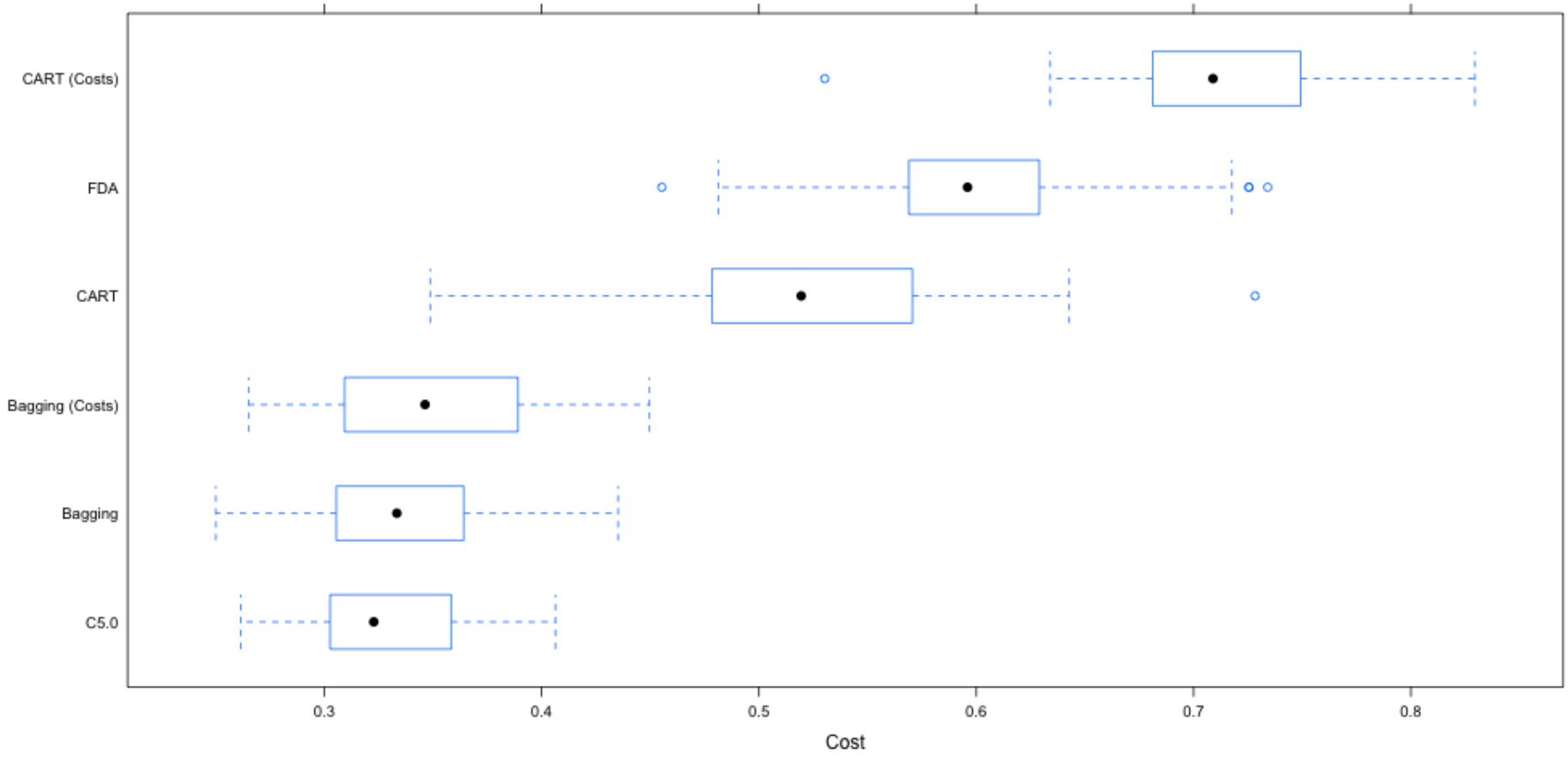
```
## C5.0
##
## 3467 samples
##    7 predictor
##    4 classes: 'VF', 'F', 'M', 'L'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 5 times)
##
## Summary of sample sizes: 3119, 3120, 3122, 3120, 3120, 3120, ...
##
## Resampling results across tuning parameters:
##
##   winnow  trials  Accuracy   Kappa      Cost       Accuracy SD  Kappa SD
##   FALSE     1     0.8094026  0.6927055  0.3835011  0.01851659   0.03001178
##   FALSE    10     0.8345537  0.7318980  0.3442725  0.01469138   0.02393878
##   FALSE    20     0.8412999  0.7428217  0.3338396  0.01412315   0.02282365
##   FALSE    30     0.8406083  0.7416276  0.3359680  0.01431617   0.02292000
```

```
##    model winnow trials  Accuracy     Kappa      Cost AccuracySD    KappaSD
## 1   tree  FALSE      1 0.8094026 0.6927055 0.3835011 0.01851659 0.03001178
## 12  tree   TRUE      1 0.8098057 0.6932152 0.3849491 0.01873836 0.03039064
## 2   tree  FALSE     10 0.8345537 0.7318980 0.3442725 0.01469138 0.02393878
## 13  tree   TRUE     10 0.8346130 0.7320788 0.3442159 0.01469821 0.02357808
## 3   tree  FALSE     20 0.8412999 0.7428217 0.3338396 0.01412315 0.02282365
## 14  tree   TRUE     20 0.8407839 0.7419558 0.3338879 0.01427739 0.02320299
## 4   tree  FALSE     30 0.8406083 0.7416276 0.3359680 0.01431617 0.02292000
## 15  tree   TRUE     30 0.8404354 0.7413244 0.3359104 0.01375501 0.02210552
## 5   tree  FALSE     40 0.8412987 0.7426118 0.3366641 