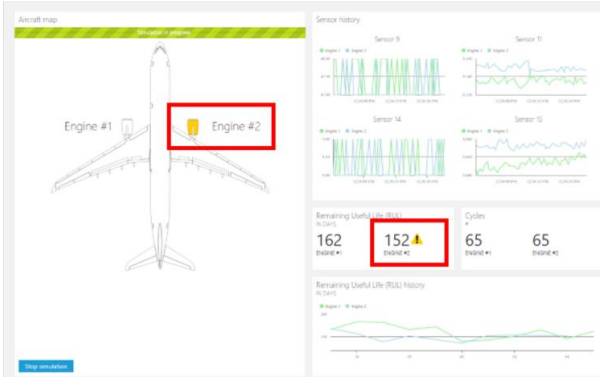
Modelling with Lasso and Random Forest

NUS Lecture

Minh Nguyen

Purposes of Data Modelling

- Inference
  - Explain the relationship among predictors and between predictors and responses.
  - Tell data insights and trigger investigation
- Prediction
  - Estimate responses given predictor values in a set of unobserved samples.



Data Structure

Sample training data

~20k rows,
100 unique engine id

id	cycle	setting1	setting2	setting3	s1	s2	s3	...	s19	s20	s21	RUL	label1	label2
1	1	-0.0007	-0.0004	100	518.67	641.82	1589.7		100	39.06	23.419			
1	2	0.0019	-0.0003	100	518.67	642.15	1591.82		100	39	23.4236			
1	3	-0.0043	0.0003	100	518.67	642.35	1587.99		100	38.95	23.3442			
...	...													
1	191	0	-0.0004	100	518.67	643.34	1602.36		100	38.45	23.1295			
1	192	0.0009	0	100	518.67	643.54	1601.41		100	38.48	22.9649			
2	1	-0.0018	0.0006	100	518.67	641.89	1583.84		100	38.94	23.4585			
2	2	0.0043	-0.0003	100	518.67	641.82	1587.05		100	39.06	23.4085			
2	3	0.0018	0.0003	100	518.67	641.55	1588.32		100	39.11	23.425			
...	...													
2	286	-0.001	-0.0003	100	518.67	643.44	1603.63		100	38.33	23.0169			
2	287	-0.0005	0.0006	100	518.67	643.85	1608.5		100	38.43	23.0848			

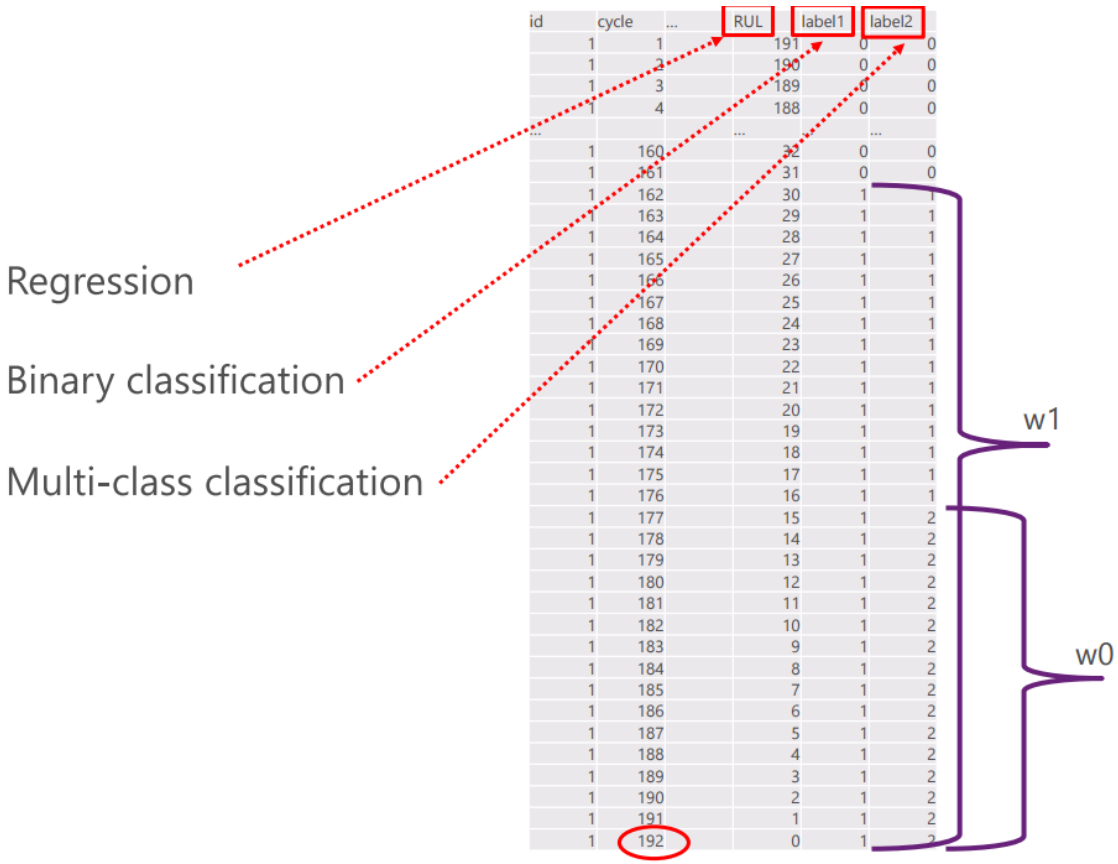
Sample testing data

~13k rows,
100 unique engine id

id	cycle	setting1	setting2	setting3	s1	s2	s3	...	s19	s20	s21
1	1	0.0023	0.0003	100	518.67	643.02	1585.29		100	38.86	23.3735
1	2	-0.0027	-0.0003	100	518.67	641.71	1588.45		100	39.02	23.3916
1	3	0.0003	0.0001	100	518.67	642.46	1586.94		100	39.08	23.4166
...	...										
1	30	-0.0025	0.0004	100	518.67	642.79	1585.72		100	39.09	23.4069
1	31	-0.0006	0.0004	100	518.67	642.58	1581.22		100	38.81	23.3552
2	1	-0.0009	0.0004	100	518.67	642.66	1589.3		100	39	23.3923
2	2	-0.0011	0.0002	100	518.67	642.51	1588.43		100	38.84	23.2902
2	3	0.0002	0.0003	100	518.67	642.58	1595.6		100	39.02	23.4064
...	...										
2	48	0.0011	-0.0001	100	518.67	642.64	1587.71		100	38.99	23.2918
2	49	0.0018	-0.0001	100	518.67	642.55	1586.59		100	38.81	23.2618
3	1	-0.0001	0.0001	100	518.67	642.03	1589.92		100	38.99	23.296
3	2	0.0039	-0.0003	100	518.67	642.23	1597.31		100	38.84	23.3191
3	3	0.0006	0.0003	100	518.67	642.98	1586.77		100	38.69	23.3774
...	...										
3	125	0.0014	0.0002	100	518.67	643.24	1588.64		100	38.56	23.227
3	126	-0.0016	0.0004	100	518.67	642.88	1589.75		100	38.93	23.274

