Foundations of Statistical and Machine Learning for Actuaries
Resampling, cross-validation and regularisation

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Schedule

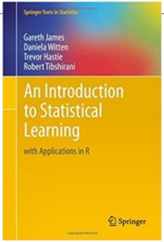
Day and Time	Presenter	Topics	Notebooks for Participant Activity
Monday Morning	Jed Jed	Welcome and Foundations; Hello to Google Colab Classical Regression Modeling	Auto Liability Claims Medical Expenditures (MEPS)
Monday Afternoon	Andrés Andrés	Resampling, cross-validation and regularisation Classification, Logistic Regression and Trees	Seattle House Sales Victoria road crash data
Tuesday Morning	Andrés Jed	(Tree-based) Ensembles methods and Interpretability Big Data, Dimension Reduction and Non-Supervised Learning	Victoria road crash data Big Data, Dimension Reduction and Non-Supervised Learning
Tuesday Afternoon	Jed Jed Fei	Neural Networks Graphic Data Neural Networks Fei Huang Thoughts on Ethics	Seattle House Prices, Claim Counts MNIST Digits Data
Wednesday Morning	Jed Jed	Recurrent Neural Networks, Text Data Artificial Intelligence, Natural Language Processing, and ChatGPT	Insurer Stock Returns
Wednesday After Lunch	Dani	Dani Bauer Insights	
Wednesday Afternoon	Andrés	Applications and Wrap-Up	

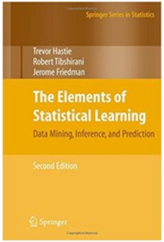
Monday Afternoon 2A - Resampling, cross-validation and regularisation

This module covers:

- General concepts of statistical learning
  - Regression vs. classification
  - Parametric vs. non-parametric models
  - Bias-variance trade-off
  - training error vs. test error
- Resampling methods: cross-validation
- Regularisation methods
  - Ridge regression
  - Lasso regression
  - Elastic net

Statistical Machine Learning: Resources



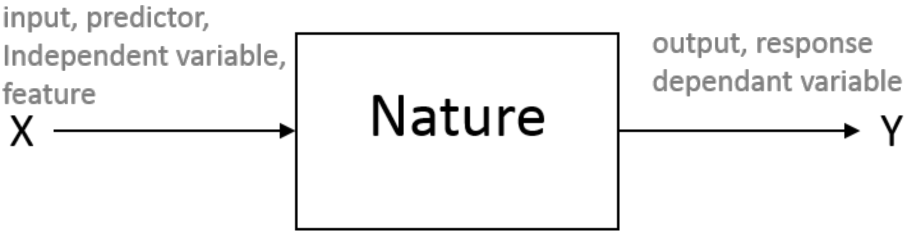


- Most of the discussion is based on this book:
  - Available at: https://www.statlearning.com/
  - Focus on intuition and practical implementation

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

The discussion builds on the UNSW Course Statistical Machine Learning for Risk and Actuarial Applications (https://unsw-risk-and-actuarial-studies.github.io/ACTL3142/)

What is statistical (machine) learning?



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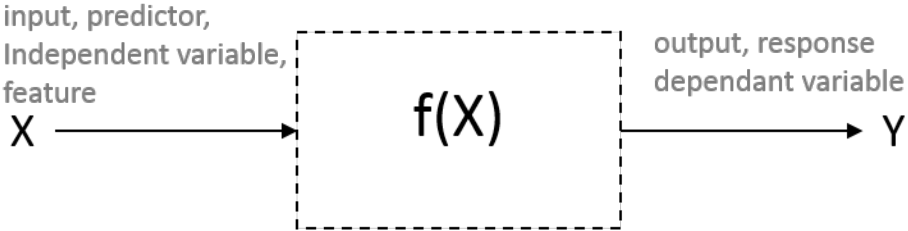