0.01425873 0.02311093
## 16  tree   TRUE     40 0.8409533 0.7420852 0.3360834 0.01393299 0.02265909
## 6   tree  FALSE     50 0.8426812 0.7449319 0.3318168 0.01246685 0.01998607
## 17  tree   TRUE     50 0.8421632 0.7441460 0.3314100 0.01238113 0.01992140
## 7   tree  FALSE     60 0.8419952 0.7437531 0.3331911 0.01335949 0.02136949
## 18  tree   TRUE     60 0.8416507 0.7432257 0.3328386 0.01318599 0.02115722
## 8   tree  FALSE     70 0.8423396 0.7443678 0.3319279 0.01406514 0.02248550
## 19  tree   TRUE     70 0.8417629 0.7434720 0.3327311 0.01430716 0.02289839
## 9   tree  FALSE     80 0.8425691 0.7446598 0.3333175 0.01330740 0.02113161
## 20  tree   TRUE     80 0.8418195 0.7434836 0.3338326 0.01354652 0.02157878
## 10  tree  FALSE     90 0.8422789 0.7442141 0.3343013 0.01415971 0.02252124
## 21  tree   TRUE     90 0.8416452 0.7432490 0.3342393 0.01408687 0.02242716
## 11  tree  FALSE    100 0.8423924 0.7443888 0.3358031 0.01398184 0.02233801
## 22  tree   TRUE    100 0.8421635 0.7440826 0.3351031 0.01386605 0.02215713
```

```
## Cross-Validated (10 fold, repeated 5 times) Confusion Matrix
##
## (entries are un-normalized counts)
##
##           Reference
## Prediction    VF     F     M     L
##         VF 164.6  17.1   1.7   0.2
##         F   11.8  83.6  11.6   1.7
##         M    0.4   6.2  27.0   2.1
##         L    0.1   0.9   0.9  16.8
```

```
##    VF F M  L
## VF  0 1 5 10
## F   1 0 5  5
## M   1 1 0  1
## L   1 1 1  0
```