Data Structure

$$y = f(X)$$

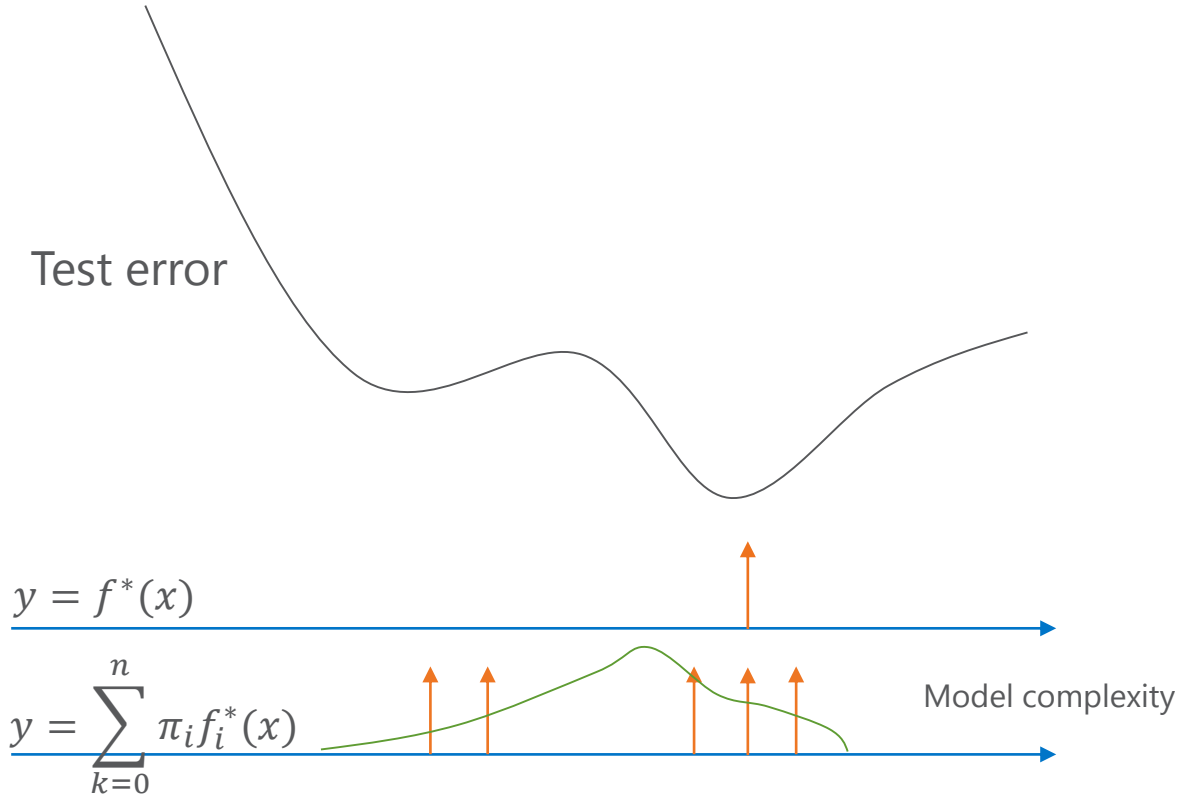


1. LASSO

Basic Model Assumptions

$$y = f(X)$$

- Two approaches to estimate f
  - Underlying model style (*)
  - Bayesian style



Ref: Chapter 5. Deep Learning. Ian Goodfellow, Yoshua Bengio and Aaron Courville

Linear Regression

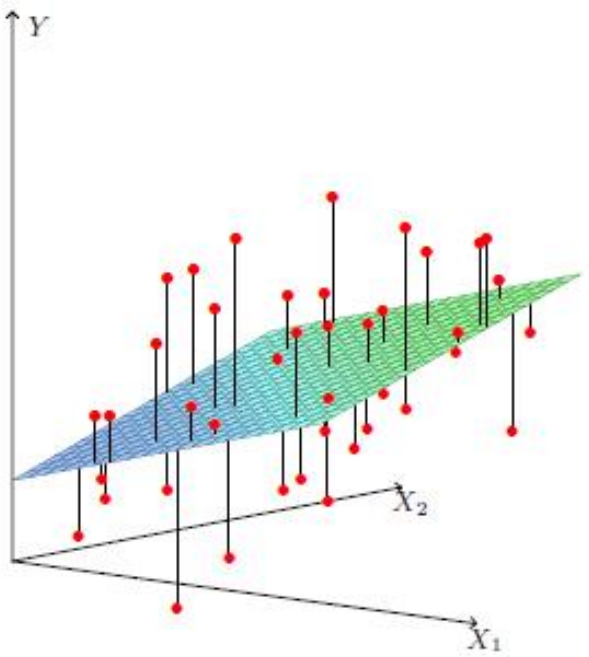
- Assumption: $f(X) = B_0 + \sum_{j=1}^{p} X_j B_j$

To find B

$$J_B = (y - XB)^T (y - XB)$$

$$\frac{\partial J_B}{\partial B} = -2X^T (y - XB)$$

$$\hat{B} = (X^T X)^{-1} X^T y$$



Ridge Regression

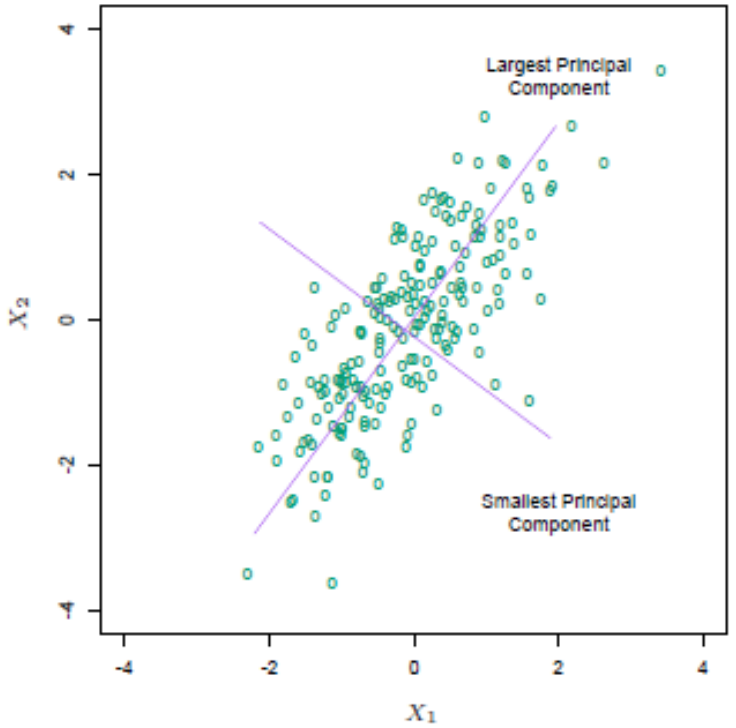
$$J_B = (y - XB)^T(y - XB) + \lambda B^T B$$
$$\hat{B} = (X^T X + \lambda I)^{-1} X^T y$$

