Random forests

RUGS Data Mining with R Workshop II

TOH Wei Zhong

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A little bit about me

- Graduated from NUS, Computational biology
  - Statistics and computing onto biology and healthcare
  - E.g. -omics
- Data scientist at NCS

Agenda for this evening

- Some materials on trees
  - Terminologies
  - Measuring performance
  - Pruning
- Ensemble modelling
  - Intuition and math
- Bagging, or bootstrap aggregating
- Random forest (RF)
  - Bagging vs. RF
  - Out-of-bag (OOB) assessment of model performance
  - Variable importance measures
  - Multidimensional scaling (MDS) plot on proximity matrix
  - Hyperparameters tuning
- Hands-on / code walkthrough

Decision trees

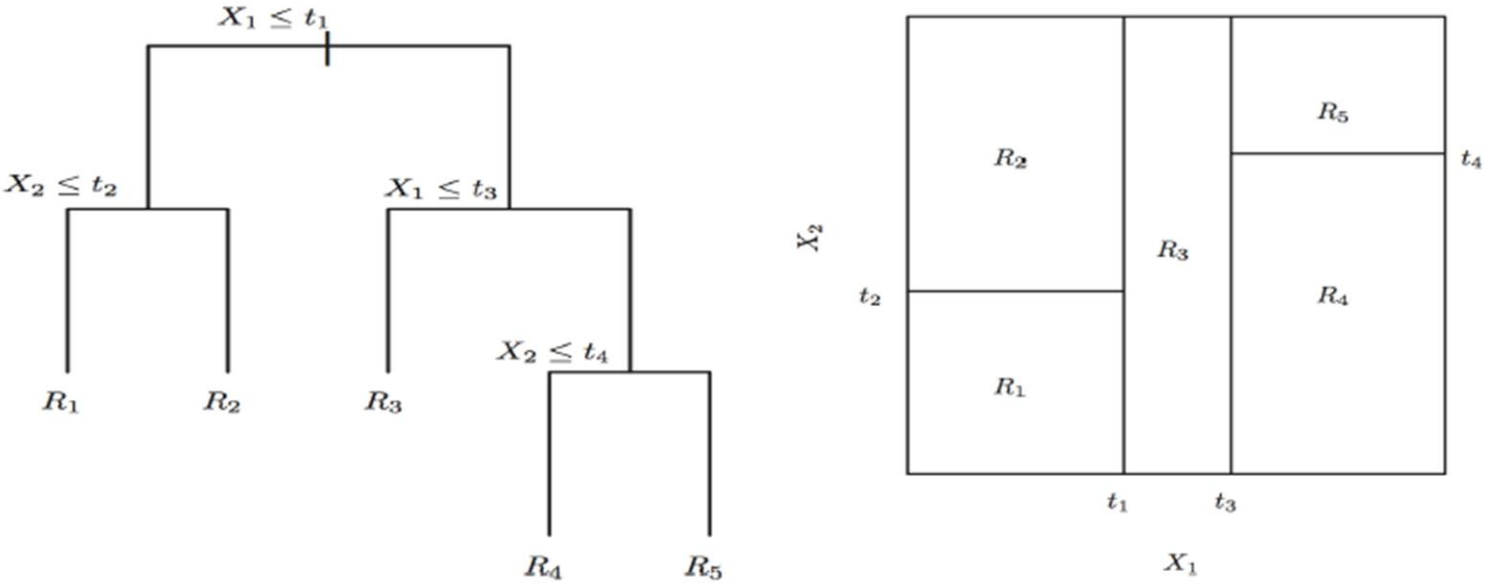
Some basic materials

Decision trees

- A simple model used in supervised learning
- CART, C4.5 – amongst top 10 most popular data mining algorithms
- Classification (response variable is categorical) and regression (response variable is continuous or numerical)
- [R] The **tree** package that we are using uses the recursive partitioning algorithm

