Introduction to Statistical Learning

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Agenda

1. Introduction to Statistical Machine Learning
   - Key concepts
   - Cross-Validation
2. Supervised learning – Regression
   - Regularisation methods
3. Supervised learning – Classification
   - Logistic regression
   - Tree-based methods
   - Ensemble Learning
4. Implementation in R

Statistical Machine Learning: Resources

- Most of the discussion is based on this book:
  - Available at: https://www.statlearning.com/
  - Focus on intuition and practical implementation

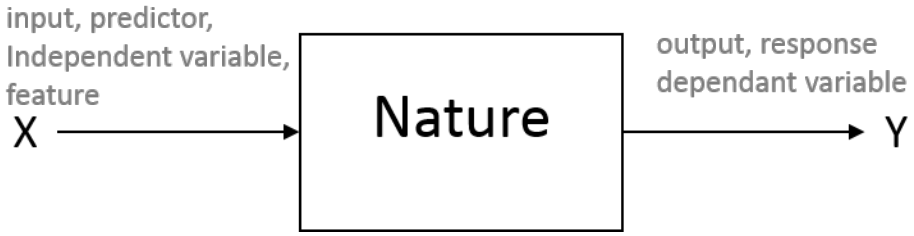
- This book can serve as reference for those interested in the math behind the methods
- Available at: http://web.stanford.edu/~hastie/ElemStatLearn/

Workshop materials

https://github.com/amvillegas/afric

Key concepts in statistical machine learning

What is statistical (machine) learning?



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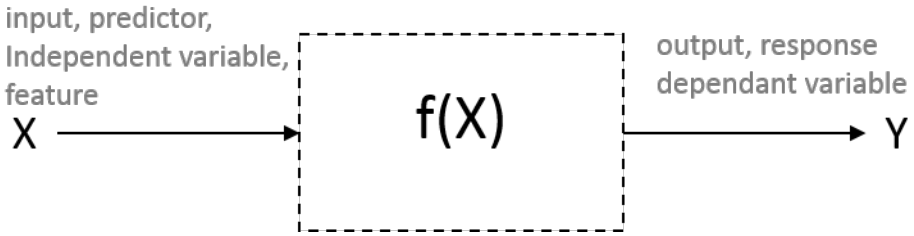

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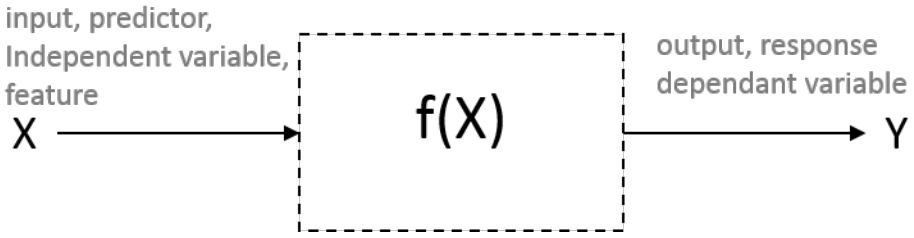


Prediction

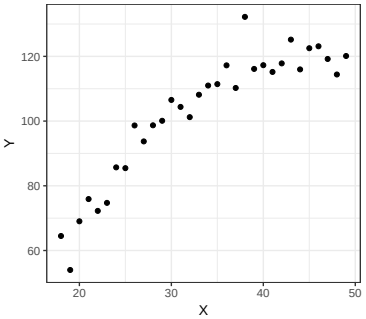
- Predict outcomes of Y given X
  - What it means isn't as important, it just needs accurate predictions
- Models tend to be more complex

Inference

- Understand how Y is affected by X
- Which predictors do we add? How are they related?
- Models tend to be simpler

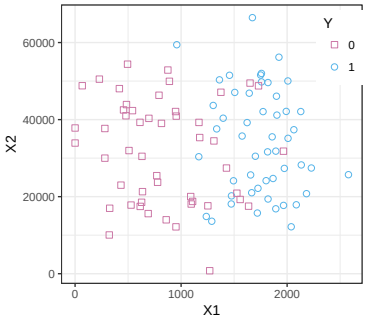
Regression vs. classification

Regression



- Y is quantitative, continuous
- Examples: Sales prediction, claim size prediction, stock price modelling

Classification



- Y is qualitative, discrete
- Examples: Fraud detection, face recognition, accident occurrence, death

More formally in regression we assume

$$Y = f(X) + \epsilon$$

- Y is the outcomes, response, target variable
- $X := (X_1, X_2, \ldots, X_p)$ are the features, inputs, predictors
- ϵ captures measurement error and other discrepancies

Our objective is to **find** an **appropriate** f for the problem at hand

How to estimate f?

Parametrics

- Make an assumption about the shape of f
- Problem reduced down to estimating a few parameters
  - Works fine with limited data, provided assumption is reasonable
- Assumption strong: tends to miss some signal

Non-parametric

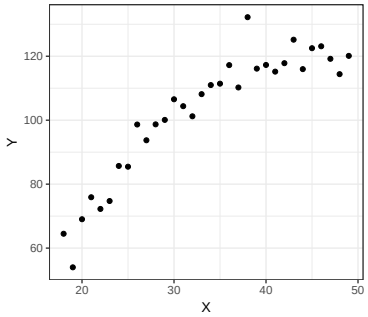
- Make no assumption about f's shape
- Involves estimating a lot of "parameters"
- Need lots of data
- Assumption weak: tends to incorporate some noise
- Be particularly careful re the risk of overfitting

Parametrics example: Linear regression

Approximately a linear relationship between X and Y

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

- The model is specified in terms of $p + 1$ parameters β_0, β_1, ..., β_p
  - Use (training) data to produce estimates $\hat{\beta}_0$, $\hat{\beta}_1$, ..., $\hat{\beta}_p$
  - **Almost never correct**, but serves as a good and interpretable approximation.

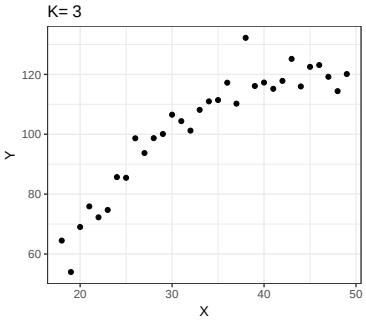


Non-parametrics example: K-nearest neighbours

KNN is one of the simplest non-parametric approaches

$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_i \in \mathcal{N}_0} y_i$$

- can be pretty good for small p and large data sets (big N)
- need to choose the size of the value of K
  - we will discuss other smoother versions such as local linear regression and splines in session 2



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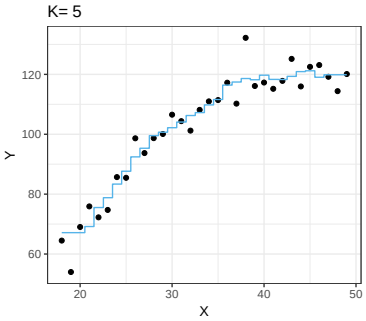

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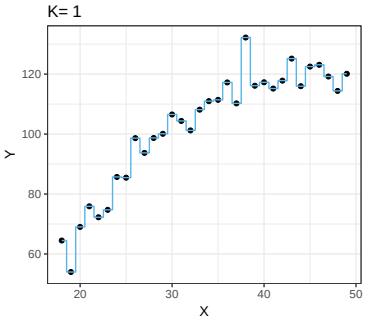
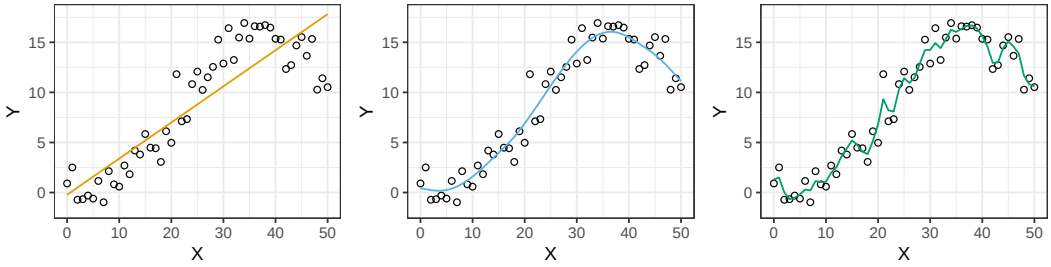


How to choose f?



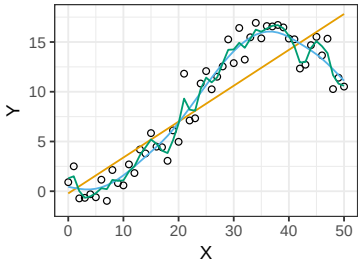
How do we decide which is the best model?

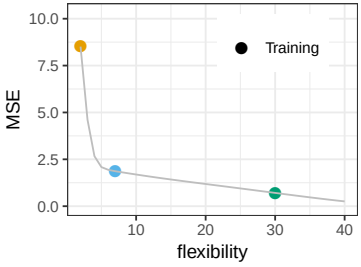
Assessing model accuracy

We fit the model $\hat{f}(x)$ to some **training** data $Tr = \{x_i, y_i\}_{i=1}^{n}$.

- We can compute the Training Mean Squared Error

$$MSE_{Tr} = \frac{1}{n} \sum_{i \in Tr} (y_i - \hat{f}(x_i))^2$$





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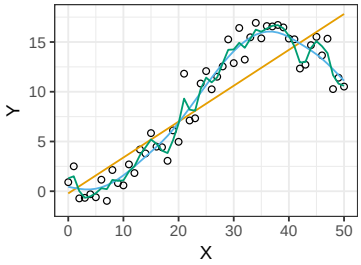
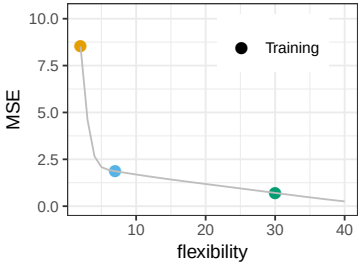
This tends to be biased to more overfit models!





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We fit the model $\hat{f}(x)$ to some **training** data $Tr = \{x_i, y_i\}_{i=1}^{n}$.

- We can compute the Training Mean Squared Error

$$MSE_{Tr} = \frac{1}{n} \sum_{i \in Tr} (y_i - \hat{f}(x_i))^2$$

This tends to be biased to more overfit models!
We should instead use some fresh **test** data $Te = \{x_i, y_i\}_{i=1}^{m}$.