Results of a variety of approaches focus on Cost metric



Dataset 2 - CPU Burn Kaggle

Description of the data

Time and ID

- **sample time** - the date and time the data was sampled.
- **m_id** - the ID of the server the data was sampled at

Process - I/O, Memory, Processes, etc.

- **appxxx_dirio, appxxx_bufio, appxxx_pgflts, appxxx_proccount, appxxx_pagesgbl, appxxx_pagespro** - data about specific application.

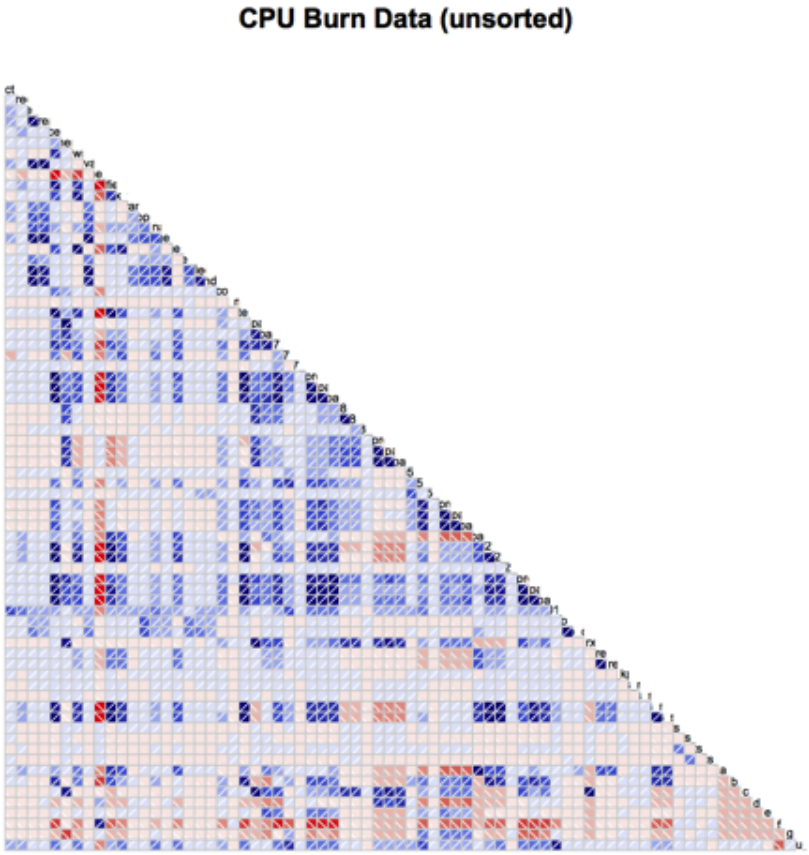
Host - Memory, CPU, I/O, Network, etc.

- **page_xxx** - data on memory usage of the server.
- **state_xxx** - data on the state the system is in.
- **syst_xxx** - data on page fault rate, number of processes, etc.
- **io_xxx** - data about general IO usage. [file IO, direct IO].
- **tcp_xxx** - data on incoming and outgoing TCP traffic.
- **lbxxx, ewxxx** - data on incoming and outgoing network traffic

Target

- cpu_01_busy - the variable we are trying to predict.