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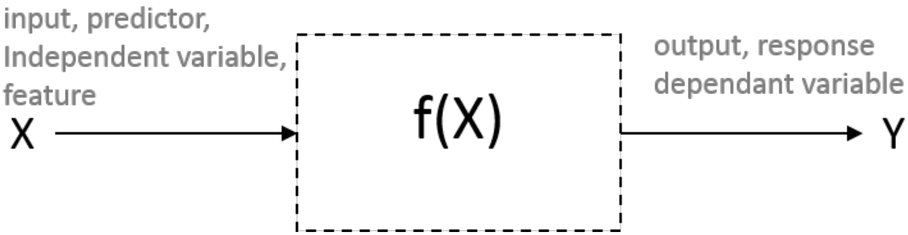


Prediction

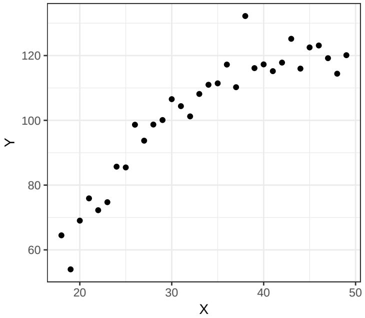
- Predict outcomes of Y given X
  - What it means isn't as important, it just needs accurate predictions
- Models tend to be more complex

Inference

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

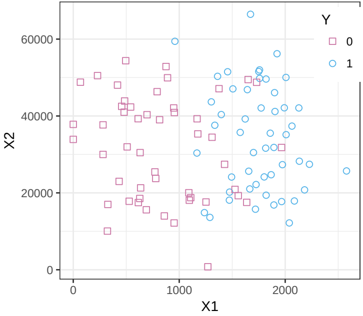
Regression vs. classification

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

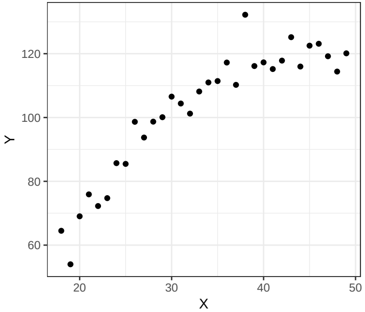
- Make no assumption about f's shape
- Involves estimating a lot of "parameters"
- Need lots of data
- Assumption weak: tends to incorporate some noise
- Be particularly careful re the risk of overfitting

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, $\ldots$, β_p
- Use (training) data to produce estimates $\hat{\beta}_0$, $\hat{\beta}_1$, $\ldots$, $\hat{\beta}_p$
- **Almost never correct**, but serves as a good and interpretable approximation.

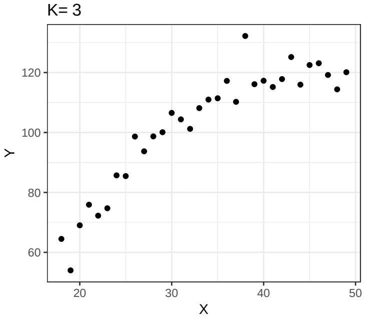


Non-parametrics example: K-nearest neighbours

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



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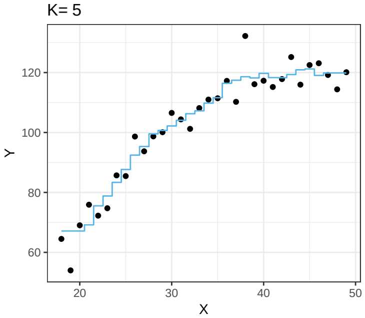