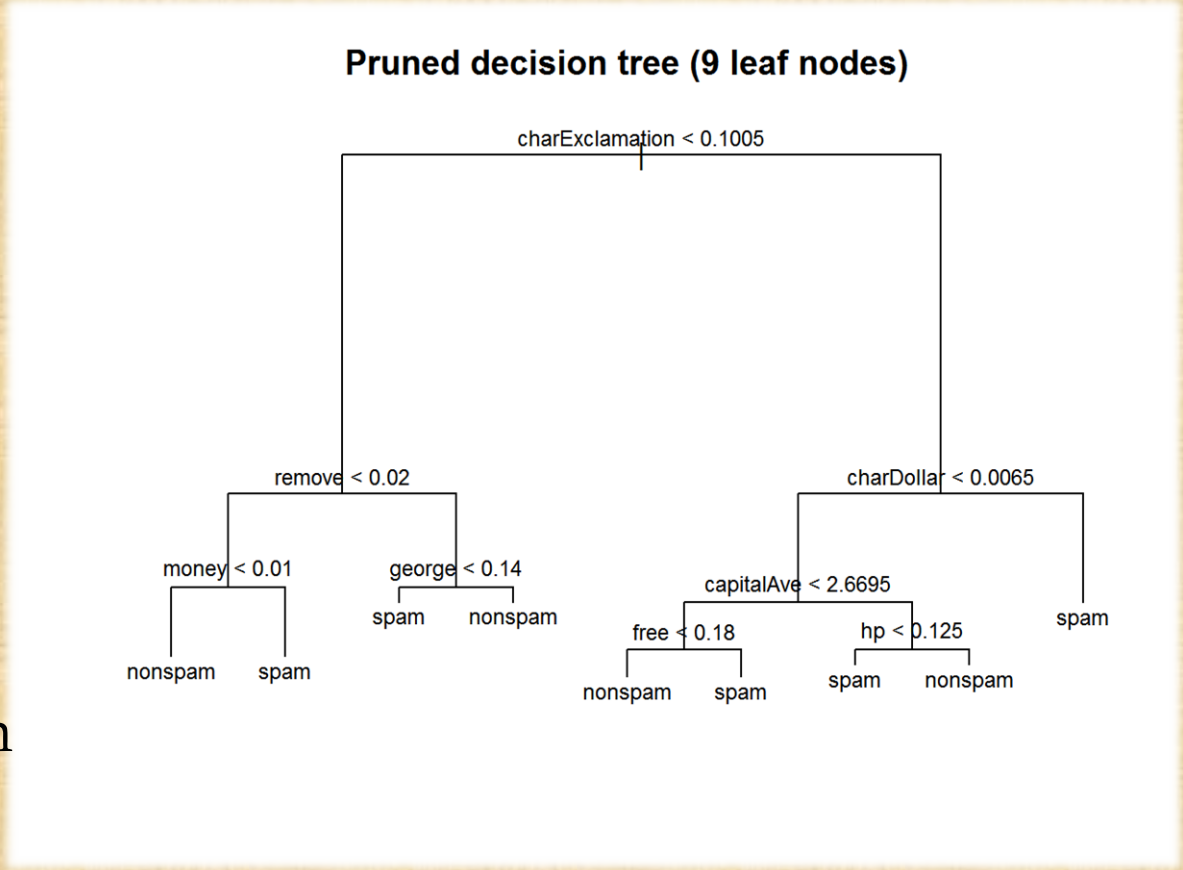
Equivalents

- Tree == Binary partitioning of dataset
- Each partition is represented by the mode (classification) or mean (regression)



Terminologies

- Depth
- Node
  - Leaf nodes
  - Non-leaf nodes
- The size of a tree sometimes refers to the number of leaf nodes
- Parents and children
- Branching factor



Assessing the performance of a supervised learning model

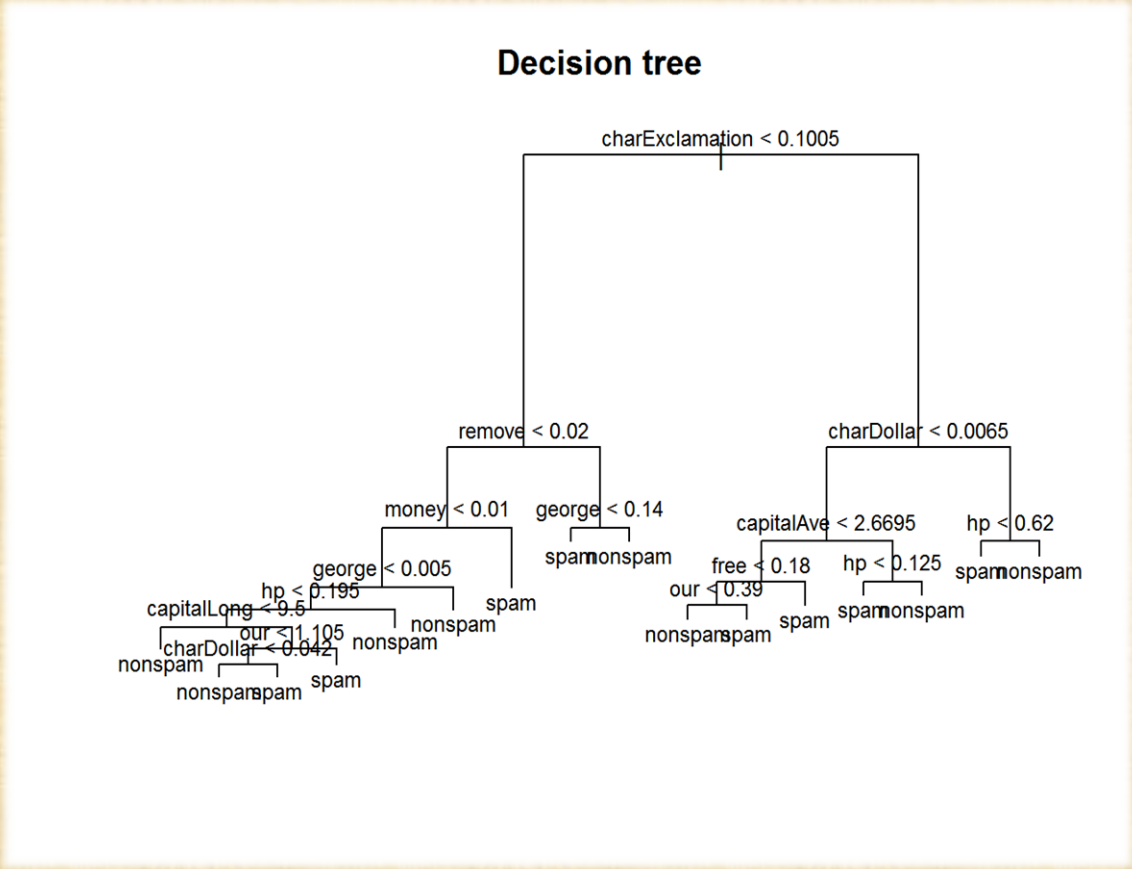
- Classification: accuracy / error rate
  - Sensitivity, specificity etc.
- Regression: mean squared error
  - $MSE = \frac{1}{n}\sum(prediction - actual)^2$