Source: http://inclass.kaggle.com/c/model-t4 kaggle

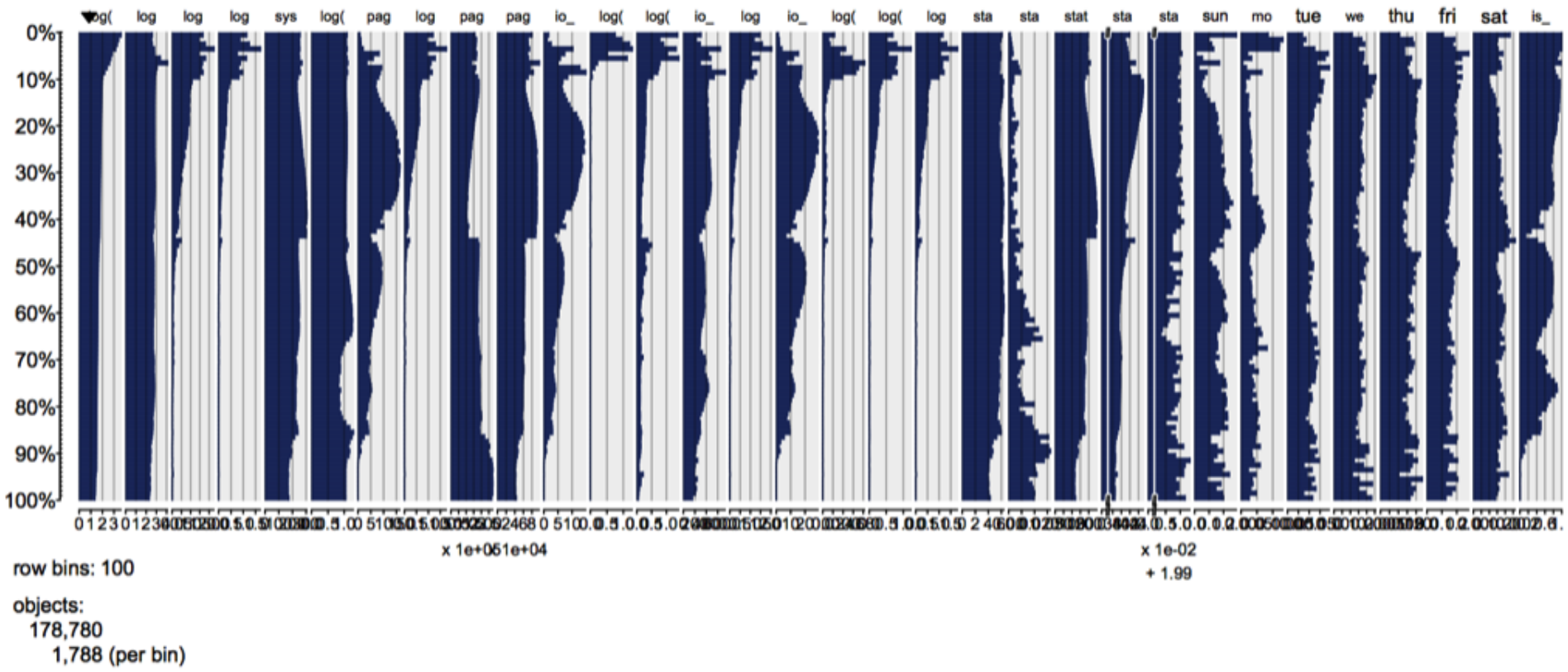


Dataset 2 - CPU Burn Kaggle

Dataset 2 - CPU Burn Kaggle

```
##   syst_direct_ipo_rate syst_buffered_ipo_rate syst_page_fault_rate
## 1                80.48                1261.97                15.55
##   syst_page_read_ipo_rate syst_process_count syst_other_states
## 1                     2.1                271                12
##   page_page_write_ipo_rate page_global_valid_fault_rate
## 1                     6.23                         4.67
##   page_free_list_size page_modified_list_size io_mailbox_write_rate
## 1              138749                  100100                  7.98
##   io_split_transfer_rate io_file_open_rate io_logical_name_trans
## 1                      0              2.82                670.32
##   io_page_reads io_page_writes page_free_list_faults
## 1          4.02          15.25                  0.98
##   page_modified_list_faults page_demand_zero_faults state_compute
## 1                      0.35                    7.47             5
##   state_mwait state_lef state_hib state_cur sun mon tue wed thu fri sat
## 1           0       212        42         2   0   0   0   1   0   0   0
##   is_cpu_busy
## 1           1
```

Dataset 2 - CPU Burn Kaggle



Dataset 2 - CPU Burn Kaggle - Feature Selection 2

```
## [1] "nearZeroVar:"
```

```
##  [1] "syst_page_read_ipo_rate"      "page_page_write_ipo_rate"
##  [3] "page_global_valid_fault_rate" "io_split_transfer_rate"
##  [5] "io_page_reads"                "io_page_writes"
##  [7] "page_free_list_faults"        "page_modified_list_faults"
##  [9] "state_mwait"                  "state_cur"
## [11] "mon"
```

```
## [1] "high correlation .75+:"
```

```
##  [1] "syst_page_fault_rate"         "page_global_valid_fault_rate"
##  [3] "syst_page_read_ipo_rate"      "io_page_reads"
##  [5] "page_modified_list_faults"    "page_free_list_size"
##  [7] "page_modified_list_size"      "syst_process_count"
##  [9] "page_page_write_ipo_rate"     "io_page_writes"
```

Dataset 2 - CPU Burn Kaggle - Feature Selection 2

```
## [1] "After removing nearZeroVar and high correlation .75+:"
```

```
##  [1] "syst_direct_ipo_rate"    "syst_buffered_ipo_rate"
##  [3] "syst_other_states"       "io_mailbox_write_rate"
##  [5] "io_file_open_rate"       "io_logical_name_trans"
##  [7] "page_demand_zero_faults" "state_compute"
##  [9] "state_lef"               "state_hib"
## [11] "sun"                     "tue"
## [13] "wed"                     "thu"
## [15] "fri"                     "sat"
## [17] "is_cpu_busy"
```

Dataset 2 - CPU Burn Kaggle - Feature Selection 3

```
## [1] "Applying BoxCox, Centering, Scaling and PCA to data:"
```