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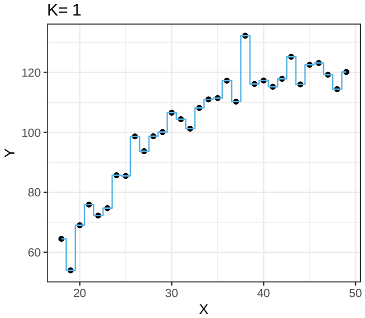
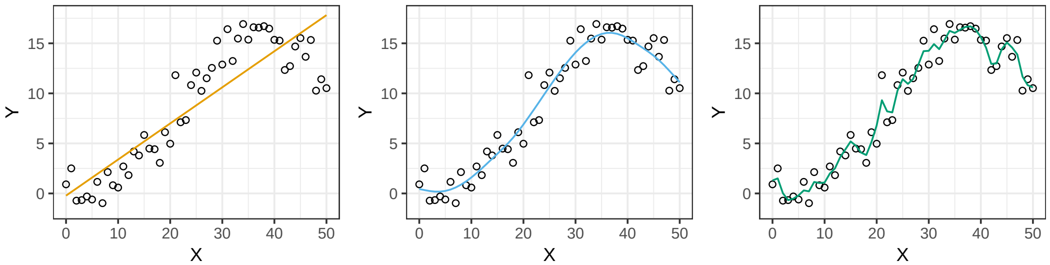


How to choose f?



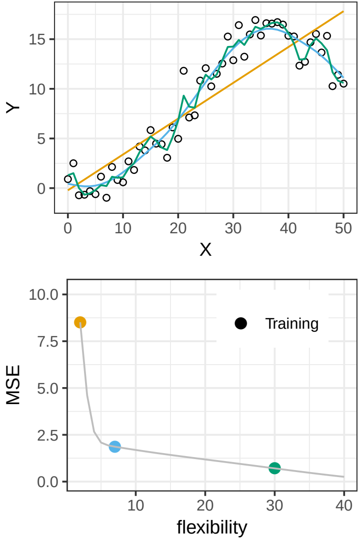
How do we decide which is the best model?

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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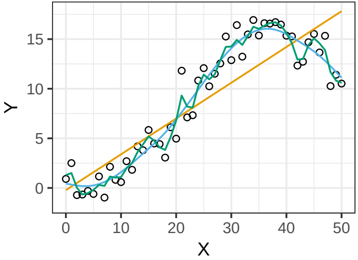
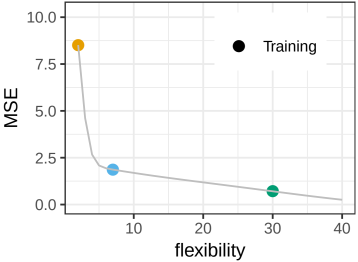
This tends to be biased to more overfit models!





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

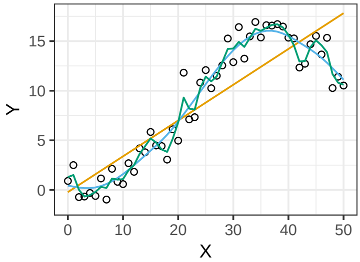
- We can compute the Training Mean Squared Error

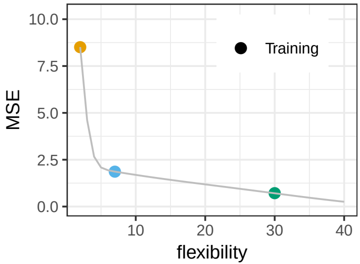
$$MSE_{Tr} = \frac{1}{n} \sum_{i \in Tr} (y_i - \hat{f}(x_i))^2$$