With $X = UDV^T$

$$\hat{B} = V(D^2 + \lambda I)^{-1} D U^T y$$

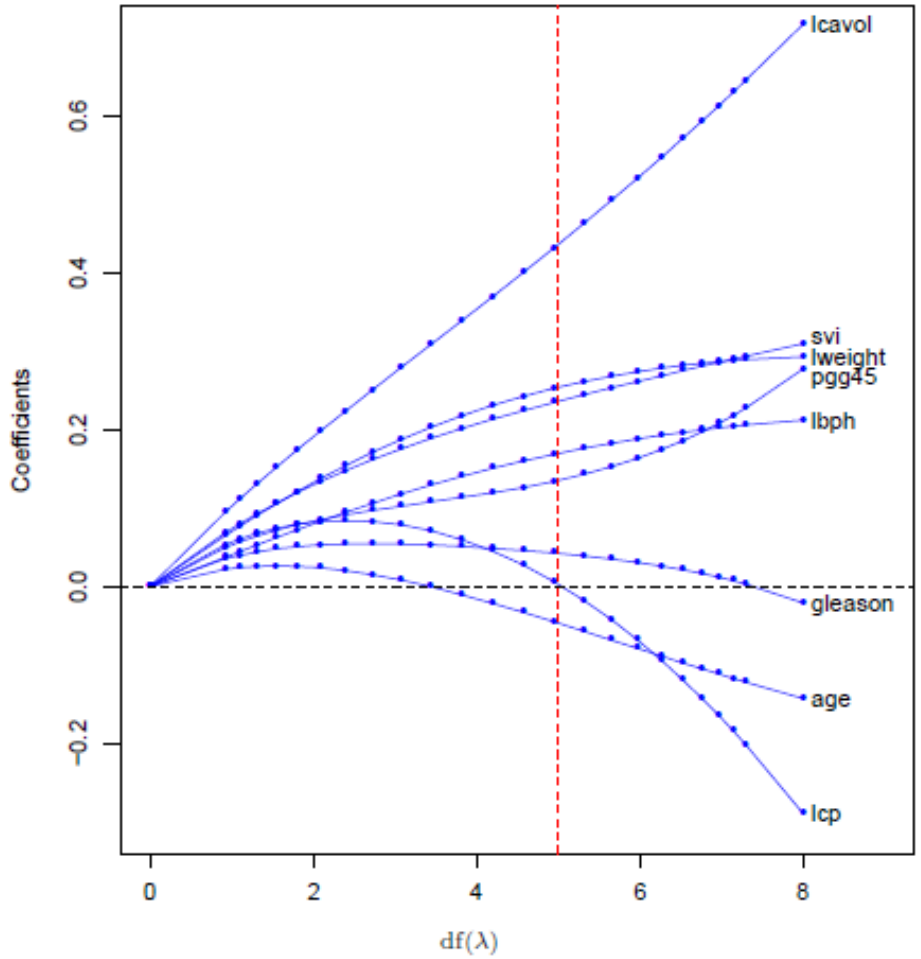
$$\hat{y} = X\hat{B} = \sum_{j=1}^{p} u_j \left(\frac{d_j^2}{d_j^2 + \lambda} \right) u_j^T y$$