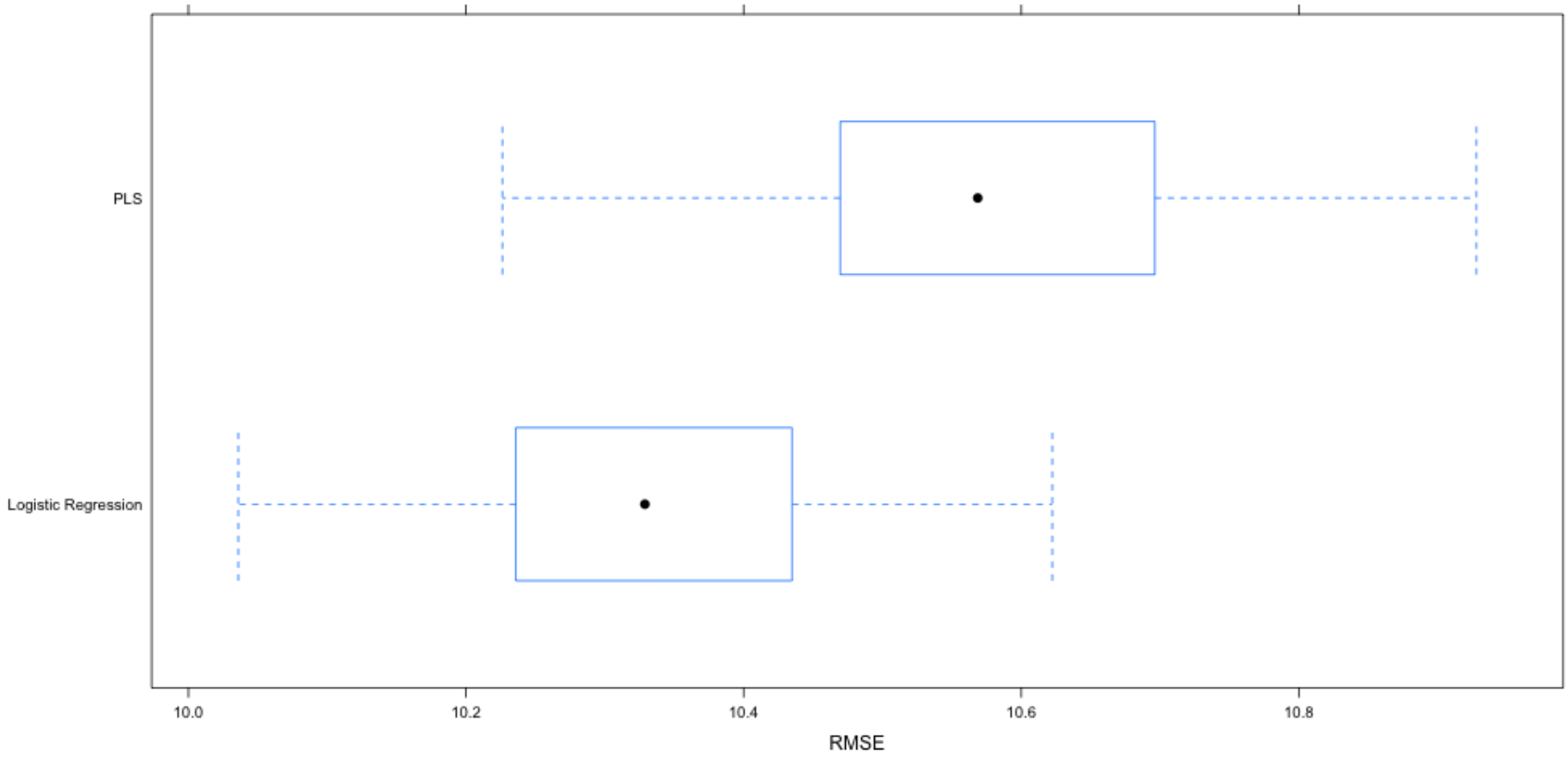
```
##
## Call:
## preProcess.default(x = cpuburn.data.df.reduced, method =
##  c("BoxCox", "center", "scale", "pca"))
##
## Created from 178780 samples and 17 variables
## Pre-processing: Box-Cox transformation, centered, scaled,
##  principal component signal extraction
##
## Lambda estimates for Box-Cox transformation:
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
##   -2.00   -0.65    0.70   -0.20    0.70    0.70      14
##
## PCA needed 15 components to capture 95 percent of the variance
```