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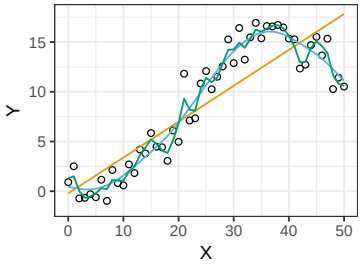
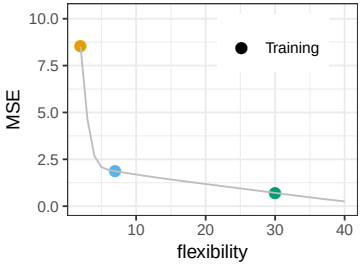
$$MSE_{Te} = \frac{1}{m} \sum_{i \in Te} (y_i - \hat{f}(x_i))^2$$





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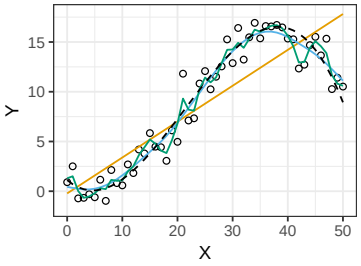
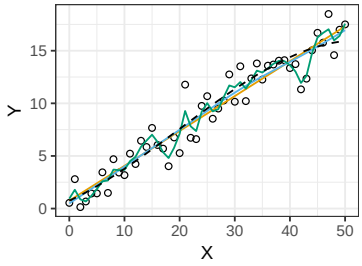
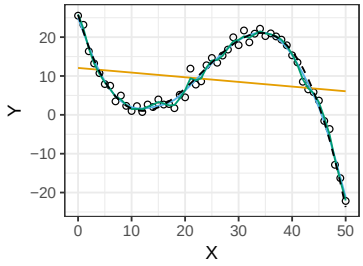
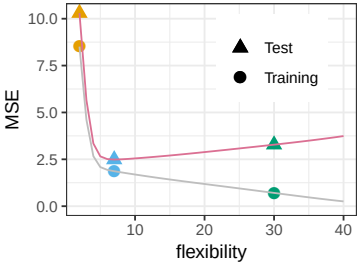
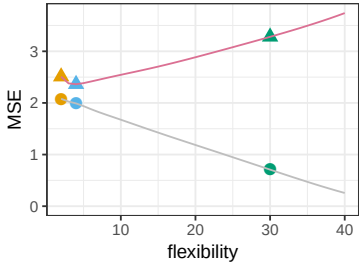
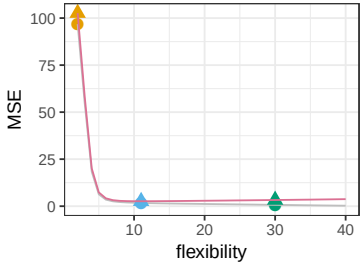












How do we calculate the test error?

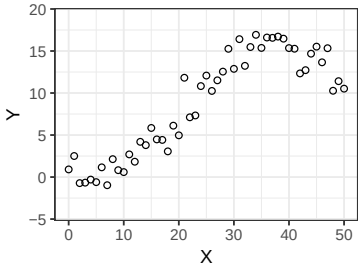
1. The best solution is to use a large designated test set
   - Often not available
2. Make a mathematical adjustment to the training error rate
   - e.g. Cp statistic, AIC and BIC
3. Fit the model to a subset of the training observations
   - Use the remaining training observations as the test set

k-fold Cross-validation

- Randomly divided the set of observations into K groups, or folds of approximately equal size
- the k^{th} fold is treated as a validation set
- the remaining $K-1$ folds make up the training set
- Repeat K times resulting K estimates of the test error

$$\text{CV}_{(K)} = \frac{1}{K}\sum_{k=1}^{K} \text{MSE}_k$$

  - In practice $K = 5$ or $K = 10$



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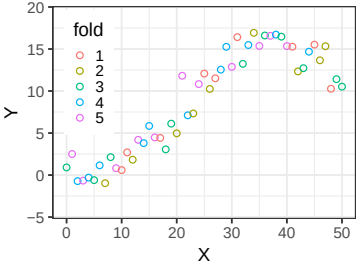
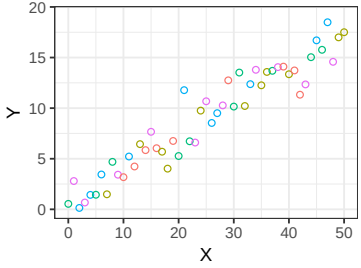
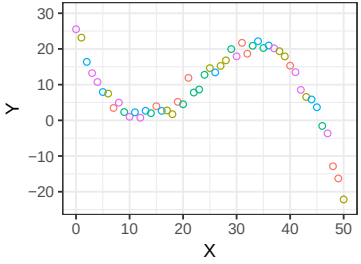
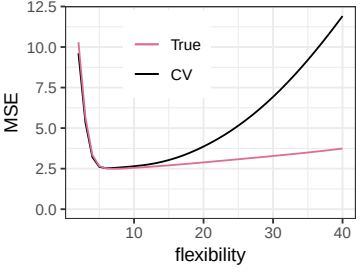
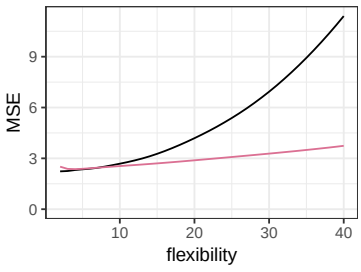
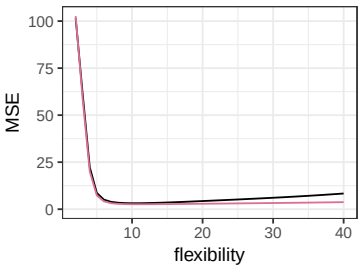












Summary of key concepts

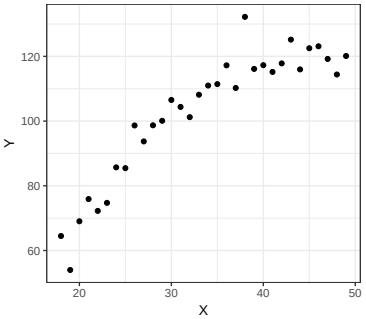
We have discussed key concepts in statistical/machine Learning

- Supervised learning vs. Unsupervised Learning
- Prediction vs. Inference
- Regression vs. Classification
- Parametric Vs. Non-Parametric
- Training MSE vs. Test MSE
- Cross-Validation

Supervised learning: regression

Regression vs. classification

Regression



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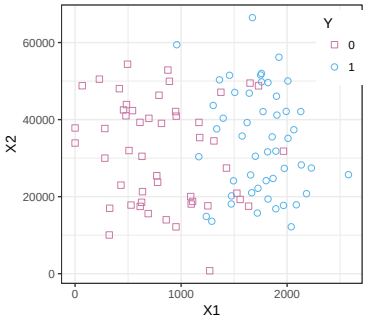
Classification



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Can we predict house prices?

Source: http://www.abc.net.au/news/2018-03-17/how-to-win-at-house-auction/9547166

Output (Y):

- House price

Input (X):

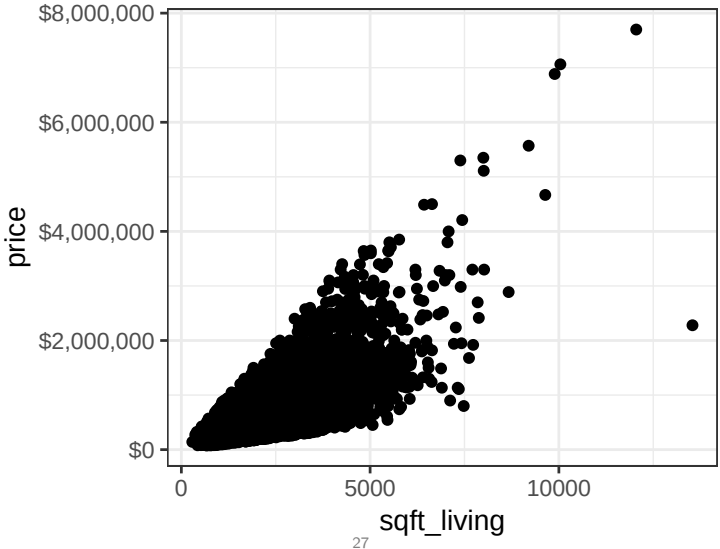
- Home area
- Land area
- # of bedrooms
- # of bathrooms
- Neighbourhood
- Year built
- ...

House Sales in King County, USA

Dataset from Kaggle of 21613 homes sold between May 2014 and May 2015. (https://www.kaggle.com/harlfoxem/housesalesprediction/home)

- `price`: Price is prediction target
- `bedrooms`: Number of Bedrooms
- `bathrooms`: Number of bathrooms/bedrooms
- `sqft_living`: square footage of the home
- `sqft_lot`: square footage of the lot
- `floors`: Total floors (levels) in house
- `yr_built`: Built Year
- `yr_renovated`: Year when house was renovated
- `waterfront`: House which has a view to a waterfront
- `sqft_above`: square footage of house apart from basement

House Sales in King County, USA



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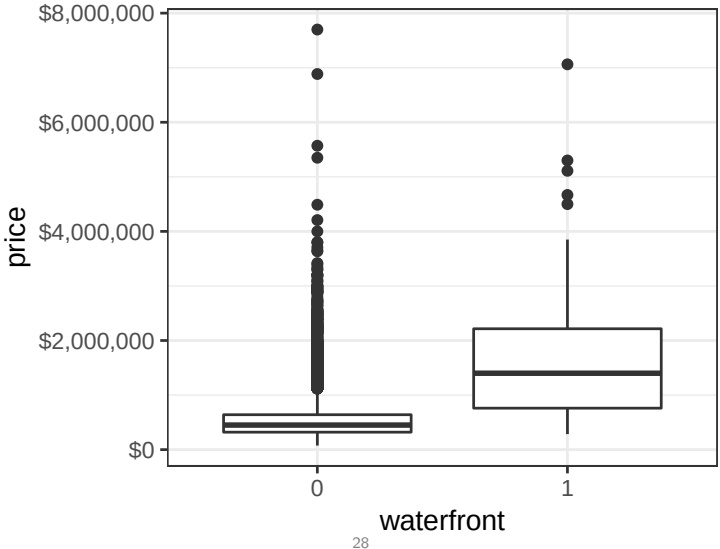