u_j columns of U, d_j diagonal elements of D



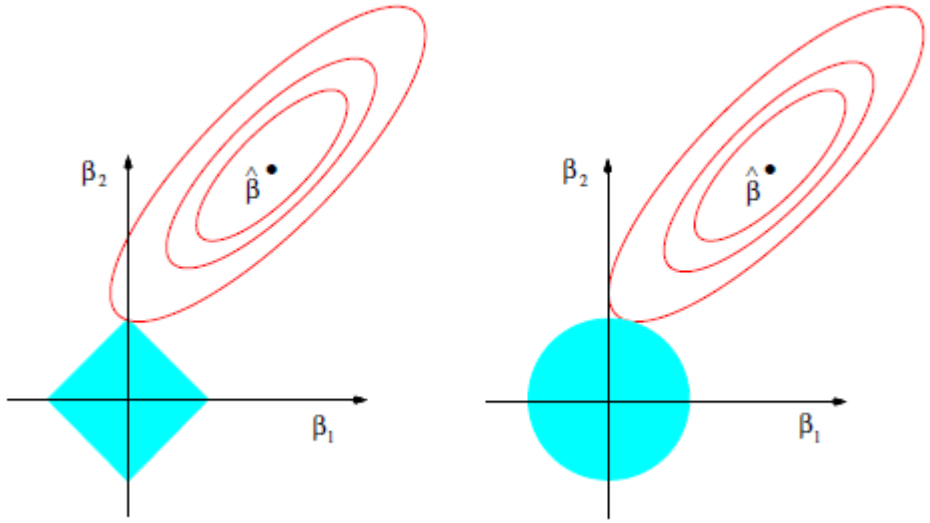
Ref: SVD Tutorial

Ridge Regression

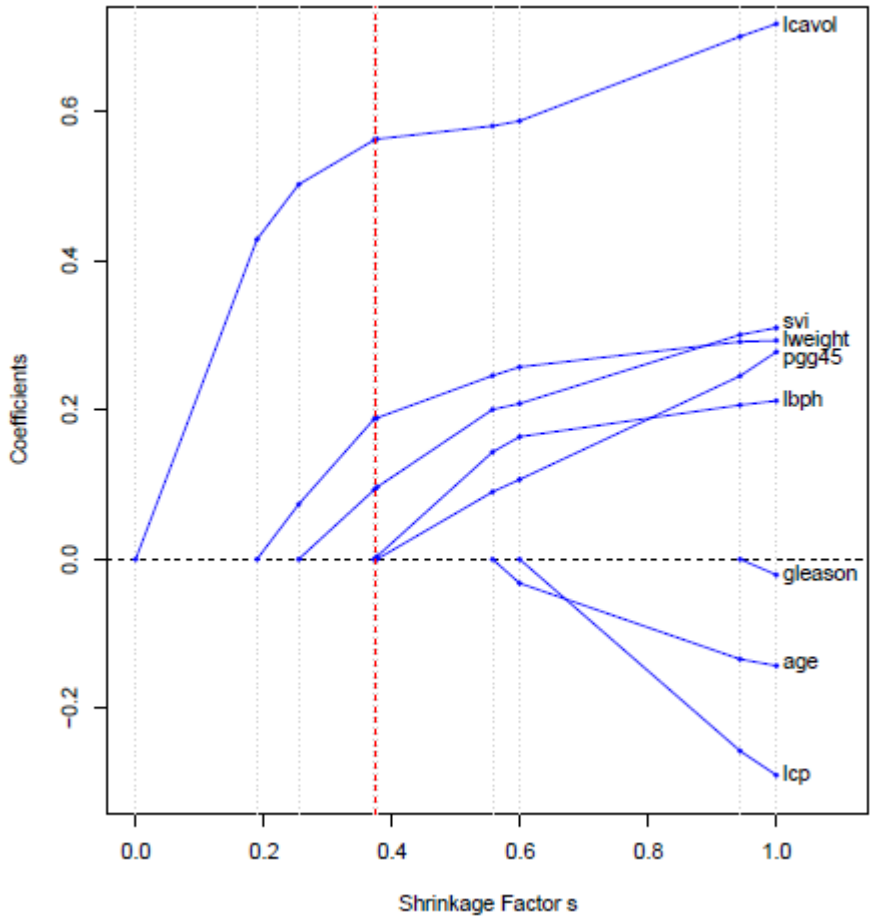


Lasso Regression

$$J_B = (y - XB)^T (y - XB) + \lambda \sum_{j=1}^{p} |B_j|$$

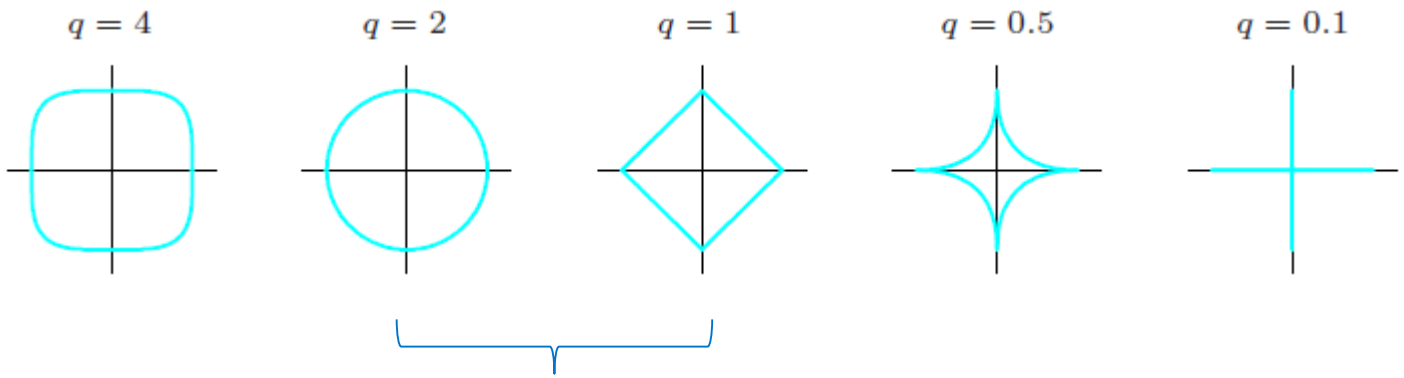


Lasso Ridge



G-Formula

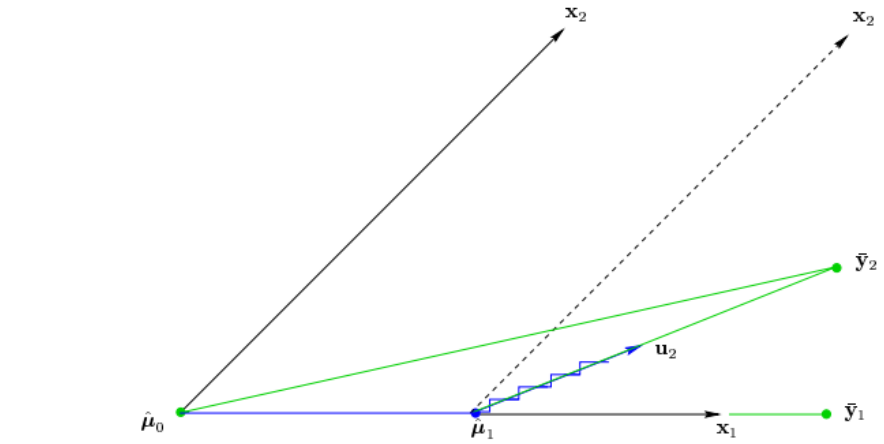
$$J_B = (y - XB)^T (y - XB) + \lambda \sum_{j=1}^{p} |B_j|^q$$

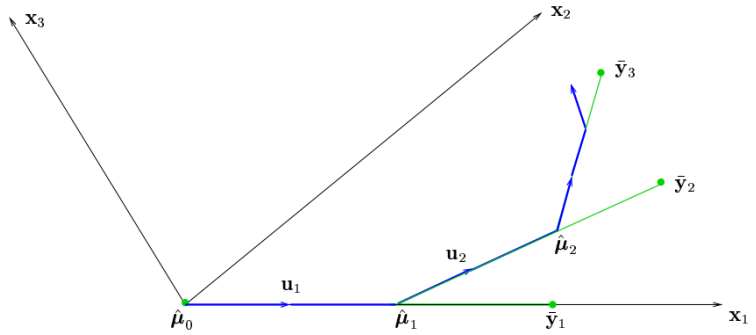


Lasso Solution – Least Angle Regression (LAR)

Algorithm 3.2 *Least Angle Regression.*

1. Standardize the predictors to have mean zero and unit norm. Start with the residual $\mathbf{r} = \mathbf{y} - \bar{\mathbf{y}}$, $\beta_1, \beta_2, \ldots, \beta_p = 0$.
2. Find the predictor $\mathbf{x}_j$ most correlated with $\mathbf{r}$.
3. Move β_j from 0 towards its least-squares coefficient $\langle \mathbf{x}_j, \mathbf{r} \rangle$, until some other competitor $\mathbf{x}_k$ has as much correlation with the current residual as does $\mathbf{x}_j$.
4. Move β_j and β_k in the direction defined by their joint least squares coefficient of the current residual on $(\mathbf{x}_j, \mathbf{x}_k)$, until some other competitor $\mathbf{x}_l$ has as much correlation with the current residual.
5. Continue in this way until all p predictors have been entered. After $\min(N-1, p)$ steps, we arrive at the full least-squares solution.



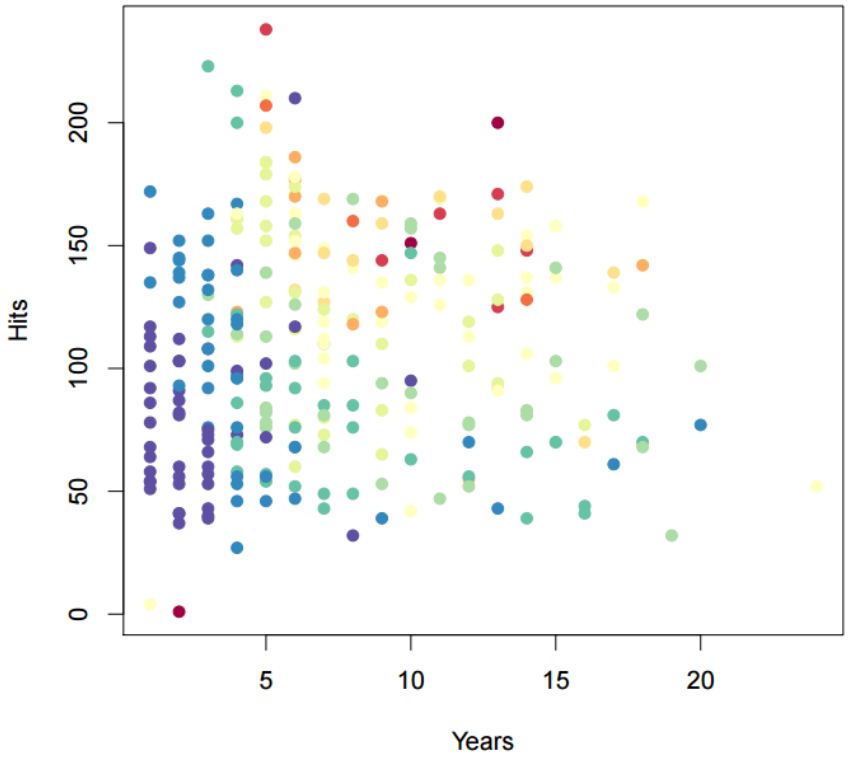


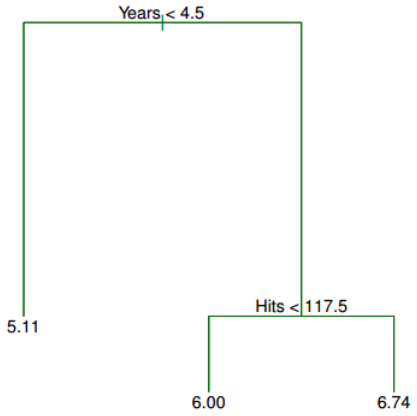
- Questions?