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

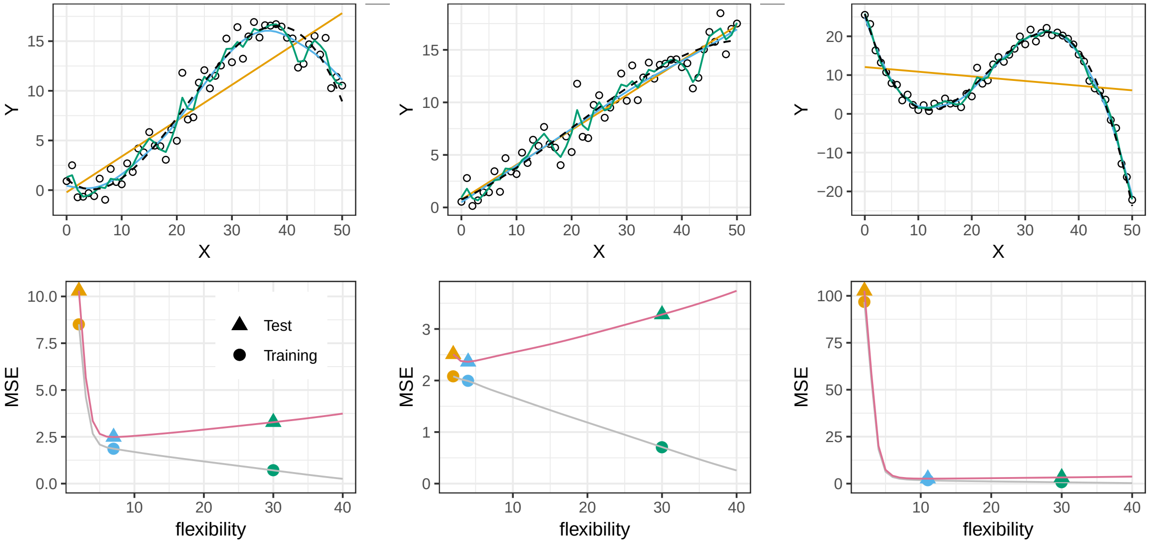
-

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





Assessing model accuracy



Bias-Variance Trade-off

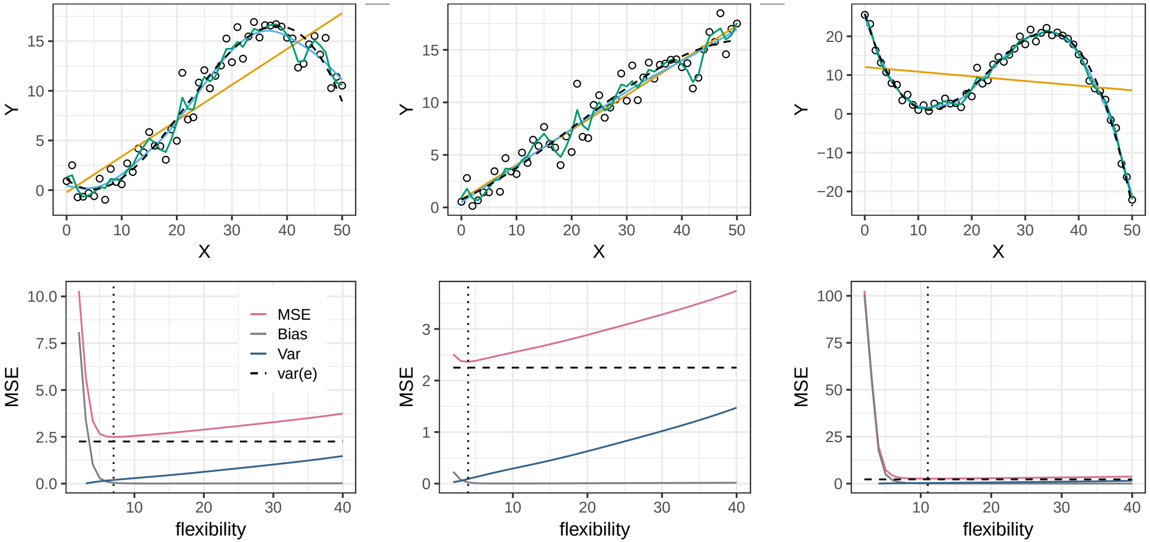
The expected test MSE can be written as:

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + Var(\epsilon)$$

- $\mathrm{Var}(\hat{f}(x_0))$: how much $\hat{f}$ would change if a different training set is used
- $[\mathrm{Bias}(\hat{f}(x_0))]^2$: how much the model is off by
- $\mathrm{Var}(\epsilon)$: irreducible error