- Also, there are two types of classification models:
  (1) Those that output classes / categories as predictions
  (2) Those that output probabilities as predictions

- (2): can use ROC-AUC as a measure of performance

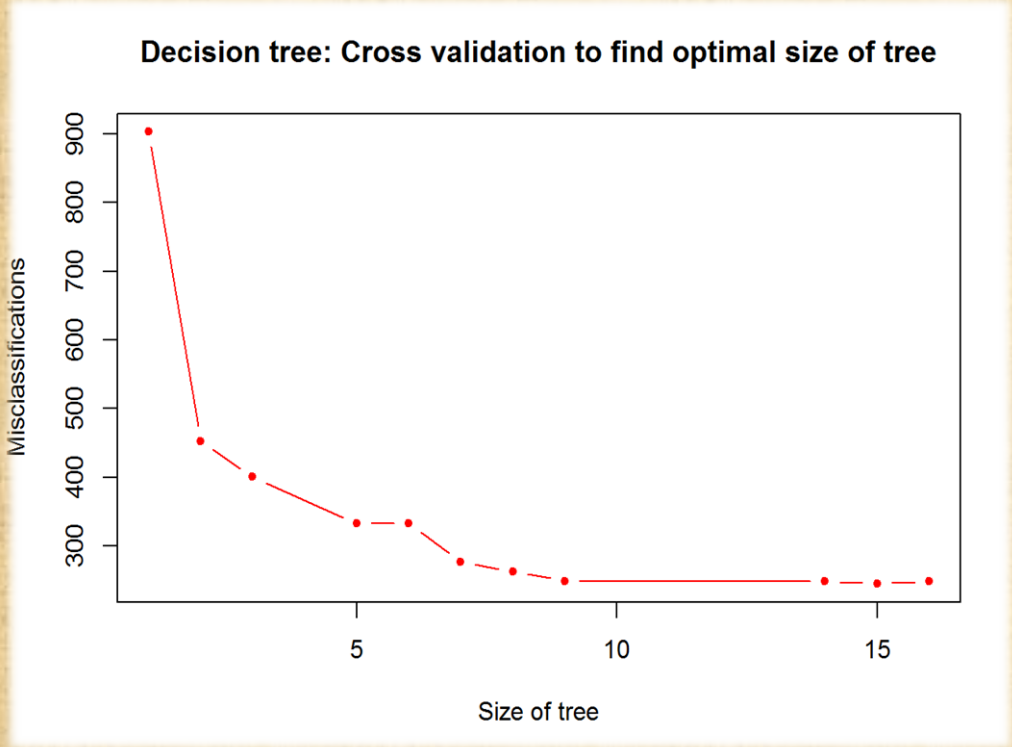
Pruning

- Typically after the construction of a decision tree, we would want to prune the tree, because the tree may be overly complicated



Pruning (2)

- Pruning refers to the process of trimming the tree to a more compact and concise one, without sacrificing much performance
- [R] The **tree** package uses cost-complexity pruning
  - Comparing the relationship between number of leaf nodes and performance of model



Pros and cons of decision trees

- Pros:
  - Very easy to interpret and communicate to others, because it is similar to how humans think and make decisions
  - Easy to construct

- Cons:
  - Generally unstable
  - Low predictive accuracy

Ensemble learning

Putting models together

Ensemble learning

- Putting multiple models / learners together in an ensemble
- Voting: can be shown mathematically that, to minimise prediction errors, for
  - Classification: use majority vote (mode)
  - Regression: use mean of all predictions

Intuition of rationale behind ensemble learning

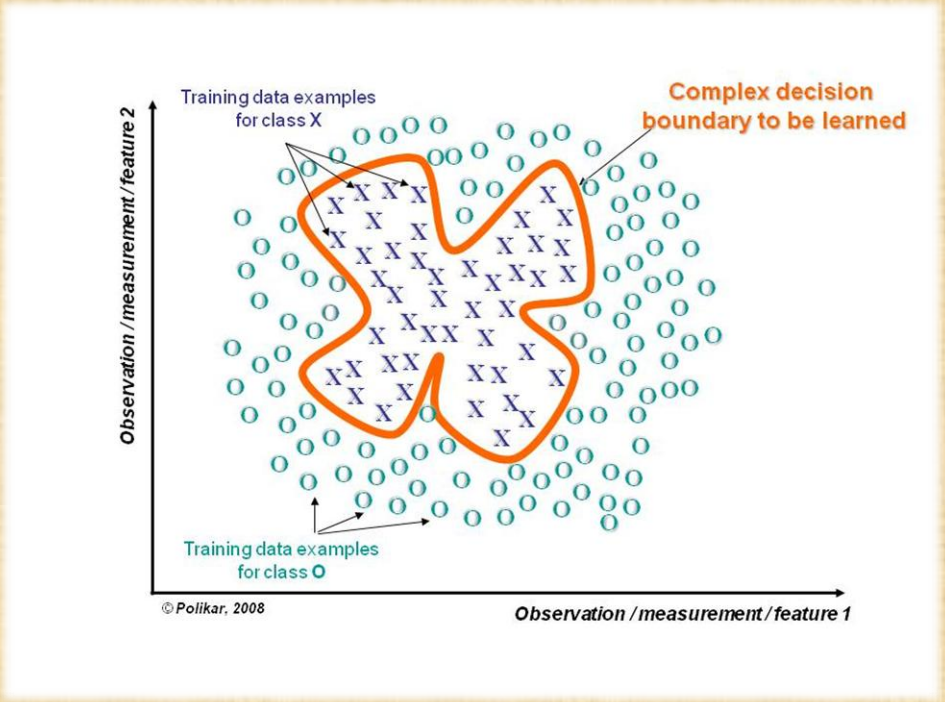
- Binary classification: a single classifier has probability $p > 0.5$ of giving the correct answer
- Let's assume $p = 0.6$
- Putting three classifiers together:
  - Predicted answer is correct if 2 out of 3 classifiers give correct answer
  - Overall probability of giving correct answer, $p^* = 0.648$
- Generally, p^* increases as number of classifiers increases
- **This result is valid only if the individual classifiers are independent, or at least uncorrelated, with each other**