Dataset 2 - CPU Burn - C50 Single Tree

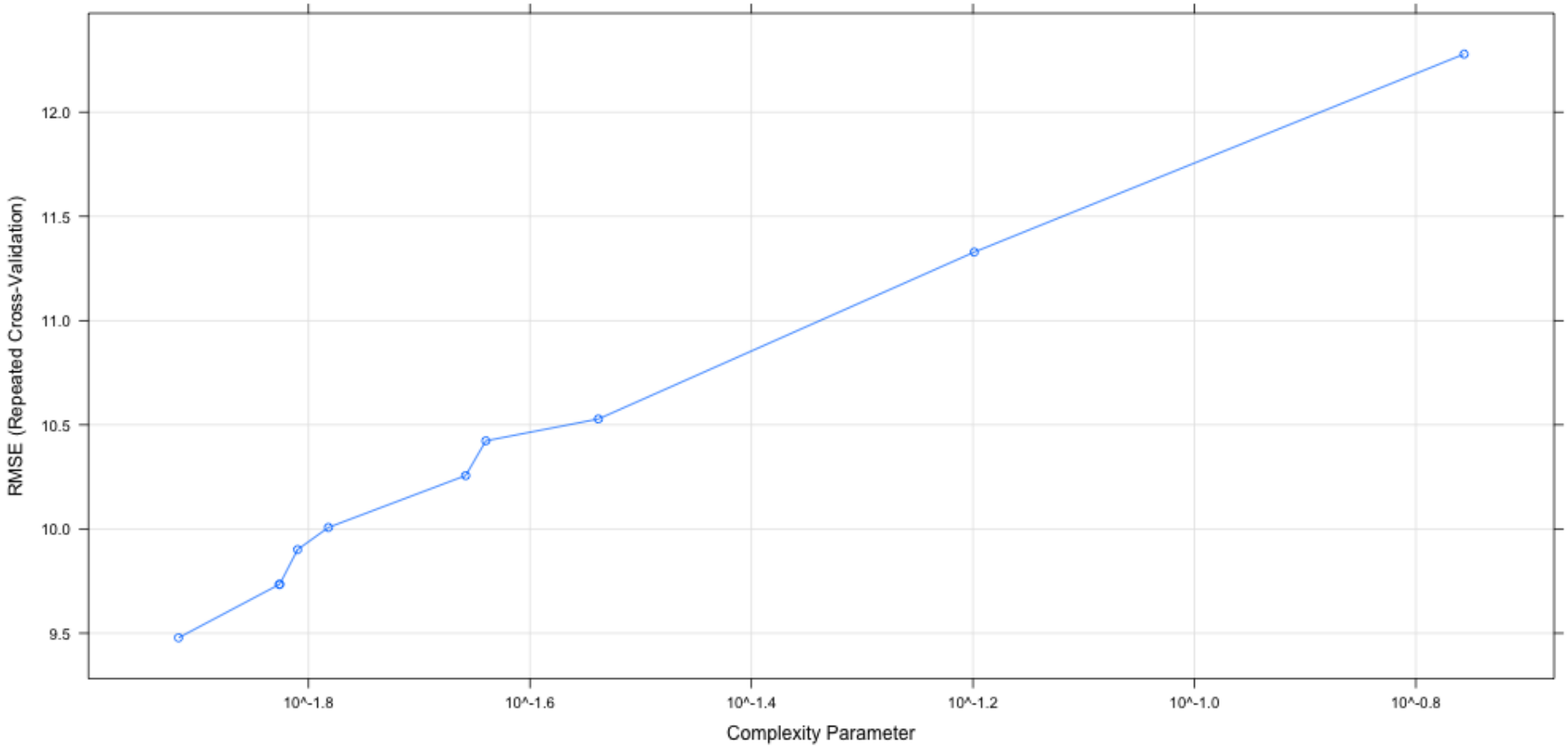
```
##   syst_direct_ipo_rate syst_buffered_ipo_rate syst_process_count
## 4                68.75                 495.10                224
## 5                47.45                 436.65                253
##   page_page_write_ipo_rate page_global_valid_fault_rate
## 4                     2.58                          1.1
## 5                     2.48                          1.1
##   page_free_list_size page_modified_list_size io_page_reads io_page_writes
## 4              200705                   54727          0.93           8.18
## 5              176726                   69647          0.93           6.22
##   page_modified_list_faults is_cpu_busy
## 4                      0.13           1
## 5                      0.12           0
```

```
##      RMSE  Rsquared
## 0.1998557 0.8284657
```

Results of Logistic Regression and PLS approaches



Results of Random Forest approach



In Summary

An idea of some of the types of classifiers available in ML.

What a confusion matrix and ROC means for a classifier and how to interpret them

An idea of how to test a set of techniques and parameters to help you find the best model for your data

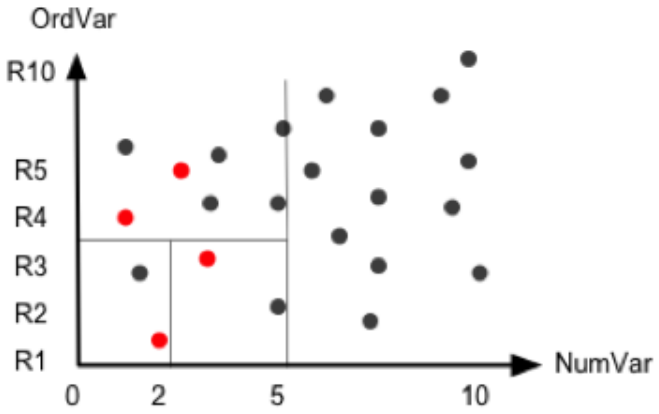
Slides, Data, Scripts will be put up on GH:
https://github.com/braz/DublinR-ML-machines

Aside - How do decision trees work ?