There is often a tradeoff between Bias and Variance

Bias-Variance Trade-off

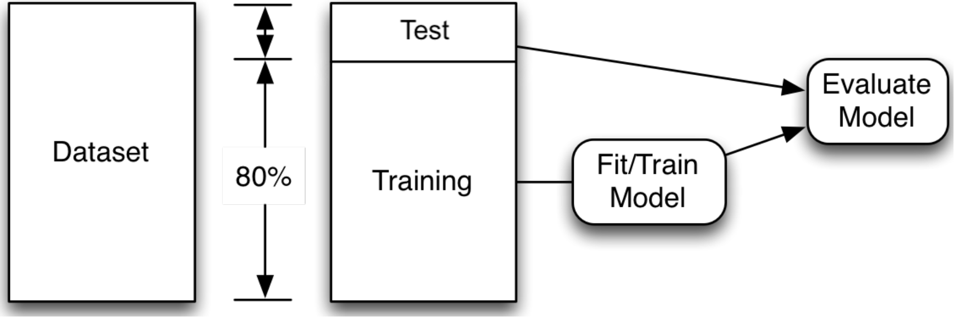


How do we calculate the test error?

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

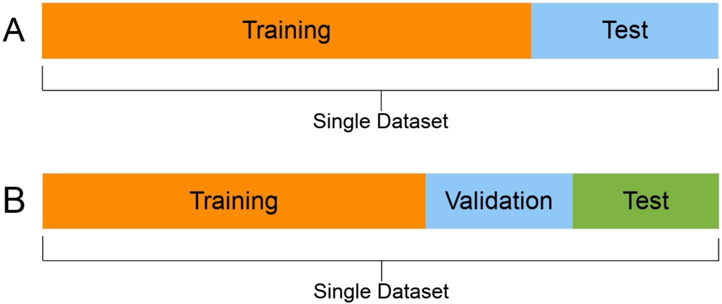
Set aside a fraction for a test set

Set aside a fraction after *shuffling*.



Adapted from: Heaton (2022), Applications of Deep Learning, Part 2.1: Introduction to Pandas.

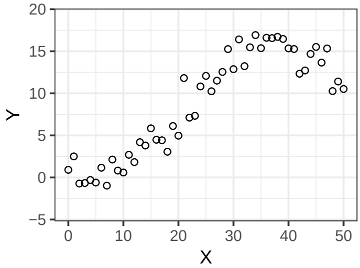
Basic ML workflow



1. For each model, fit it to the *training set*.
2. Compute the error for each model on the *validation set*.
3. Select the model with the lowest validation error.
4. Compute the error of the final model on the *test set*.

Source: Wikipedia.