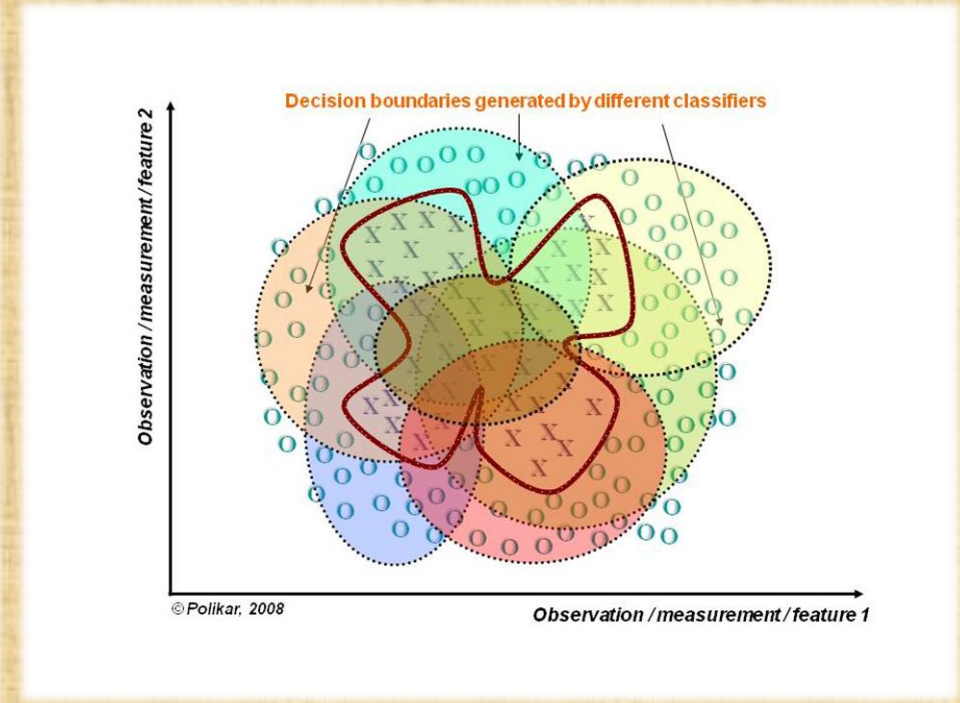
Mathematical rationale

- Each classifier c signifies a Bernoulli random variable, with mean of p, variance of $p(1-p)$
- Putting 3 classifiers together and assuming independence,
  - $(ens.) = \frac{1}{3}(c_1 + c_2 + c_3)$
  - $E(ens.) = p$ (unbiased)
  - $Var(ens.) = \frac{1}{3}p(1-p) < p(1-p) = Var(c)$
- Without independence, we need to consider pairwise covariance terms: $Var(ens.)$ increases

- Analogous for a regression problem: $Var(ens.)$ increases

Another way to look at it





Bagging

Bootstrap aggregating

Bagging

- Voting only works well if the individual models are uncorrelated, or at least less correlated with one another
- Bagging, a.k.a. **b**ootstrap **ag**gregating, aims to alleviate this problem
- Idea: build decision trees on different subsets of the training data. Each subset is known as a "bag"
- Each bag is a sample from the training data, **with replacements**
- Each decision tree gives a vote, overall classification / regression is based on the votes
- **Size of each bag is the same as the sample size of the dataset**