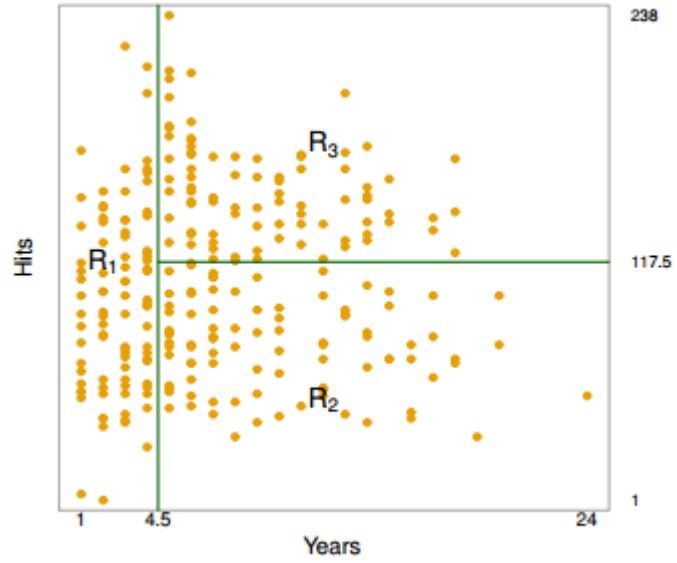
2. RANDOM FOREST

Decision Tree

Salary is color-coded from low (blue, green) to high (yellow,red)