Simple linear regression

- Approximately a linear relationship between X and Y

$$Y = \beta_0 + \beta_1 X + \epsilon$$

- Use (training) data to produce estimates $\hat{\beta}_0$ and $\hat{\beta}_1$
  - Make predictions given $X = x$

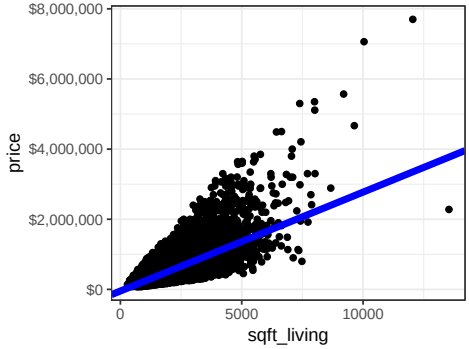
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

- Minimise the residual sum of squares (RSS)

$$\mathrm{RSS} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x)^2$$

Simple linear regression: House prices

$$\texttt{price} = \beta_0 + \beta_1 \times \texttt{sqft\_living}$$



	Variable	estimate	std.error	p.value
1	(Intercept)	-47116.08	4923.34	0.00
2	sqft_living	281.96	2.16	0.00

Multiple linear regression

- Extend the simple linear regression model to accommodate multiple predictors

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$

- β_j: the average effect on Y of a one unit increase in X_j, holding all other predictors fixed

Multiple linear regression: House prices

	Variable	estimate	std.error	p.value
1	(Intercept)	6289259.59	156282.14	0.00
2	bedrooms	-67820.03	2534.30	0.00
3	bathrooms	67280.69	4247.65	0.00
4	sqft_living	281.71	5.22	0.00
5	sqft_lot	-0.29	0.04	0.00
6	floors	43248.82	4526.50	0.00
7	yr_built	-3221.70	80.97	0.00
8	yr_renovated	6.69	4.74	0.16
9	waterfront	740322.15	20947.07	0.00
10	sqft_above	19.19	5.30	0.00

Shortcomings of linear regression

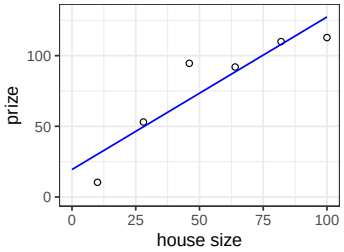
1. **Prediction accuracy**: the linear regression fit often does not predict well, especially when p (the number of predictors) is large
2. **Model Interpretability**: linear regression freely assigns a coefficient to each predictor variable. When p is large, we may sometimes seek, for the sake of interpretation, a smaller set of **important variables**
3. **Non-linearities**: linear assumption is almost **always an approximation** – sometimes bad.

Generalisations of the Linear Model

We discuss methods that expand the scope of linear models and how they are fit:

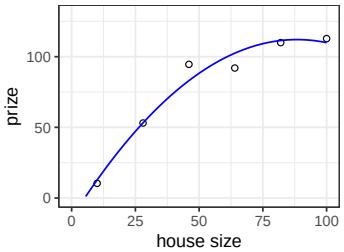
- *Regularised fitting:* Ridge regression and lasso
- *Classification problems:* logistic regression
- *Interactions:* Tree-based methods, bagging, random forests and boosting (these also capture non-linearities)

Motivation: Linear Regression House prices



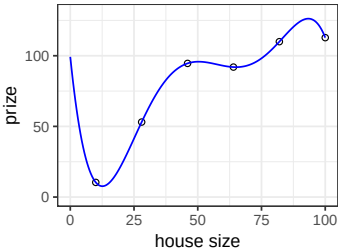
$$y = \beta_0 + \beta_1 x$$

- Underfit
- High bias



$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

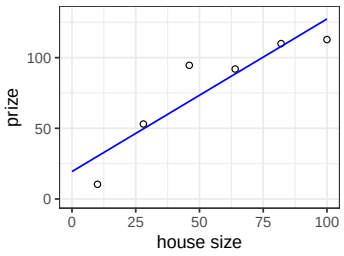
- Just right



$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$$

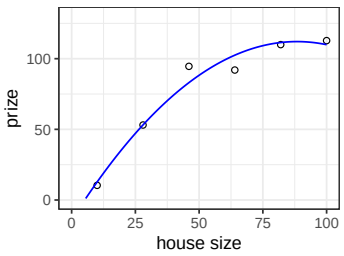
- Overfit
- High variance

Motivation: Linear Regression House prices



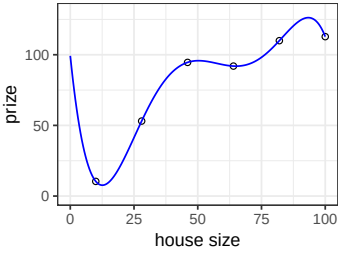
$$y = \beta_0 + \beta_1 x$$

- Underfit
- High bias



$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

- Just right



$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$$

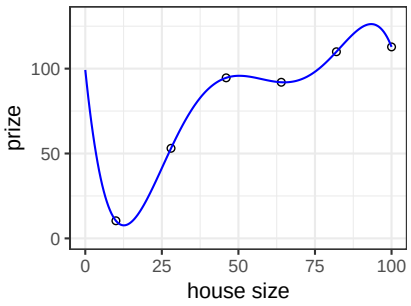
- Overfit
- High variance

Overfitting: We have too many features, the model may fit the training set well ($RSS \approx 0$), but fail to generalise to new cases (predict prices of new example)

Overfitting with many features

Not unique to polynomial regression but also if lots of inputs (p large)

- x_1 = Home area
- x_2 = Land area
- x_3 = # of bedrooms
- x_4 = # of bathrooms
- x_5 = Neighbourhood
- x_6 = Year built
- x_7 = Average income in the neighbouhood
- x_8 = Kitchen size
- $\vdots$
- x_{100}



Addressing Overfitting

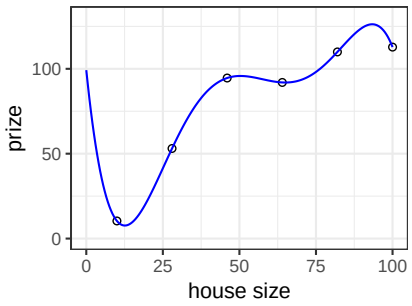
There are several several options

1. Reduce number of features/variable

- Manually
- Subset selection algorithm

2. Regularisation

- Keep all the features, but reduce magnitude of parameters β_i
  - Works well when we have a lot of features, each of which contributes a bit to predicting y



Addressing overfitting via regularisation

$$\text{Total cost} = \begin{matrix}\text{Measure} \\ \text{of Fit}\end{matrix} + \begin{matrix}\text{Measure of Magnitude} \\ \text{of Coefficient}\end{matrix}$$

Addressing overfitting via regularisation

$$\text{Total cost} = \underbrace{\text{Measure of Fit}}_{\text{RSS}} + \text{Measure of Magnitude of Coefficient}$$

Addressing overfitting via regularisation

$$\text{Total cost} = \underbrace{\text{Measure of Fit}}_{\text{RSS}} + \underbrace{\text{Measure of Magnitude of Coefficient}}_{\beta_1^2+\beta_2^2+\cdots+\beta_p^2}$$

Ridge Regression

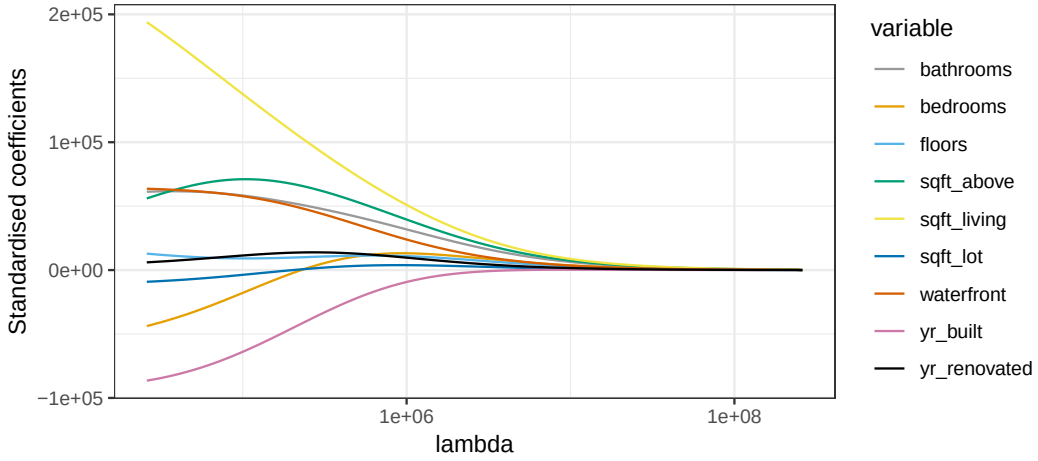
Minimise on β:

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right) + \lambda\sum_{j=1}^{p}\beta_j^2 = RSS + \lambda\sum_{j=1}^{p}\beta_j^2$$

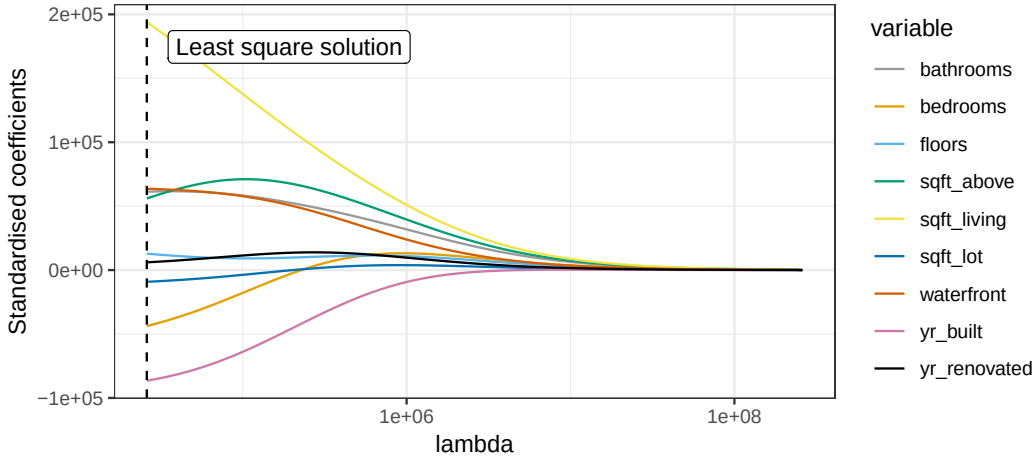
λ: Tuning parameter = balance of fit and magnitude

- $\lambda \to \infty$: Parameter estimates heavily penalised, coefficients pushed to zero, model is $y_i = \hat{\beta}_0$
  - $\lambda = 0$: Parameter estimates not penalised at all, reduces to simple linear regression - obtain the best model which includes all parameters.