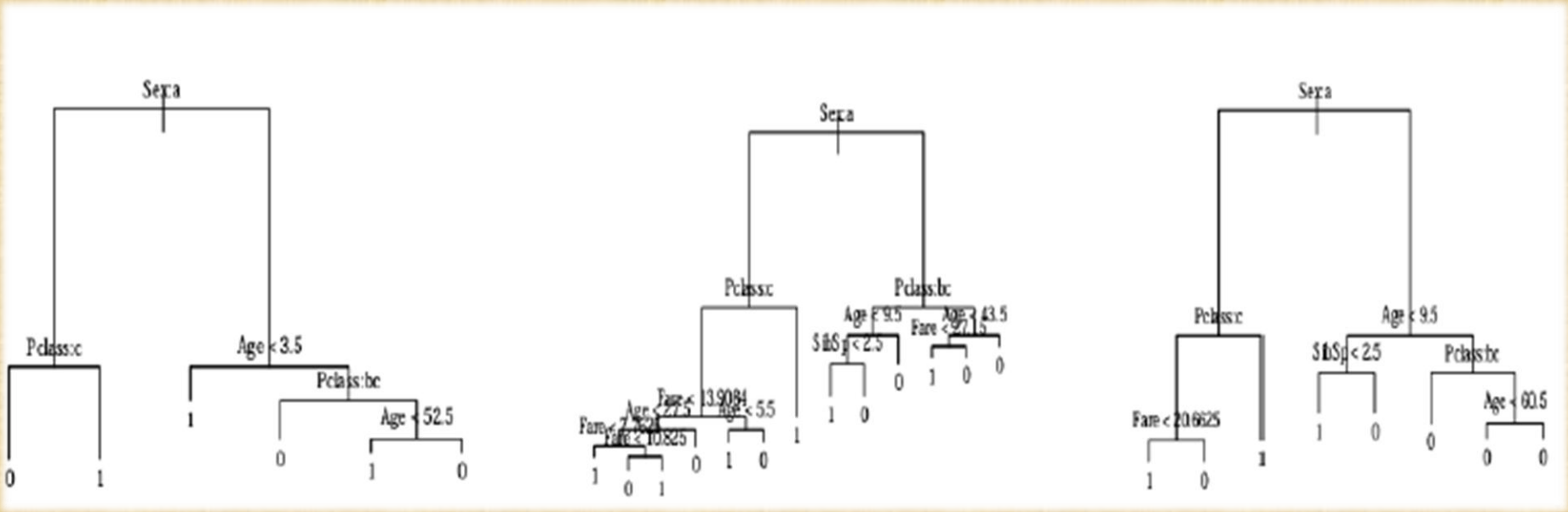
Bagging (2)

Bagging: sample **with** replacement, one tree each

ID	V_1	V_2	V_3	…	V_M	RESPONSE
1						
2						
3						
4						
…						
N						

Not good enough

- Bagging is an attempt to reduce the amount of correlation / similarity in the individual trees




Random forest
Random subspace sampling

Random forest

- To further reduce correlation / similarity between trees, RF uses a technique called "**random subspace sampling**"
- For each tree, for each node, instead of choosing one variable from all variables to split on, choose one from only a random subset of variables
- "Space" refers to feature space, i.e. all variables in training data

Bagged forest vs. random forest

Random subspace sampling: sample **without** replacement, choose one to split on for each tree, each node

ID	V_1	V_2	V_3	…	V_M	RESPONSE
1						
2						
3						
4						
…						
N						

Bagged forest: bagging

Random forest: bagging + random subspace sampling

Bagging: sample **with** replacement, one tree each

Bagged forest vs. random forest (2)

Tree

-> (ensemble learning + bagging) bagged forest

-> (random subspace sampling) random forest

- The only difference between bagged forest and random forest is the use of a subset of variables to do splitting on
- [R] Only the **mtry** argument differs

Pros and cons of random forest

- Pros:
  - One of the top-performing models in supervised learning
  - With some basic understanding of sampling and bootstrapping, RF can be easy to communicate. The intuition of voting as a mechanism to make decisions is simple
  - Able to derive variable importance measures
- Cons:
  - Computationally intensive

More about random forest

- Out-of-bag (OOB) assessment of model performance
- Variable importance measures
- Multidimensional scaling (MDS) plot on proximity matrix
- Hyperparameters tuning

Out-of-bag assessment of model performance

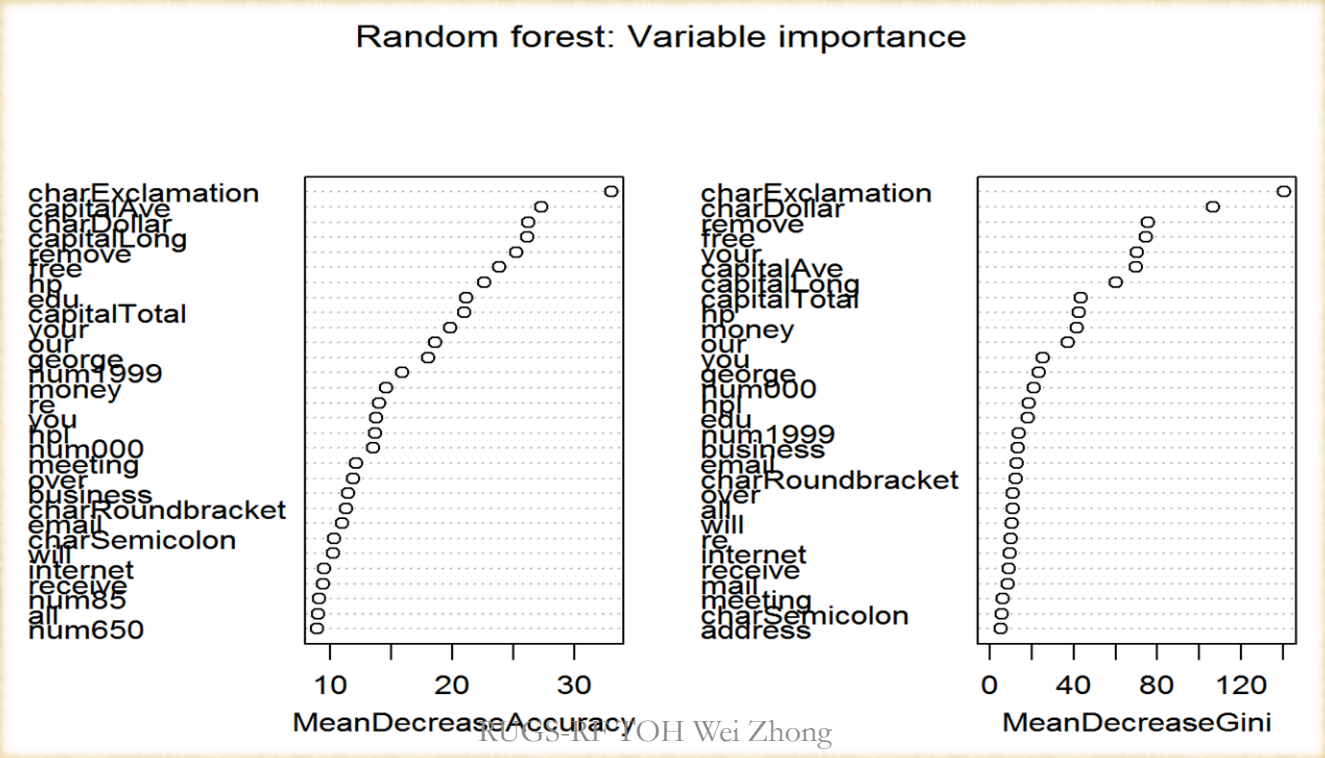
- Similar to cross validation
- Recall that in bagging, we have multiple bags – each bag is a subset of samples in the dataset
- Individual models are then built on each bag
- For a given bag, there are samples in the dataset that is either in the bag or out of bag (OOB)