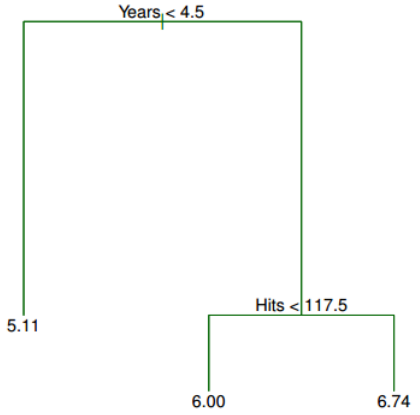


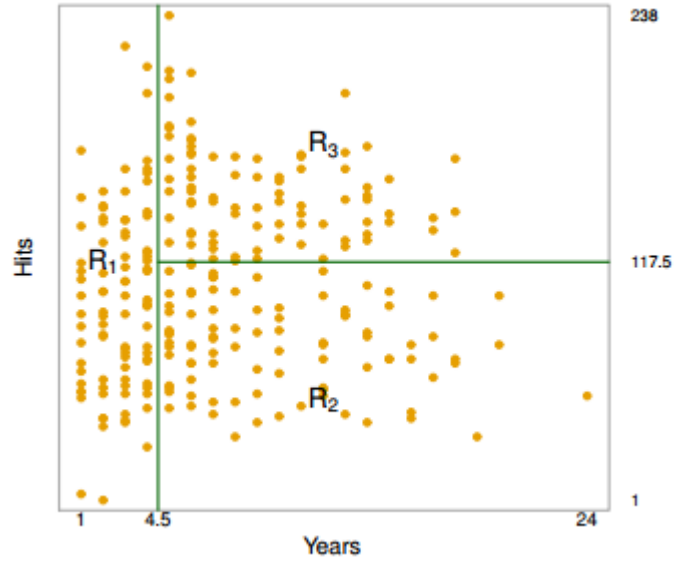
Decision Tree

An approach that is known as recursive binary splitting

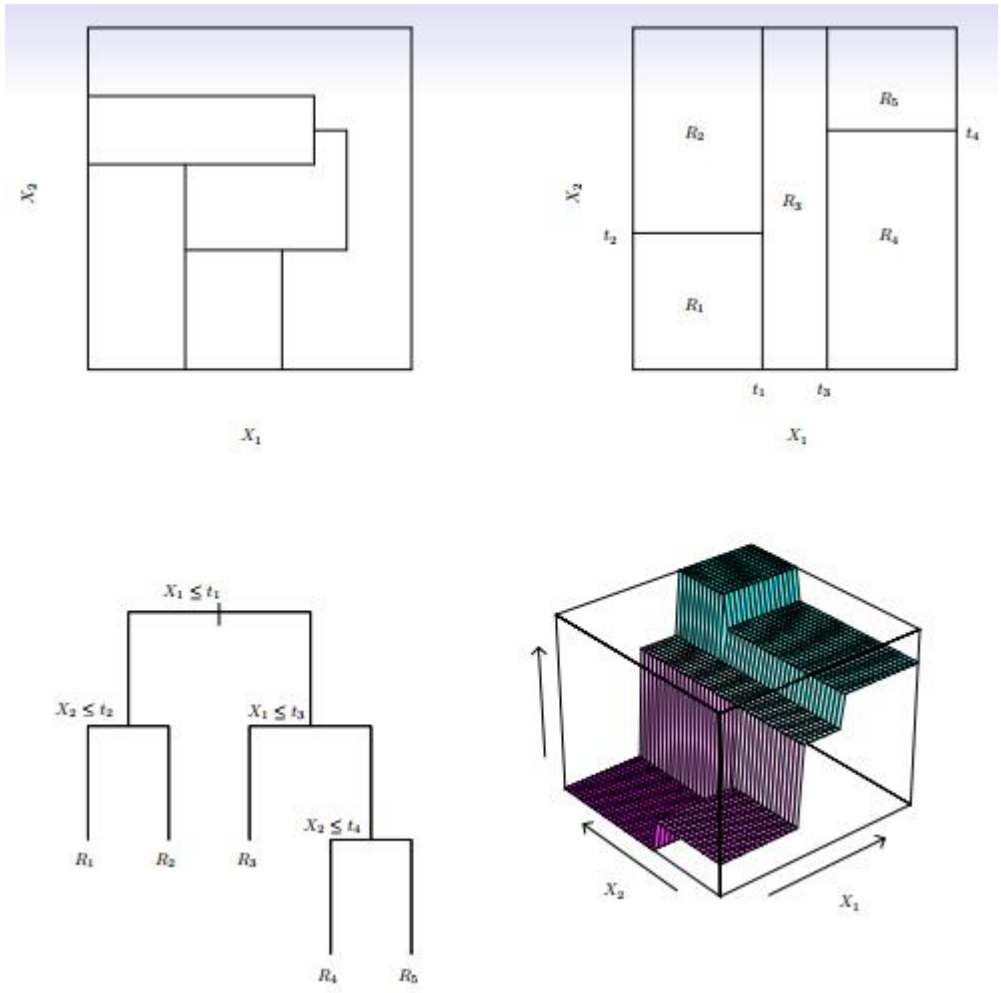
- **Top-down**,
- **Greedy**

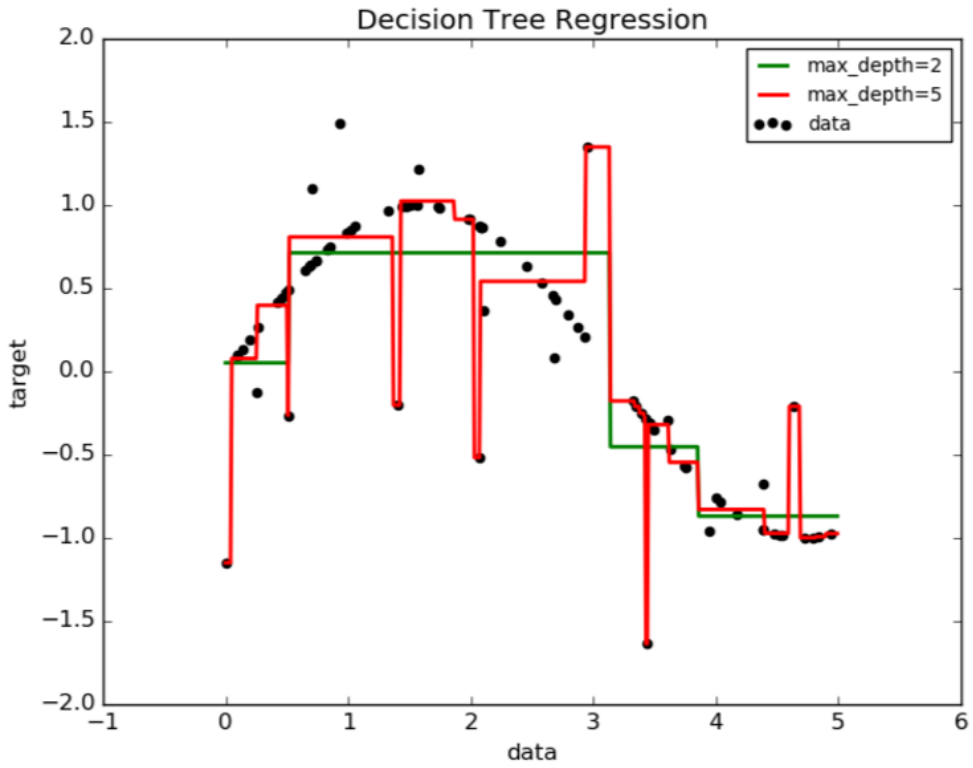
Predict the response for a given test observation using the mean of the training observations in the region





Tree Complexity and Overfitting





Tree Pruning

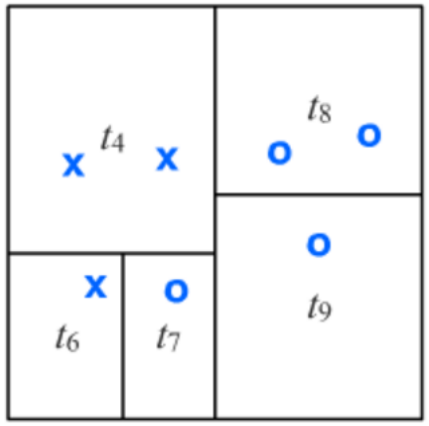
- Motivation: Simple tree is too biased. Complex tree is overfitting.
- Naïve solution: grow the tree only so long as the decrease in the RSS due to each split exceeds some (high) threshold.
  - Result in smaller trees, but is too **short-sighted**: a seemingly worthless split early on in the tree might be followed by a very good split

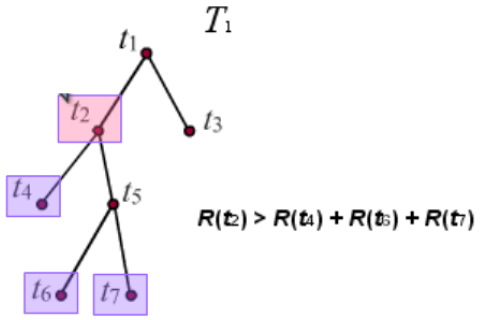
XOR

P	Q	$P\ xor\ Q$
1	1	0
1	0	1
0	1	1
0	0	0

Tree Pruning

- Motivation: Simple tree is too biased. Complex tree is overfitting.
- Better solution: grow a large tree, then merge back nodes to obtain a smaller tree of the right size link





0.25 > 0 + 0 + 0

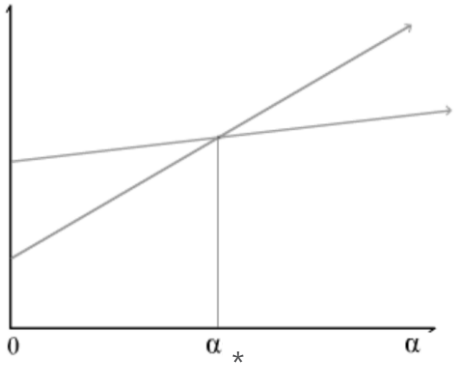
Cost complexity pruning (or Weakest link pruning)

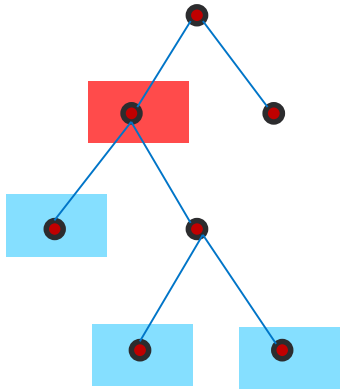
- Define T_t a branch rooted at a node t, and and $\tilde{T}_t$ is its set of terminal nodes.
- Let α be a regularization parameter.

$$R_\alpha(t) = R(t) + \alpha * 1$$

$$R_\alpha(T_t) = \sum_{t' \; in \; \tilde{T}_t} R(t') + \alpha * \left|\tilde{T}_t\right|$$

$$\alpha_* = \frac{R(t) - R(T_t)}{\left|\tilde{T}_t\right| - 1}$$





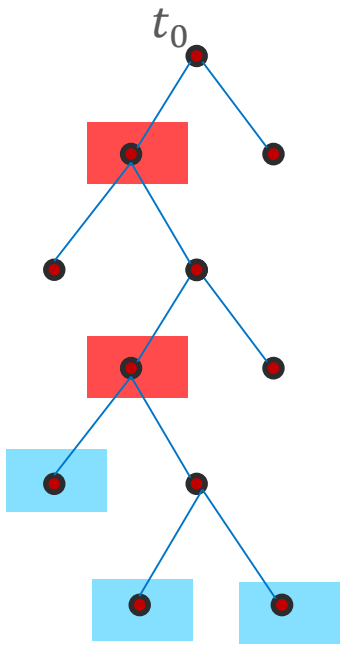
Cost complexity pruning (or Weakest link pruning)

1. Construct a large tree T_0.
2. Find a node t that minimizes the function $g(\mathrm{t}) = \frac{R(t)-R(T_t)}{|\tilde{T}_t|-1}$. Let $\alpha_1 = \mathrm{g}(t)$ and remove all sub-nodes under t to produce T_1.
3. Repeat step 2 to find two sequences

$\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_{|T|}$

$T_1 > T_2 < T_3 > \cdots > t_0$

Note: $R(t)$ can be stored.



Single Decision Tree

Algorithm 8.1 *Building a Regression Tree*

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.