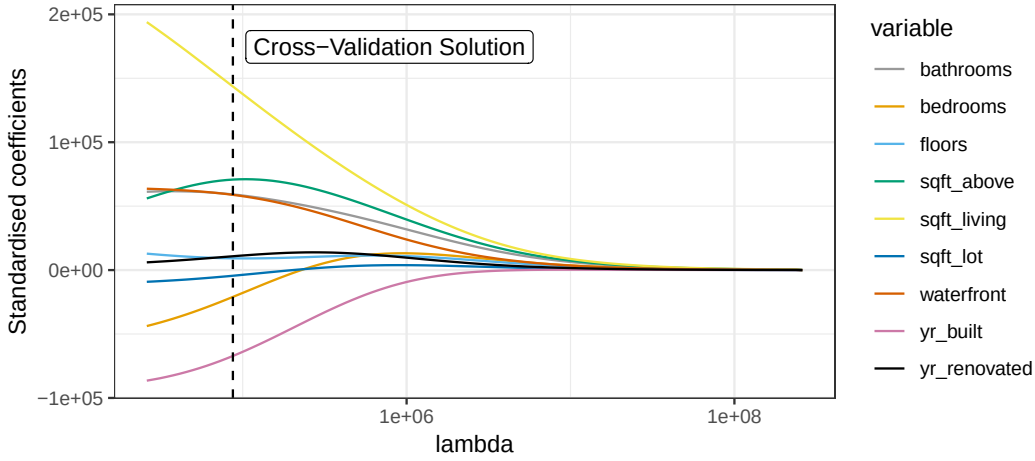
Ridge Solutions paths: The house data



Ridge Solutions paths: The house data



Ridge Solutions paths: The house data

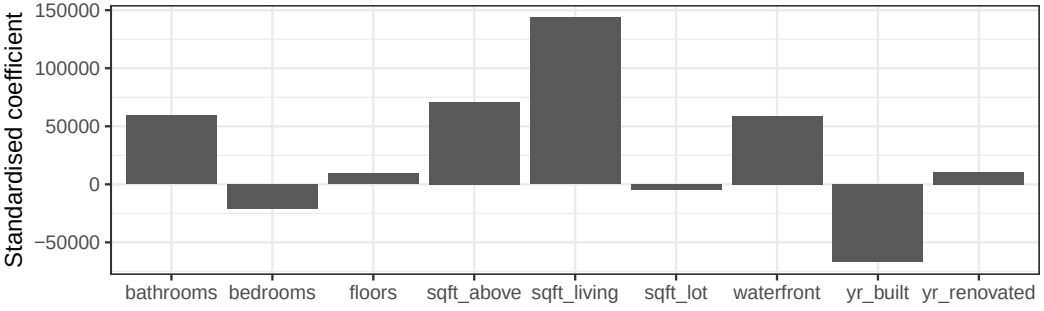


Ridge Cross-Validation Solution: The house data

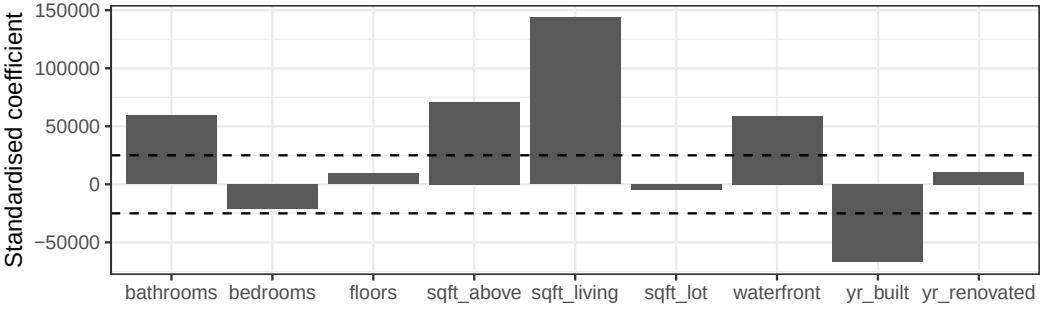
Variable	Estimate
(Intercept)	4461371.36
bedrooms	-23152.81
bathrooms	76655.13
sqft_living	155.79
sqft_lot	-0.11
floors	17043.10
yr_built	-2290.26
yr_renovated	27.11
waterfront	675263.65
sqft_above	85.58

Contains all variables so **still harder to interpret!**

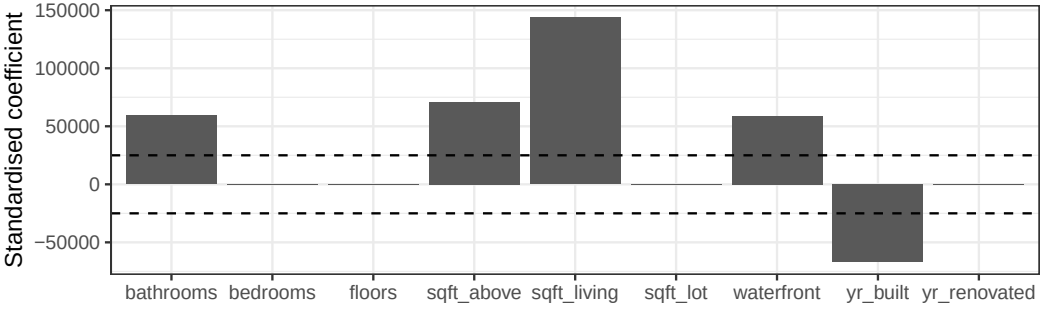
Thresholding ridge coefficients?



Thresholding ridge coefficients?



Thresholding ridge coefficients?



Feature selection via regularisation

$$\text{Total cost} = \underbrace{\text{Measure of Fit}}_{\text{RSS}} + \underbrace{\text{Measure of Magnitude of Coefficient}}_{|\beta_1|+|\beta_2|+\cdots+|\beta_p|}$$

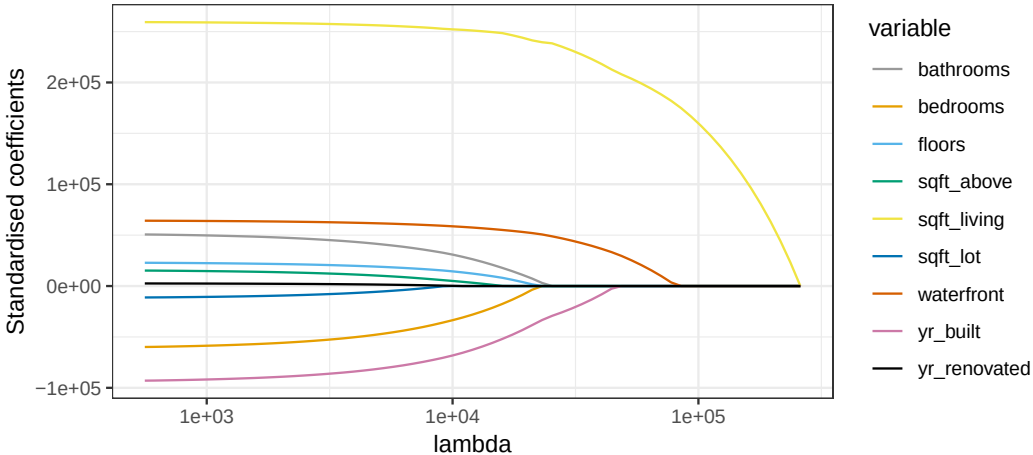
Lasso regression

Minimise on β:

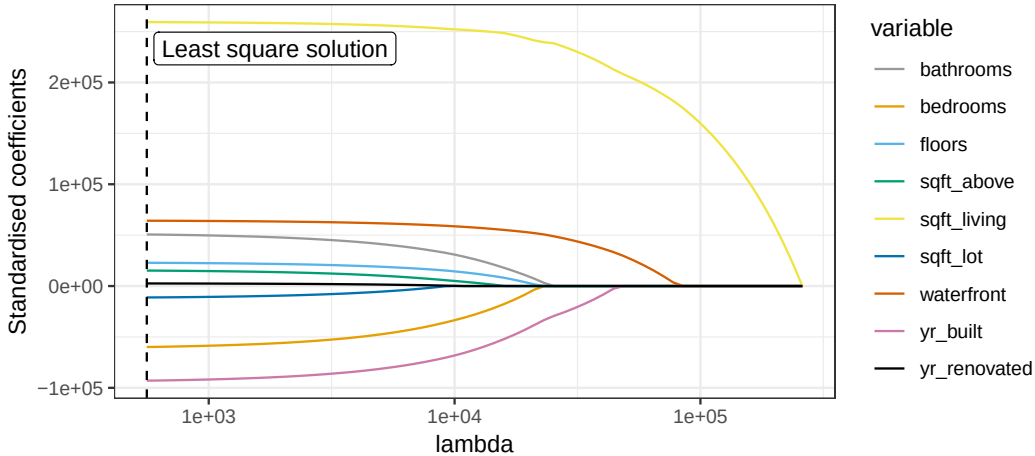
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right) + \lambda\sum_{j=1}^{p}|\beta_j| = RSS + \lambda\sum_{j=1}^{p}|\beta_j|$$

- Only difference: penalties placed on absolute value of coefficient estimates
- Can force some of them to exactly zero: significantly easier to interpret model
- Has the effect of also performing some variable selection