Out-of-bag assessment of model performance (2)

- For each sample s_i, take the set of models in the ensemble that did not use s_i in its construction. Call this sub-ensemble E_{-i}
- We then get a prediction of s_i, using E_{-i}, by voting
- The prediction of s_i using E_{-i} may incur
  - A classification error $(err.)_i$
  - A regression error ε_i
- The OOB error estimate of the entire ensemble is then
  - $(err.rate)_{OOB} = \frac{1}{n}\sum(err.)_i$
  - $MSE_{OOB} = \frac{1}{n}\sum {\varepsilon_i}^2$

Variable importance

- To assess relative variance importance in RF model,
  - Mean decrease in accuracy (MDA)
  - Mean decrease in Gini (MDG)



Mean decrease in accuracy

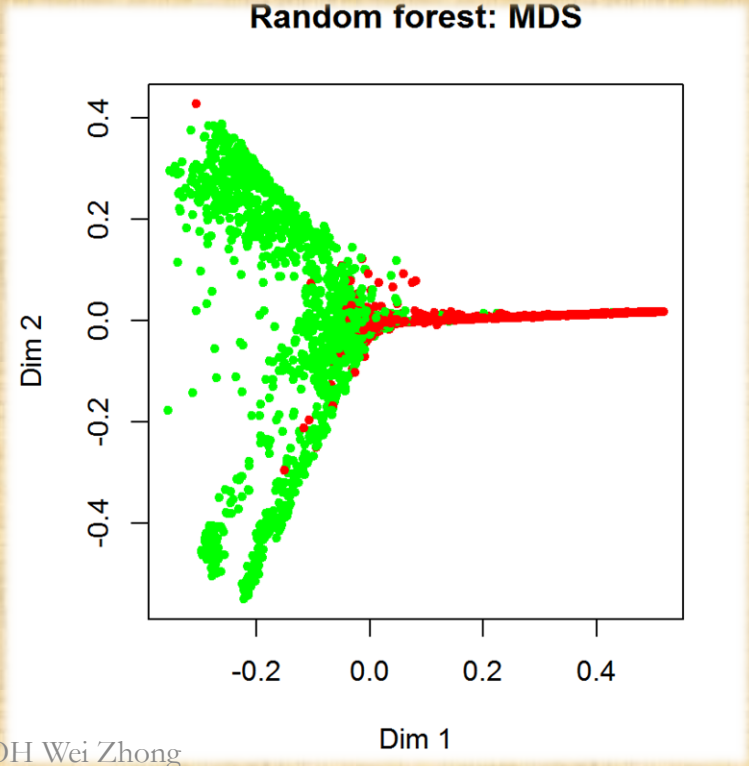
- For each tree T_k in the ensemble, take its OOB samples (samples that were not used in the construction of T_k). Call them $(oob)_k$
- Run all $(oob)_k$ down T_k, and get a classification accuracy
- Now, for each variable v_j in $(oob)_k$, randomly shuffle its values. Run the v_j-shuffled-$(oob)_k$ down T_k
- Measure the decrease in accuracy for v_j on T_k, call it $(da)_{jk}$. Repeat for all j, k
- To get MDA for v_j,
  - $(mda)_j = \frac{1}{\boldsymbol{ntree}} \sum (da)_{jk}$
- Analogous to regression: use MSE

Mean decrease in Gini

- In the construction of each tree T_k in the ensemble, for each split, the variable used reduces the Gini impurity criterion
- Simply add up the Gini decreases accumulated by each variable, and divide by **ntree**

Multidimensional scaling plot on proximity matrix

- Very good tool to visualize samples in the dataset in relations to each other, in the context of the RF model
- Two things here:
  - Multidimensional scaling
  - Proximity matrix