k-fold Cross-validation

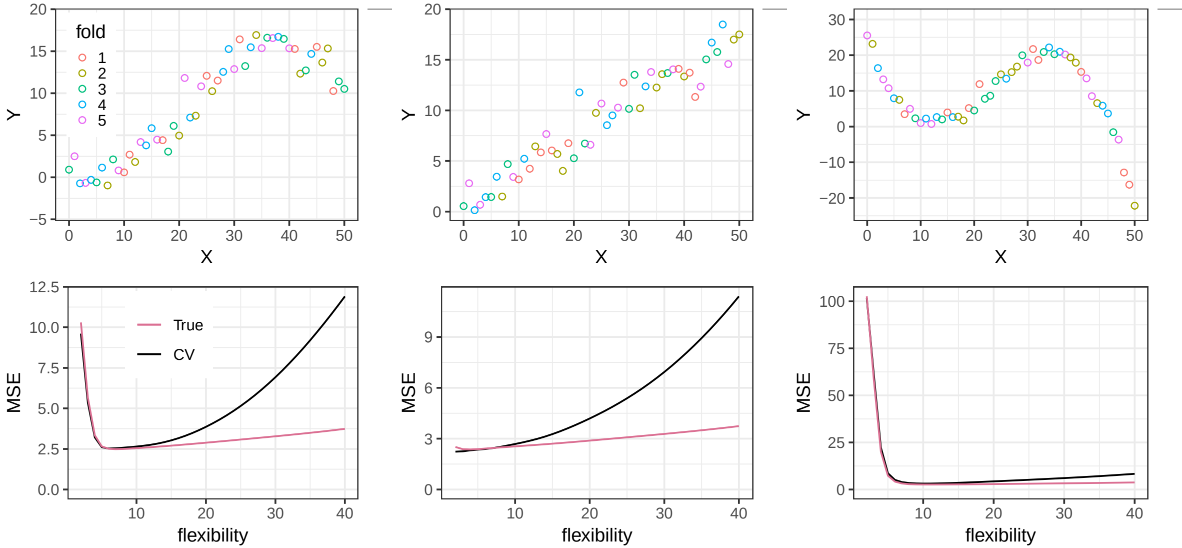


- Randomly divided the set of observations into K groups, or folds of approximately equal size
- the k^{th} fold is treated as a validation set
- the remaining $K-1$ folds make up the training set
- Repeat K times resulting K estimates of the test error

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

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

k-fold Cross-validation



Regularisation

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):

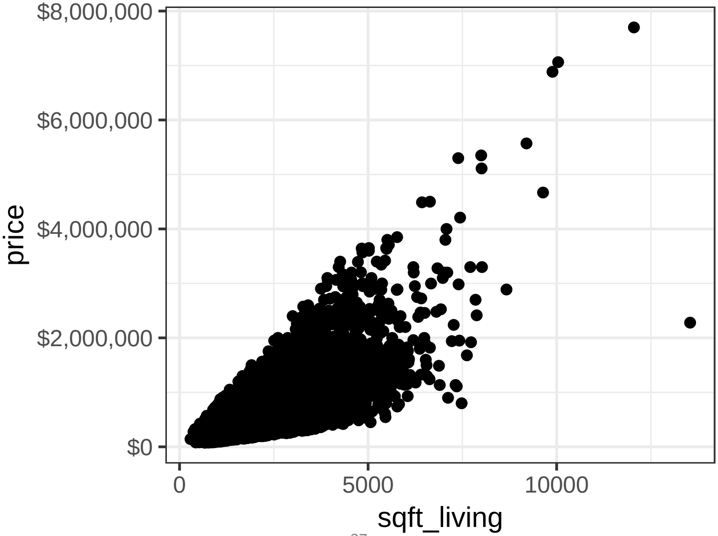
- Home area
- Land area
- # of bedrooms
- # of bathrooms
- Neighbourhood
- Year built
- ...

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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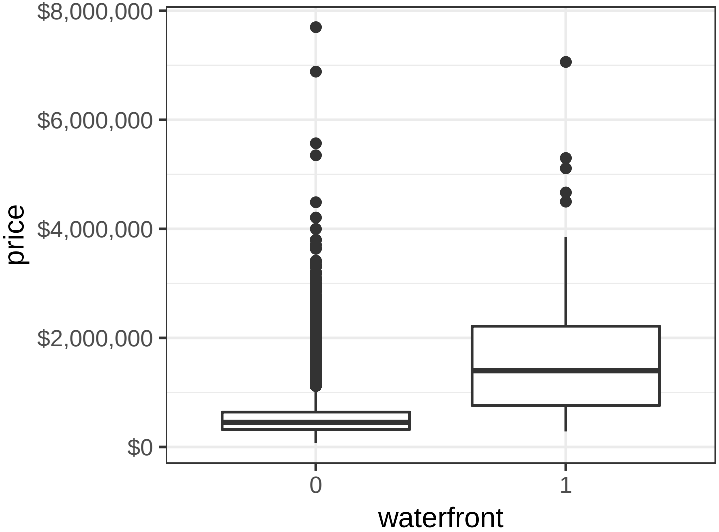


Simple linear regression

- 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 $X = x$

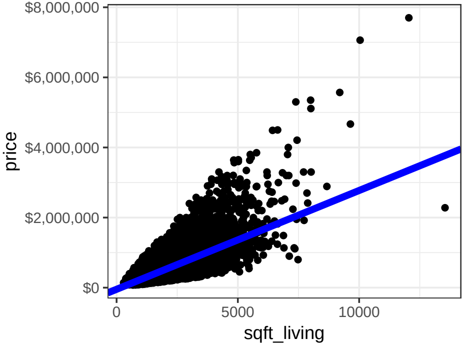
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