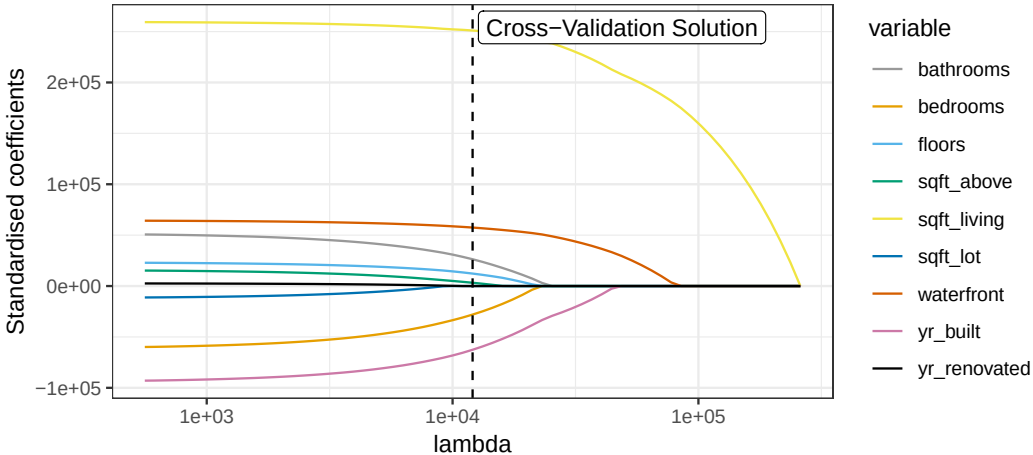
Lasso Solutions paths: The house data



Lasso Solutions paths: The house data



Lasso Solutions paths: The house data

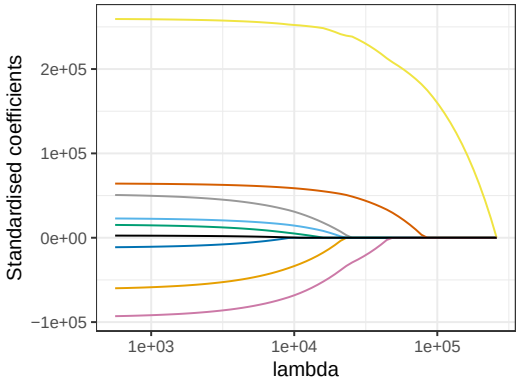


Lasso Cross-Validation Solution: The house data

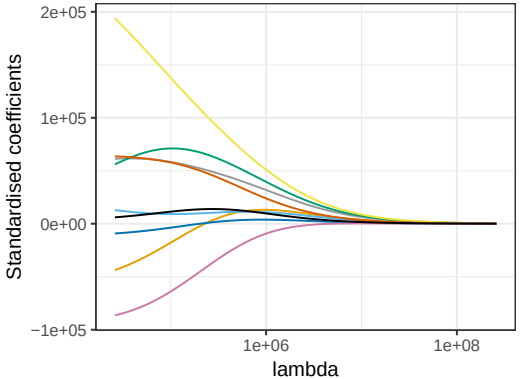
Variable	estimate
(Intercept)	4166939.79
bedrooms	-30936.45
bathrooms	34095.80
sqft_living	272.38
sqft_lot	–
floors	22706.47
yr_built	-2134.77
yr_renovated	–
waterfront	659380.22
sqft_above	3.90

Lasso vs. Ridge

Lasso



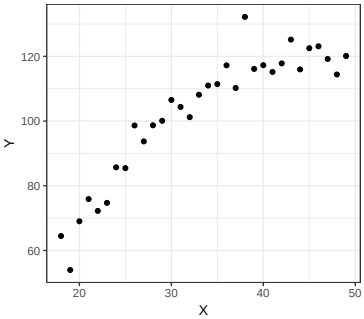
Ridge



Supervised learning: classification, logistic regression and tree-based methods

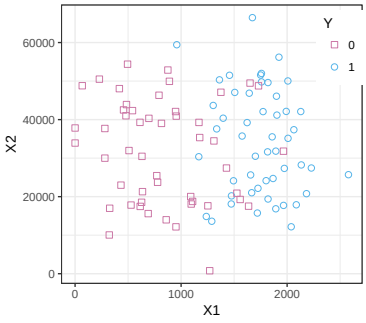
Regression vs. classification

Regression



- Y is quantitative, continuous
- Examples: Sales prediction, claim size prediction, stock price modelling

Classification



- Y is qualitative, discrete
- Examples: Fraud detection, face recognition, accident occurrence, death

Classification problems

- Coding in the binary case is simple:

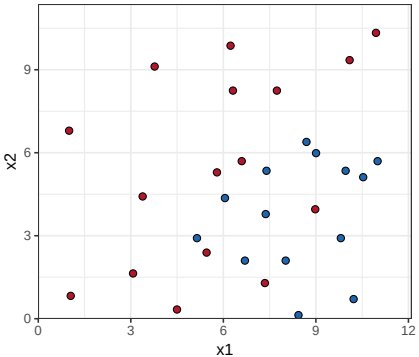
$$Y \in \{0, 1\} \Leftrightarrow Y \in \{\bullet, \bullet\}$$

- Our objective is to find a good predictive model f that can:
  1. Estimate the probability $\Pr(Y = 1|X) \in \{0, 1\}$

$$f(X) \rightarrow \bullet\bullet\bullet\bullet\bullet\bullet\bullet\bullet\bullet$$

  2. Classify observation

$$f(X) \rightarrow \hat{Y} \in \{\bullet, \bullet\}$$



Can we predict if a road accident will be fatal?

Output (Y):

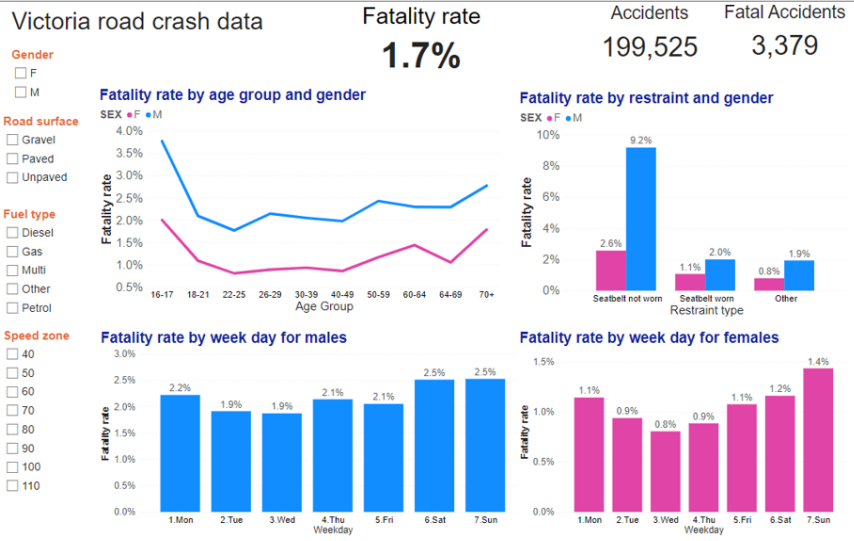
- The accident is fatal; the accident is not fatal

Input (X):

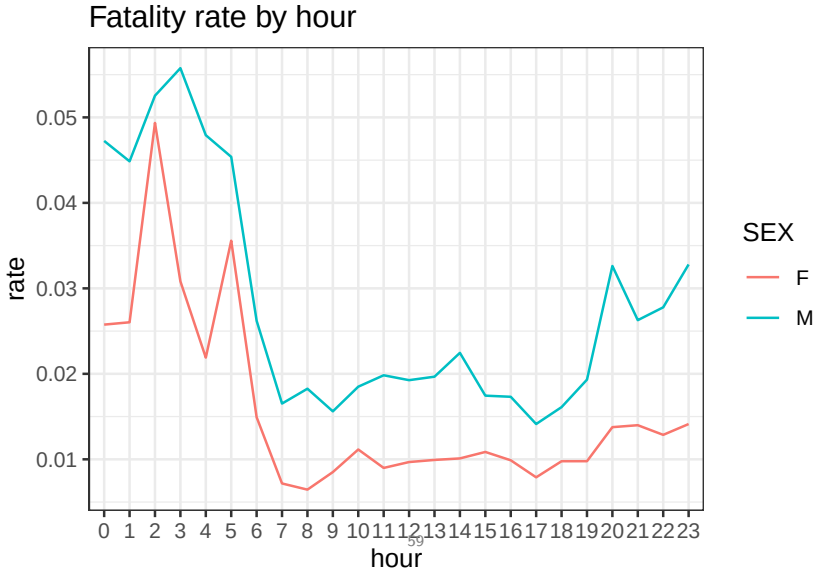
- Age of Driver
- Sex of Driver
- Time of the accident
- Weather conditions
- Type of vehicle
- ...

Source: https://discover.data.vic.gov.au/dataset/crash-stats-data-extract

VicRoads Crash Data



VicRoads Crash Data



Logistic regression

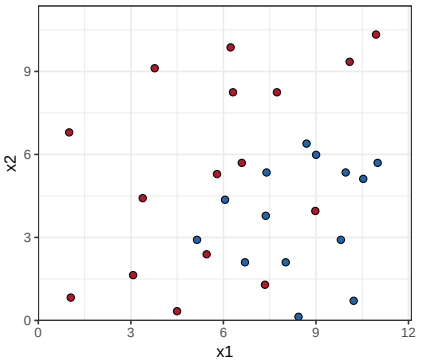
- Perform regression on:

$$\Pr(Y = 1|X) = p(X) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}{1 + e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}$$

- In other words:

$$\underbrace{\ln\left(\frac{p(X)}{1-p(X)}\right)}_{\text{log-odds}} = \underbrace{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}_{\text{linear model}}$$

- Use (training) data and maximum-likelihood estimation to produce estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots \hat{\beta}_p$

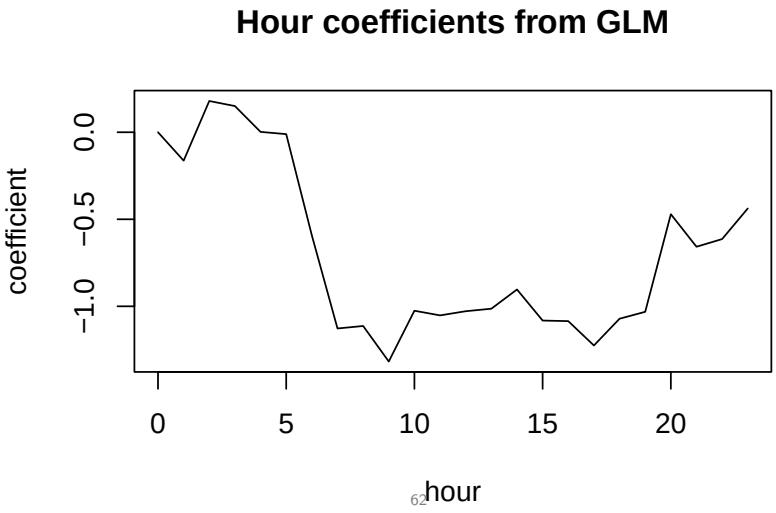


Logistic regression: VicRoads Crash Data

	Estimate	Pr(>|z|)
(Intercept)	-3.49	$< 2e-16^{***}$
SEXM	0.67	$< 2e-16^{***}$
SEXU	-0.38	0.59
HELMET_BELT_WORNSeatbelt not worn	1.50	$< 2e-16^{***}$
HELMET_BELT_WORNSeatbelt worn	0.12	0.01^{*}
AGE_GROUP18-21	-0.31	0.17
AGE_GROUP22-25	-0.50	0.03^{*}
⋮	⋮	⋮
AGE_GROUP70+	0.21	0.35
Weekday2.Tue	-0.13	$0.09^{\cdot}$
Weekday3.Wed	-0.20	0.01^{**}
Weekday4.Thu	-0.06	0.40
Weekday5.Fri	-0.10	0.14
Weekday6.Sat	0.00	1.00
Weekday7.Sun	0.02	0.79

Interpretation: The odds of an accident with a male driver being fatal are $\exp(0.67) = 1.95$ times higher than those of a female driver.