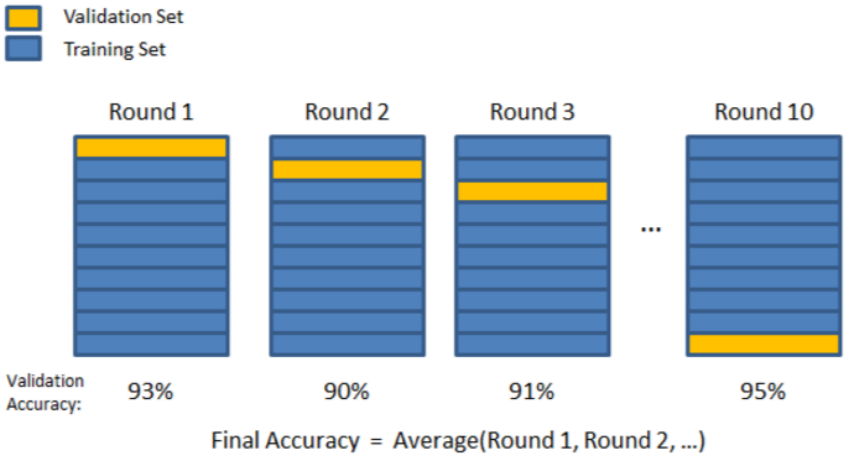
3. Use K-fold cross-validation to choose α. That is, divide the training observations into K folds. For each $k = 1, \ldots, K$:

   (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.

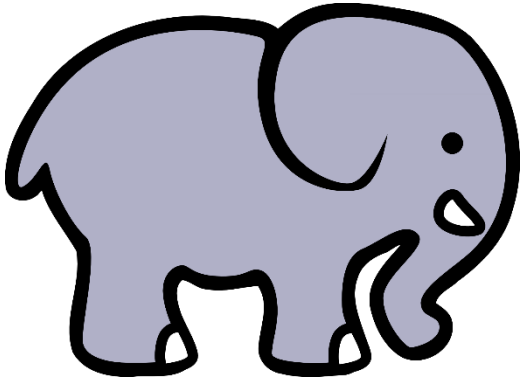
   (b) Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

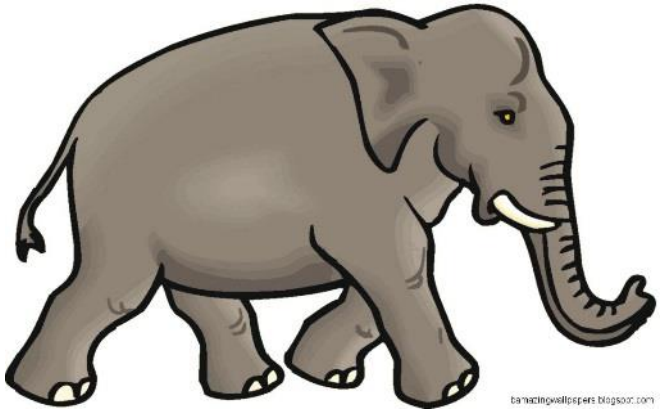
   Average the results for each value of α, and pick α to minimize the average error.

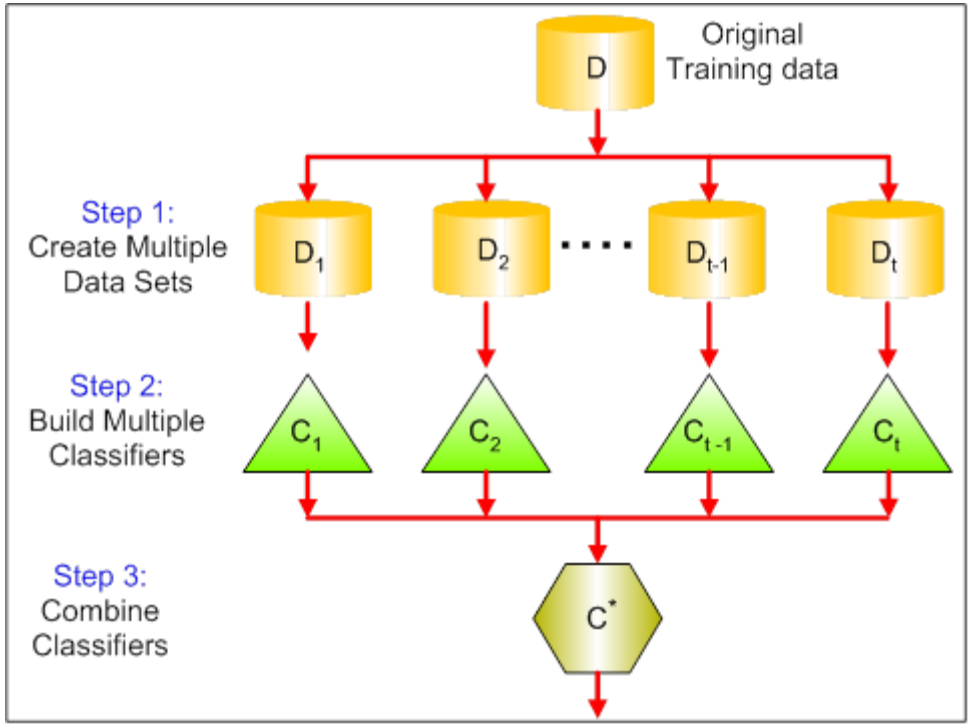
4. Return the subtree from Step 2 that corresponds to the chosen value of α.



Bagging





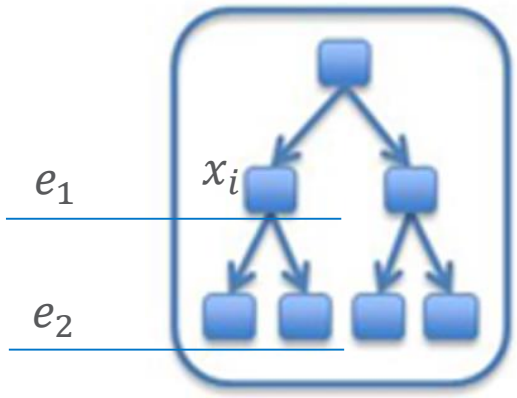


Bagging – Prediction

- Averaging predictions from multiple trees, each is constructed on one part of a training data set. Famous method: Bootstrap (sampling with replacement).