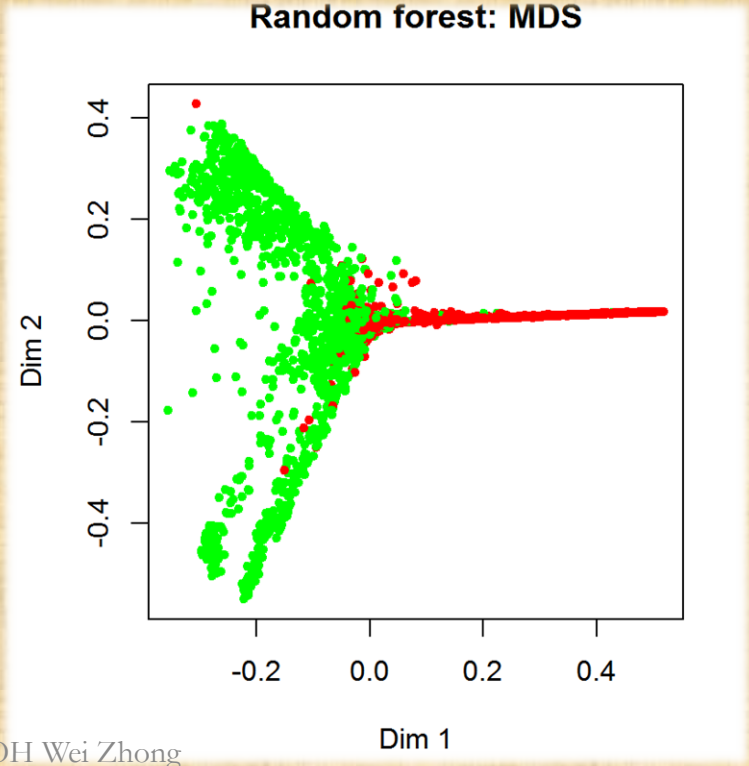


Proximity matrix in RF

- Create a n-by-n identity matrix (n is the number of samples). Call it P
- For each sample s_i, run it down all trees in E_i
  - s_i will end up in particular leaf nodes in each tree in E_i
- Take another sample s_j, run it down in E_j
- Each time s_i and s_j end up in the same leaf node, increment P_{ij} and P_{ji} by 1
- Finally, standardise by dividing the off-diagonal elements of P by **ntree**
- This gives the proximity matrix P

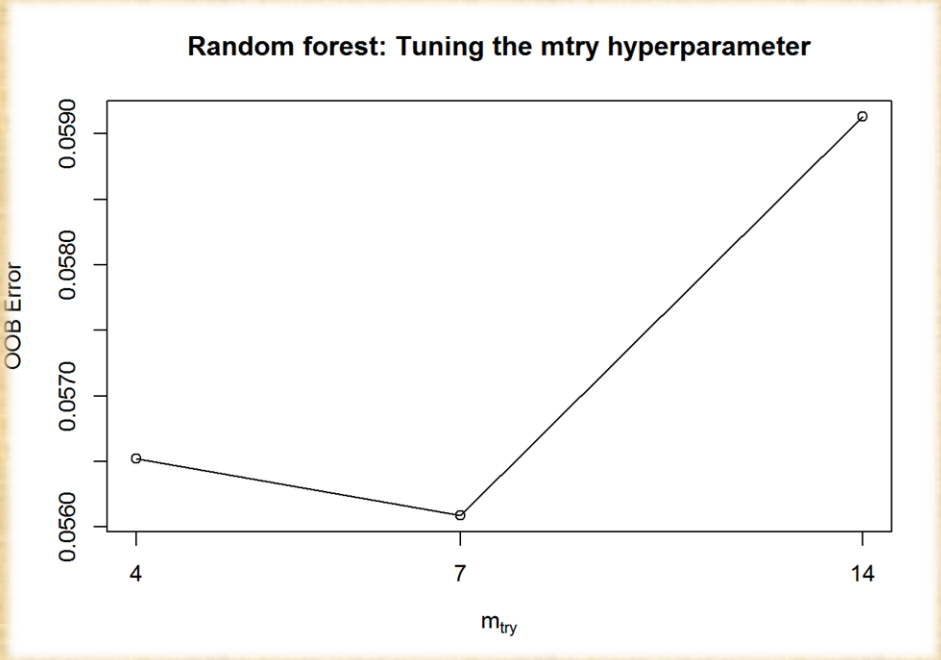
Multidimensional scaling plot on proximity matrix