Logistic regression: VicRoads Crash Data



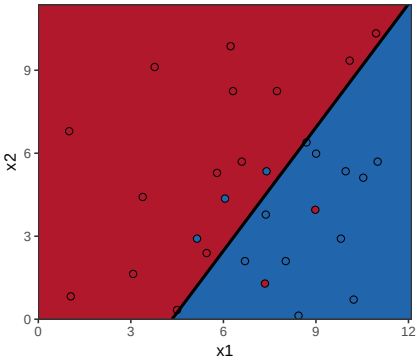
Assessing accuracy in classification problems

- We assess model accuracy using the error rate

$$\text{error rate} = \frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$$

- In our toy example with a 50% threshold

$$\text{training error rate} = \frac{5}{30} = 0.1667$$

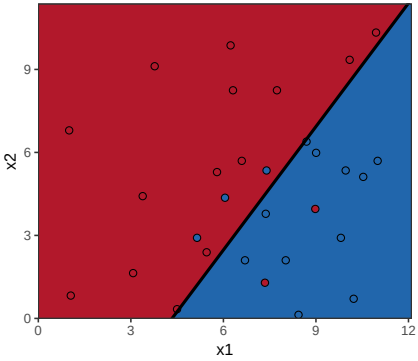


Confusion matrix (50% Threshold)

- Confusion matrix

	$Y = 0$	$Y = 1$	Total
$\hat{Y} = 0$	12	3	15
$\hat{Y} = 1$	2	13	15
Total	14	16	30

- True-Positive Rate $= \frac{13}{16} = 0.875$
- False-Positive Rate $= \frac{2}{14} = 0.1428$

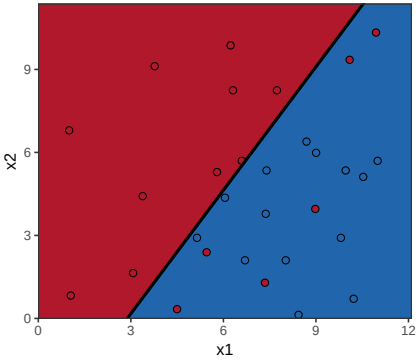


Confusion matrix (25% Threshold)

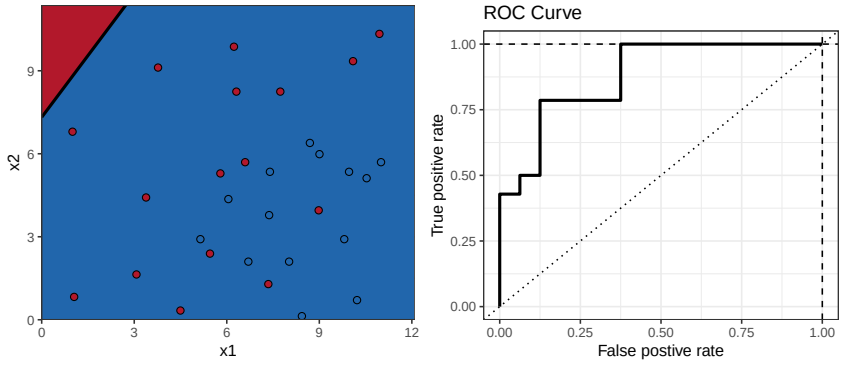
- Confusion matrix

	$Y = 0$	$Y = 1$	Total
$\hat{Y} = 0$	10	0	10
$\hat{Y} = 1$	6	16	22
Total	14	16	30

- True-Positive Rate $= \frac{16}{16} = 1$
- False-Positive Rate $= \frac{6}{14} = 0.4286$

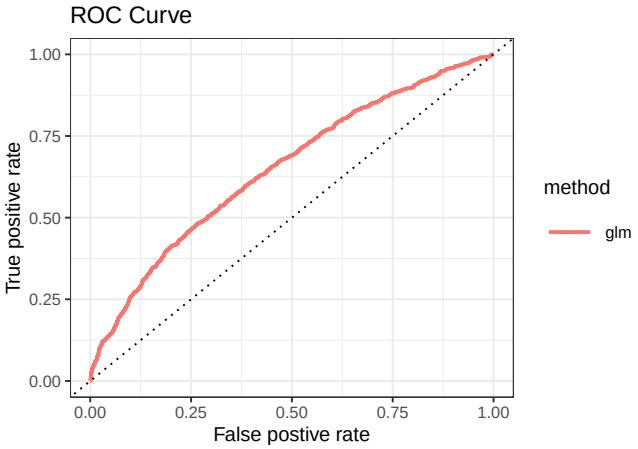


ROC Curve and AUC



- ROC Curve: Plots the true-positive rate against the false-positive rate
- A good model will have its ROC curve hug the top-left corner more
- AUC is the area under the ROC curve: For this toy example AUC=0.8795

Accuracy: VicRoads Crash Data



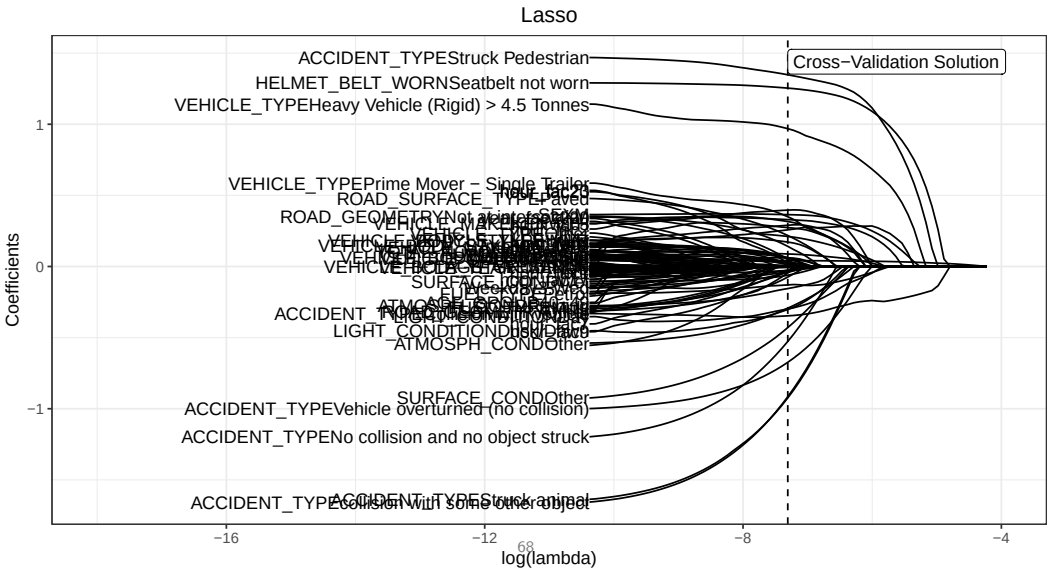
On Test Data

- Confusion matrix

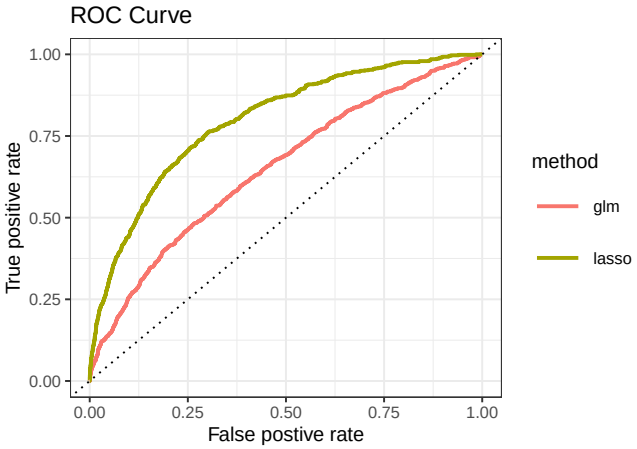
	$Y = 0$	$Y = 1$
$\hat{Y} = 0$	39324	676
$\hat{Y} = 1$	0	0

- Error Rate $= 0.01695$
- Accuracy $= 0.98305$
- AUC=0.6498

Logistic + Lasso: VicRoads Crash Data



Logistic + Lasso: VicRoads Crash Data (ROC)



AUC

Method	Train	Test
glm	0.663	0.650
lasso	0.809	0.797

Tree based methods

Tree-based methods

- Stratify / Segment the predictor space into a number of simple regions
- The set of splitting rules can be summarised in a tree

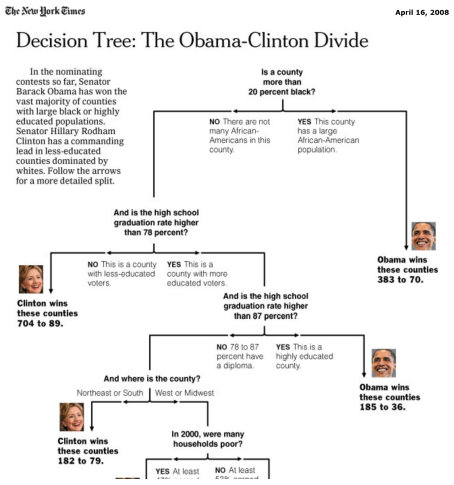
Bagging, random forests, boosting

- Ensemble methods
- Produce multiple trees
- Improve the prediction accuracy of tree-based methods
- Lose some interpretation