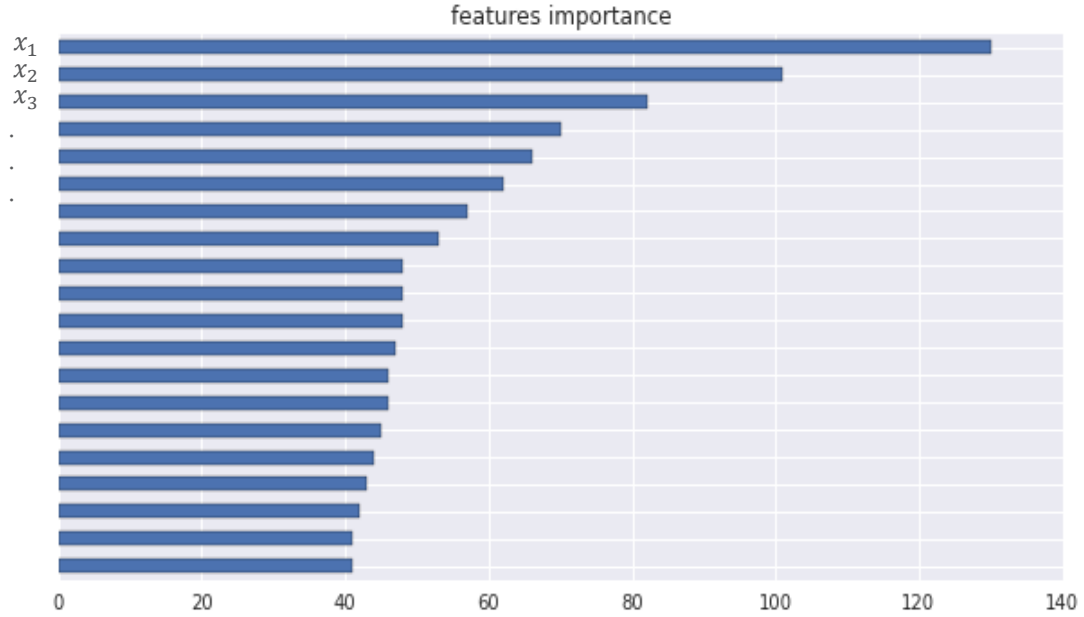
Bagging – Variable Importance

At each tree

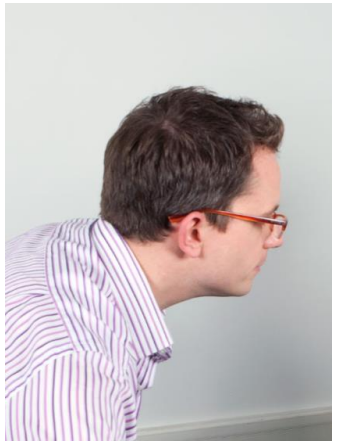


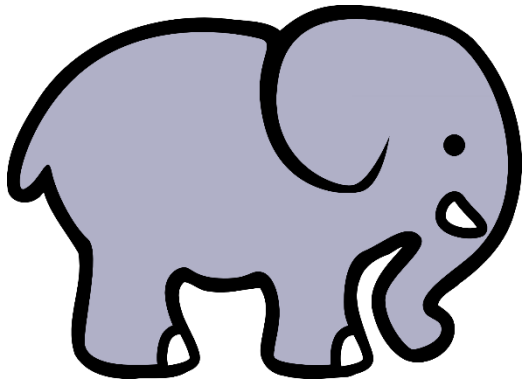
Importance of x_i
$= e_1 - e_2$

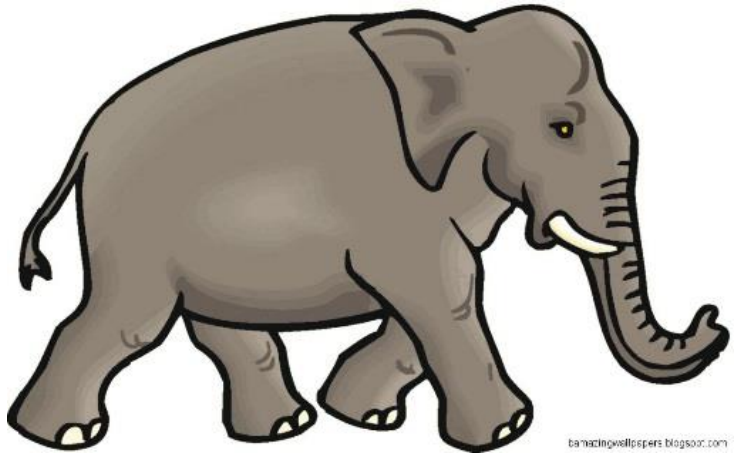
Sum-up



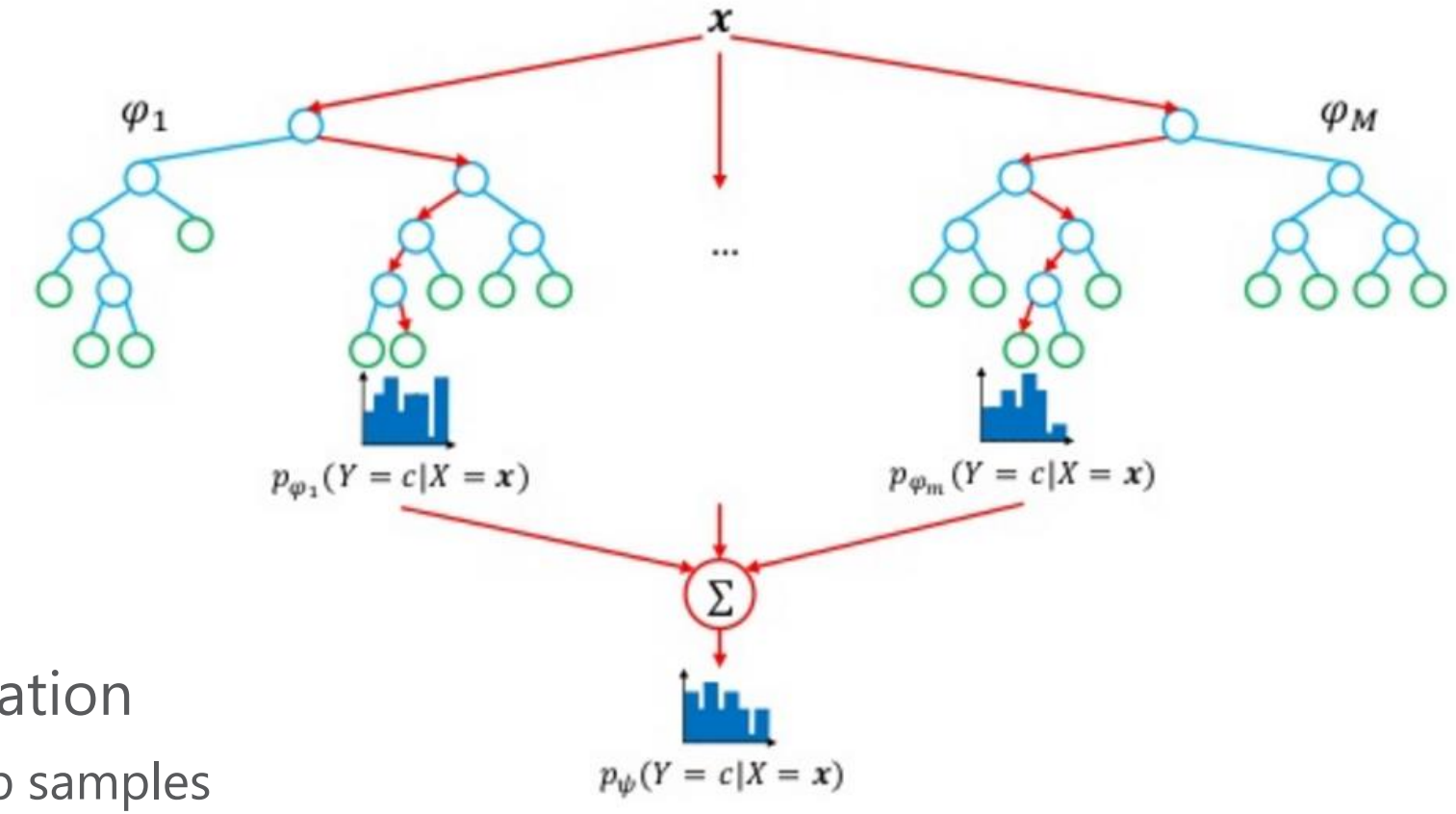
Random Forest







Random Forests



- Randomization
  - Bootstrap samples
  - Variable selection for each tree


Micron®