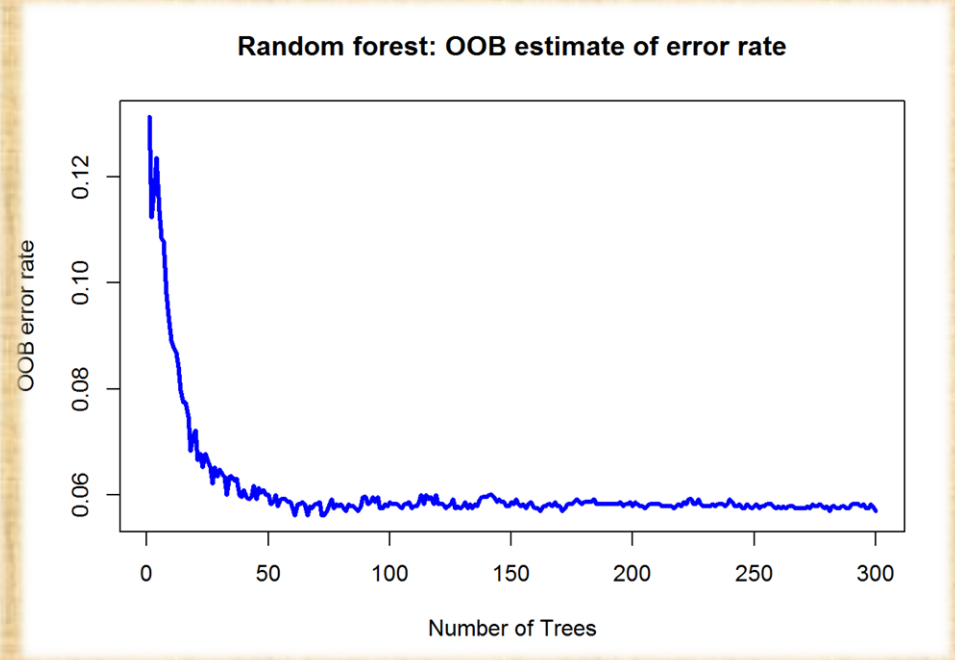
- With the proximity matrix P, do principal components analysis (PCA)
- Plot PC1 and PC2



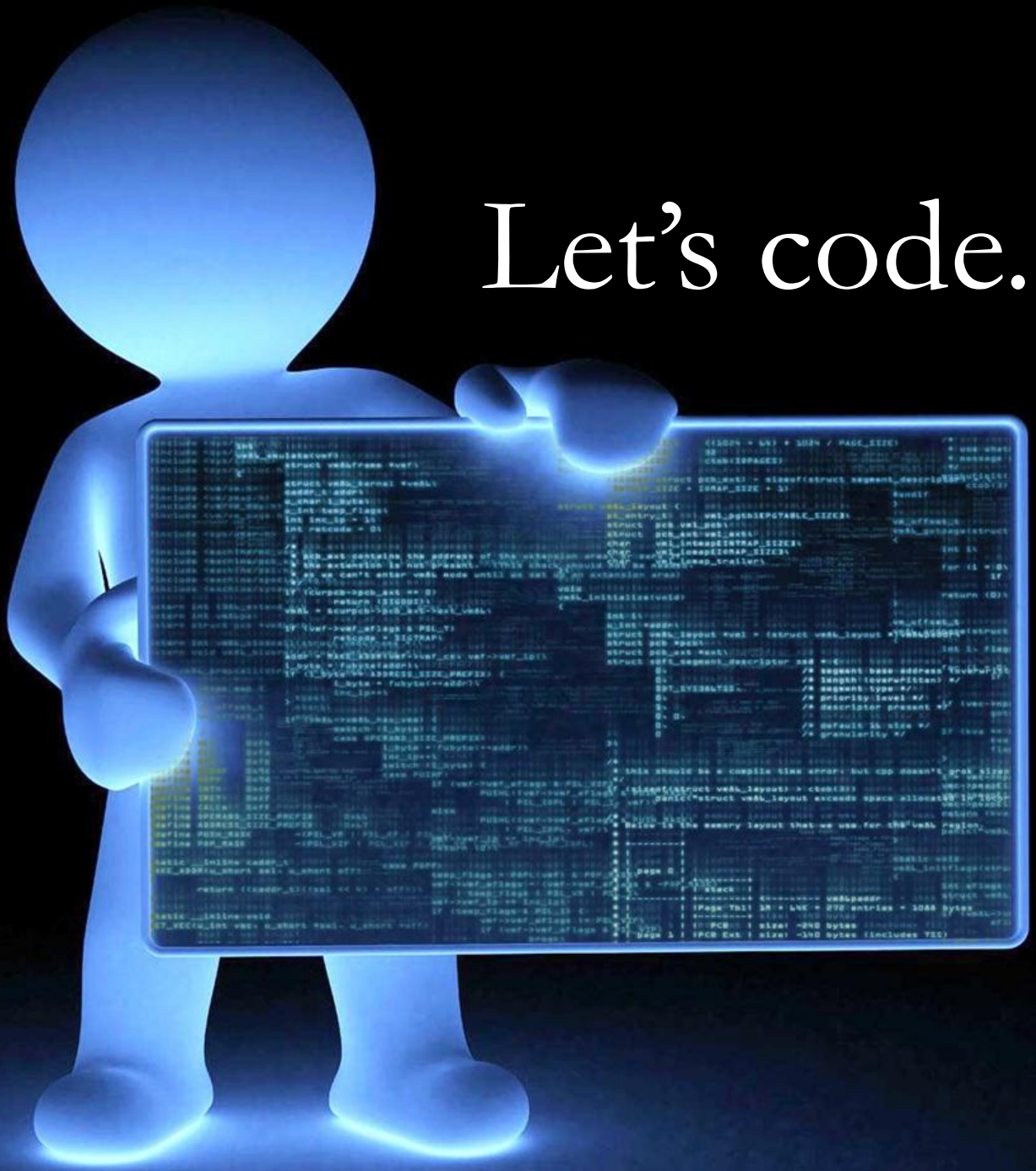
Tuning of RF parameters in R

- **mtry**: number of variables to try from for each split
- **ntrees**: number of trees in ensemble





Let's code.



What's next?

- Gradient boosting
- Ensemble of ensembles
- Model stacking

} Well-liked by Kagglers


Thanks!
Questions?
github.com/singator/rugs
sg.linkedin.com/in/tohweizhong
tohweizhong@u.nus.edu