Tree based methods: Motivation

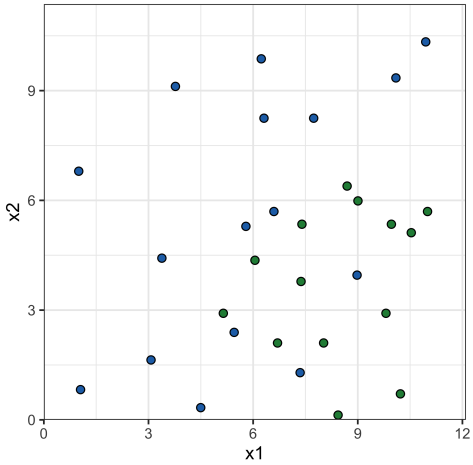
Trees are

- Simple
- Useful for interpretation
- Very common



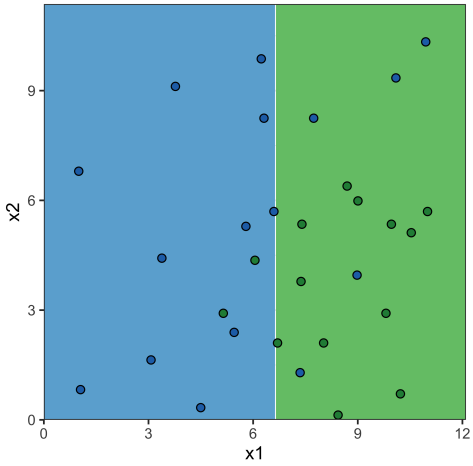
Source: New York Times (2008), Decision Tree: The Obama-Clinton Divide.

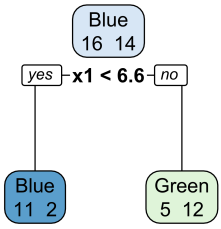
Growing a Tree I



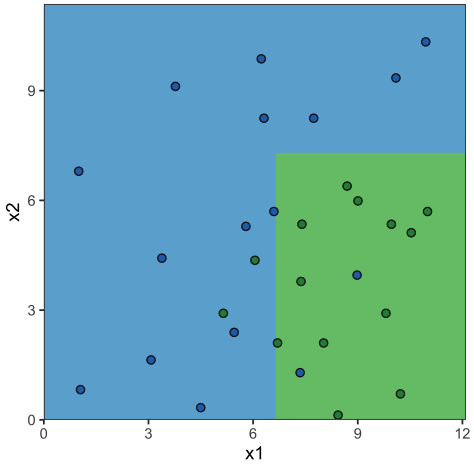
Blue
16 14

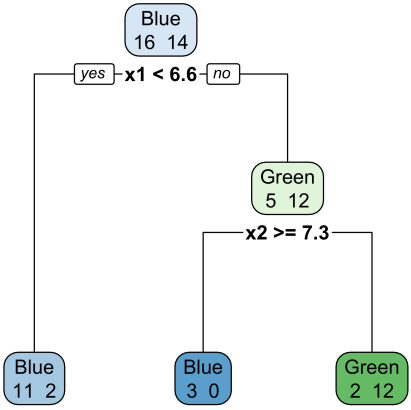
Growing a Tree II



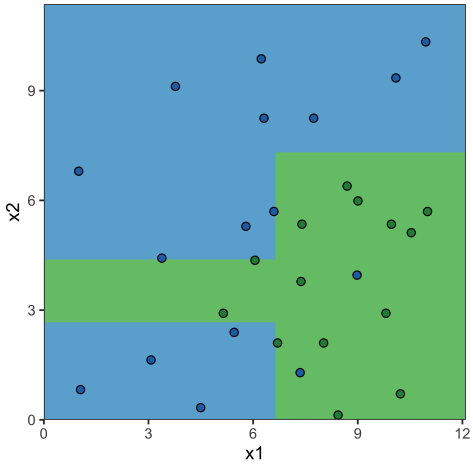


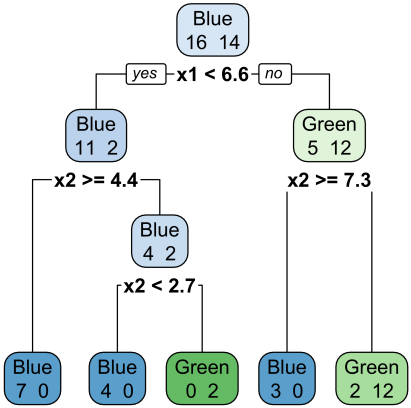
Growing a Tree III



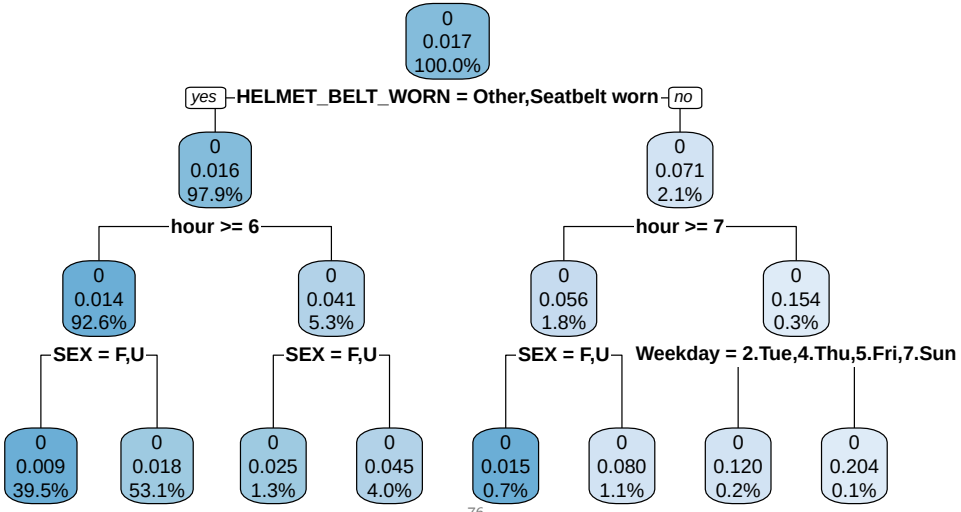


Growing a Tree IV

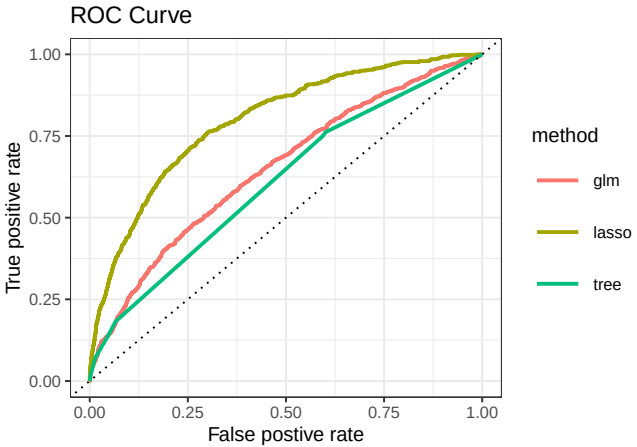




Tree: VicRoads Crash Data



Tree: VicRoads Crash Data (ROC)



AUC

Method	Train	Test
glm	0.663	0.650
lasso	0.809	0.797
tree	0.629	0.610

Advantages and disadvantages of Trees

Advantages

- Easy to explain
- (Mirror human decision making)
- Graphical display
- Easily handle qualitative predictors

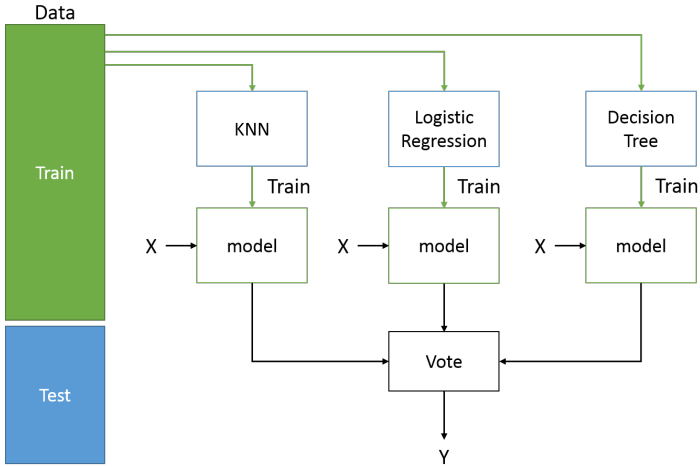
Disadvantages

- Low predictive accuracy compared to other regression and classification approaches
- Can be very non-robust

Is there a way to improve the predictive performance of trees?