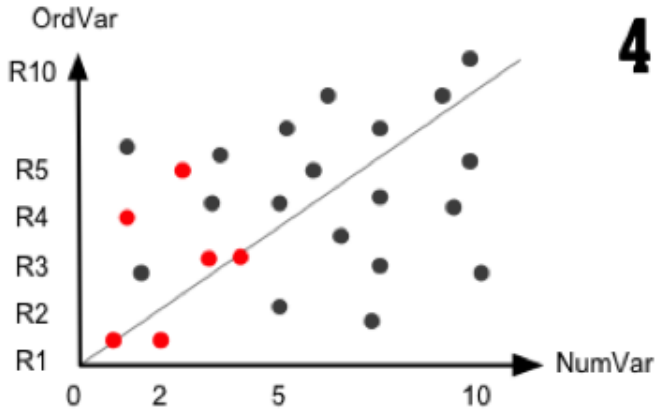
1

NumVar	OrdVar	CatVar
1	R2	Good
1.5	R4	Bad
2	R1	Bad
2.5	R5	Good
3	R3	Good
3.5	R3	Bad
⋮	⋮	⋮

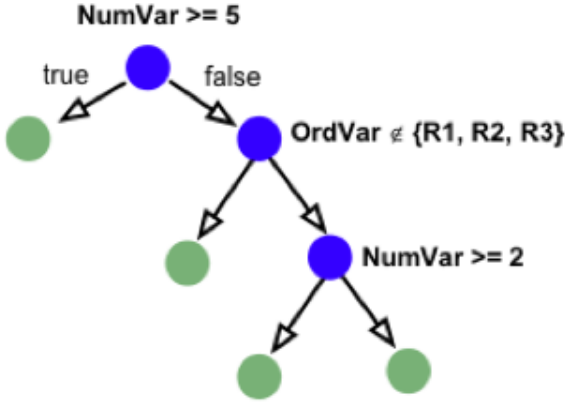
3



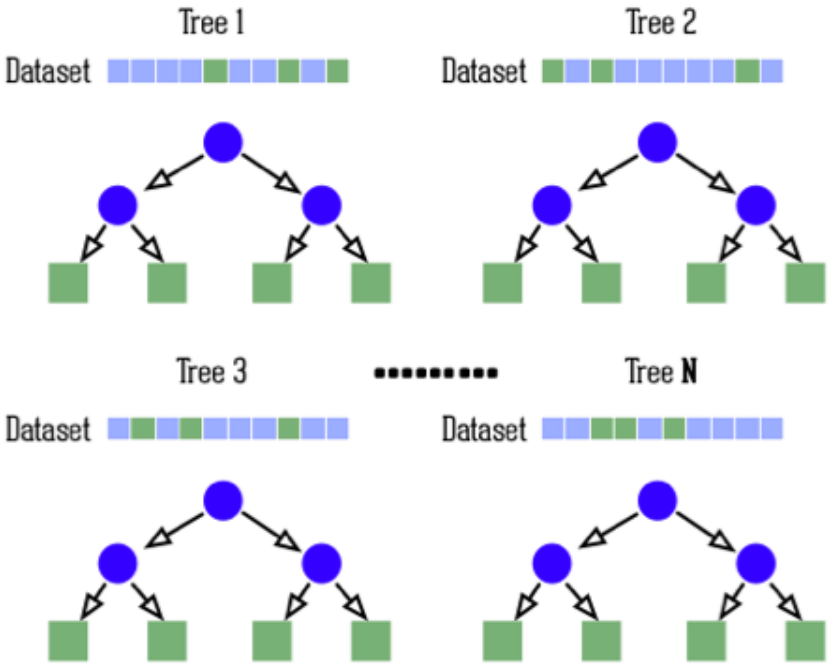
2



4



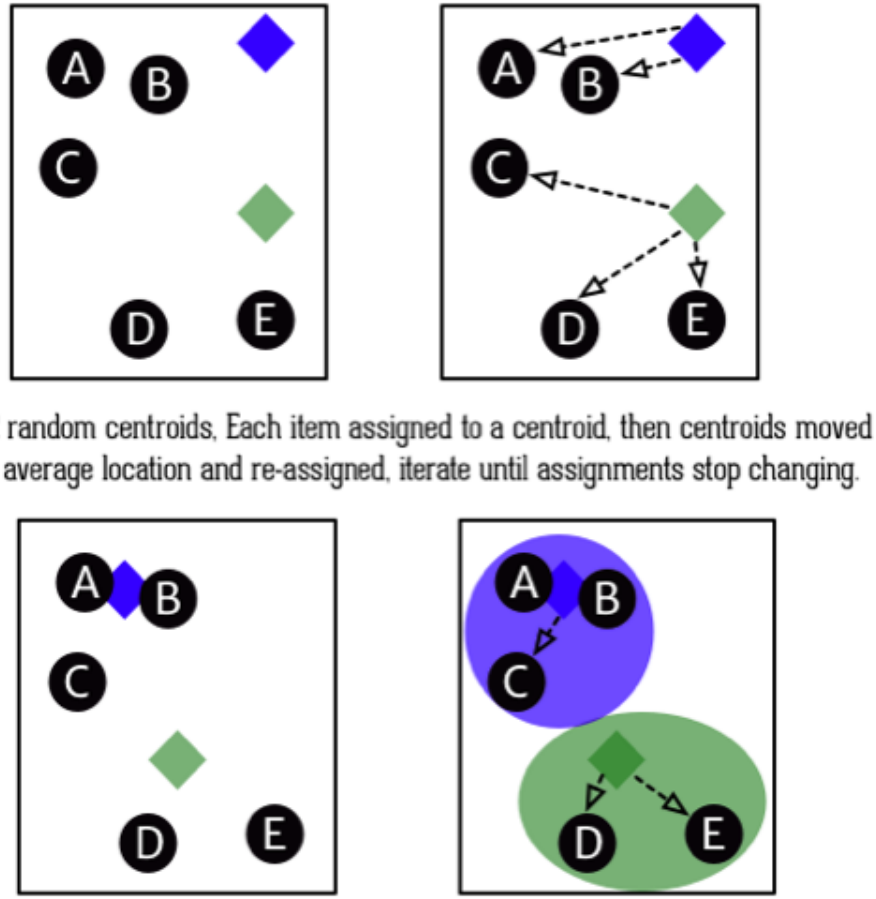
Aside - How does a random forest work ?



Traverse each tree and at each node in a tree:

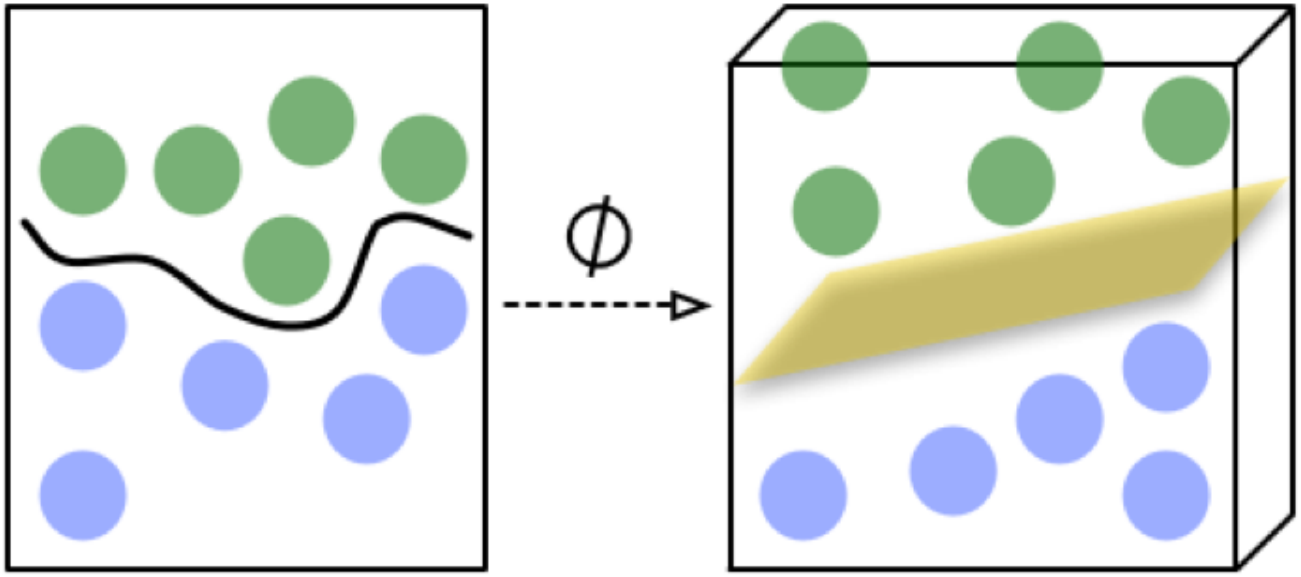
i. Select **m** random predictor variables from available set
ii. Use the variable with best split [use objective function]
iii. Move to next node in tree

Aside - How does k nearest neighbors work ?



K=2 random centroids. Each item assigned to a centroid, then centroids moved to average location and re-assigned, iterate until assignments stop changing.

Aside - How do support vector machines work ?



A list of number [a n-dimensional vector] and transform the points into higher dimensions so it is easier to separate them using a [n-1] dimensional hyperplane.