- Ensemble methods
- Bagging, random forest, boosting

Ensamble methods



Ensembles tend to have lower error and produce less overfitting

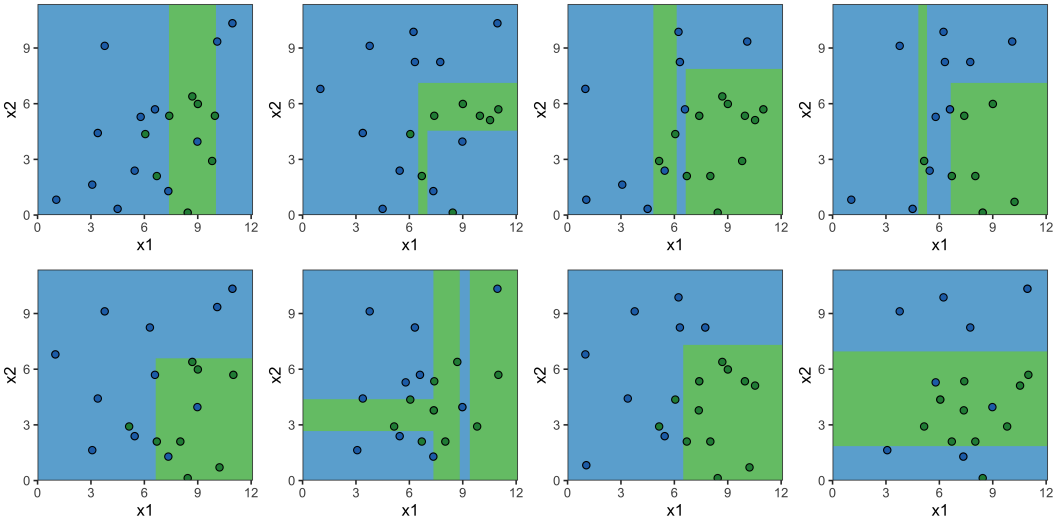
Bootstrap Aggregation (Bagging)

- A **general-purpose** procedure to reduce the variance of a statistical learning method
  - particularly useful and frequently used in the context of decision trees

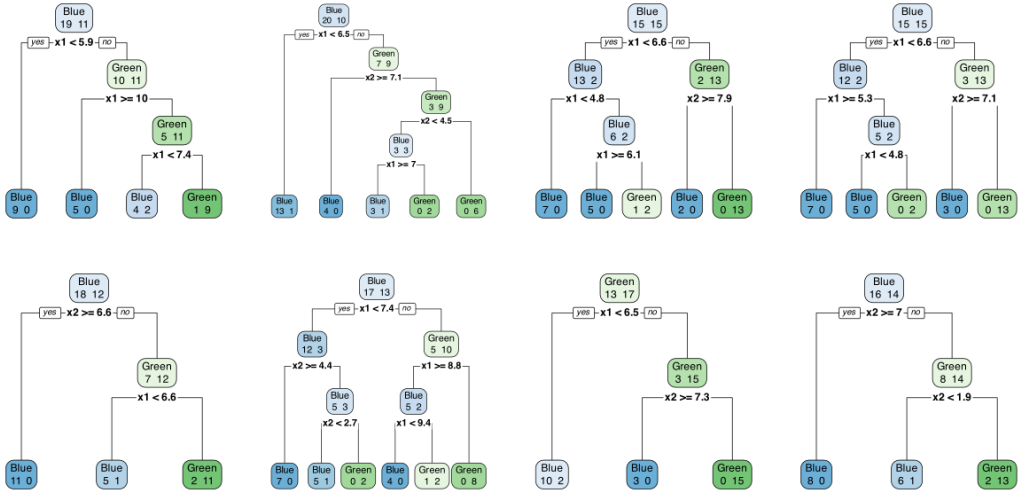
Bagging procedure

- Bootstrap
  - sample with replacement repeatedly
  - generate B different bootstrapped training data sets
- Train
  - train on the bth bootstrapped training set to get $\hat{f}^{*b}(x)$
- Aggregate
  - Take a majority vote of all of the trained models

Bagging: Illustration



Bagging: Illustration



Random forest

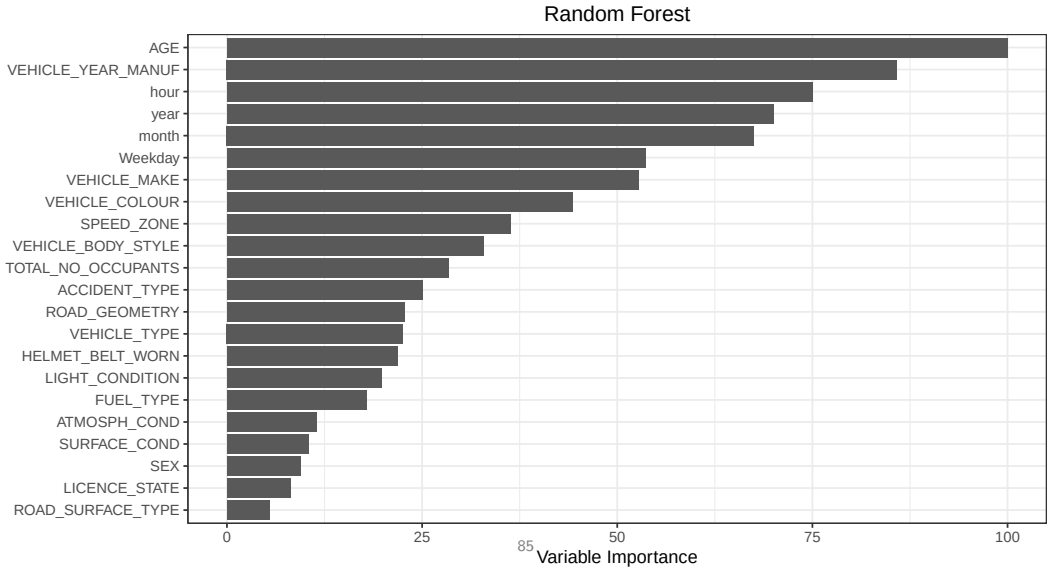
Random forests decorrelates the bagged trees

- At each split of the tree, a fresh random sample of m predictors is chosen as split candidates from the full set of p predictors
- Strong predictors are used in (far) fewer models, so the effect of other predictors can be properly measured.
  - Reduces the variance of the resulting trees
- Typically choose $m \approx \sqrt{p}$
- Bagging is a special case of a random forest with $m = p$

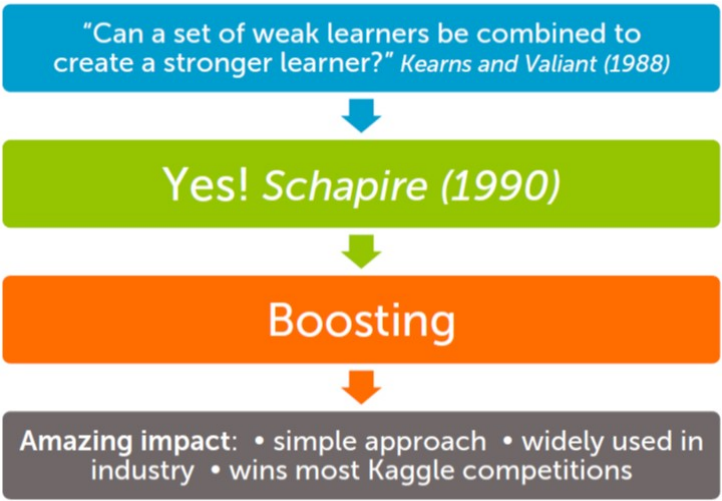
Bagging/Random Forest: Variable Selection and Importance

- Bagging and Random Forest can lead to difficult-to-interpret results, since, on average, no predictor is excluded
- Variable importance measures can be used
  - Bagging classification trees: Gini index reduction for each split (measure of node purity)
- Pick the ones with the highest variable importance measure

Random forest: Variable Importance VicRoads Data



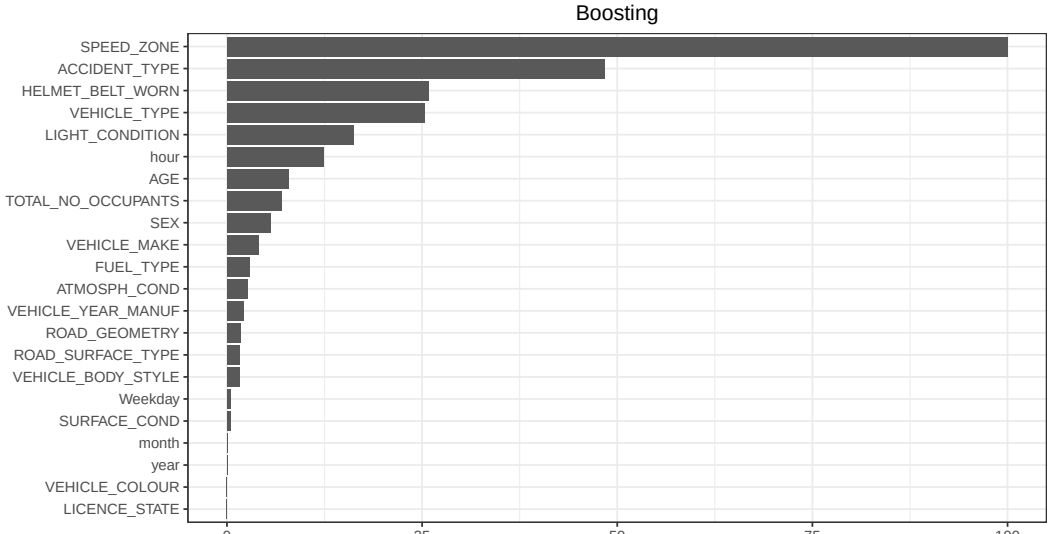
Boosting motivation



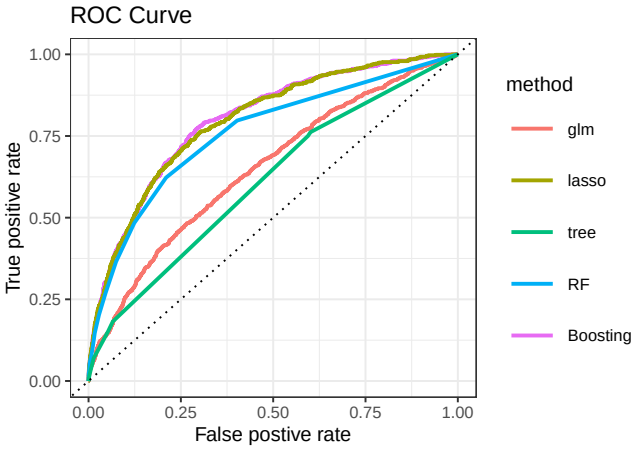
Boosting procedure

- A general approach that can be applied to many statistical learning methods for regression or classification
- Involves combining a large number of decision trees
  - trees are grown sequentially
  - using the information from previously grown trees
  - no bootstrap - instead each tree is fitted on a modified version of the original data (sequentially)
- Unlike standard trees, boosting learns slowly - by focusing on the residuals and hence focusing on areas the previous tree did not perform well.

Boosting: Variable Importance VicRoads Data



Comparison of methods: VicRoads Crash Data



AUC

Method	Train	Test
glm	0.663	0.650
lasso	0.809	0.797
tree	0.629	0.610
RF	0.676	0.759
Boosting	0.813	0.800

Summary of key concepts in classification problems

We have discussed key concepts in classification problems

- Logistic Regression
- Assessing model accuracy
  - Confusion matrix
  - ROC curve
  - AOC
- Tree-based methods
  - Bagging
  - Random Forest
  - Boosting

Summary of session

1. Introduction to Statistical Machine Learning
2. Supervised learning – Regression
3. Supervised learning – Classification

Thank you!

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