- 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

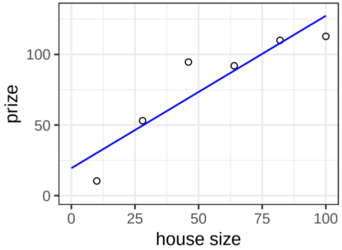
1. **Prediction accuracy**: the linear regression fit often does not predict well, especially when p (the number of predictors) is large
2. **Model Interpretability**: linear regression freely assigns a coefficient to each predictor variable. When p is large, we may sometimes seek, for the sake of interpretation,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

Generalisations of the Linear Model

Methods that expand the scope of linear models:

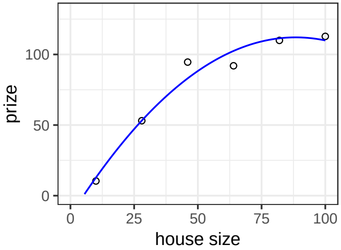
- *Regularised fitting:* Ridge regression and lasso
- *Non-linearity:* splines and generalized additive models; nearest neighbor methods
- *Classification problems:* logistic regression
- *Interactions:* Tree-based methods, bagging, random forests and boosting (these also capture non-linearities)

Motivation: Linear Regression House prices



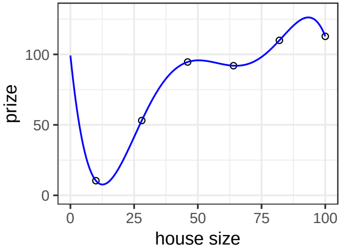
$$y = \beta_0 + \beta_1 x$$

- Underfit
- High bias



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

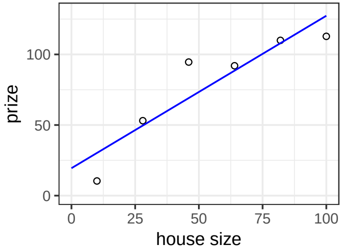
- Just right



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

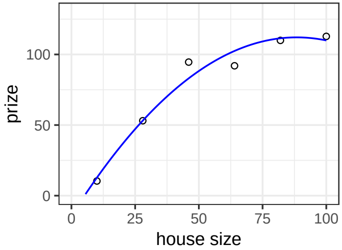
- Overfit
- High variance

Motivation: Linear Regression House prices



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

- Underfit
- High bias



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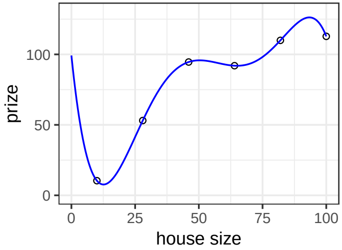


$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$$

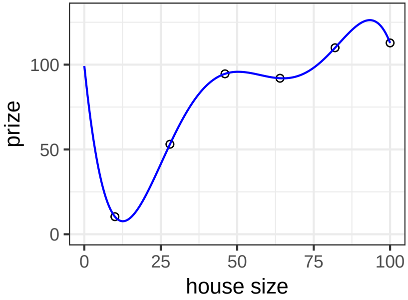
- Overfit
- High variance

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)

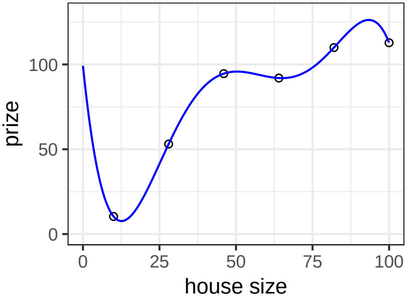
- x_1 = Home area
- x_2 = Land area
- x_3 = # of bedrooms
- x_4 = # of bathrooms
- x_5 = Neighbourhood
- x_6 = Year built
- x_7 = Average income in the neighbouhood
- x_8 = Kitchen size
- $\vdots$
- x_{100}



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

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

Addressing overfitting via regularisation

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

Addressing overfitting via regularisation

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

Ridge Regression I

Minimise on β:

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

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 regression II

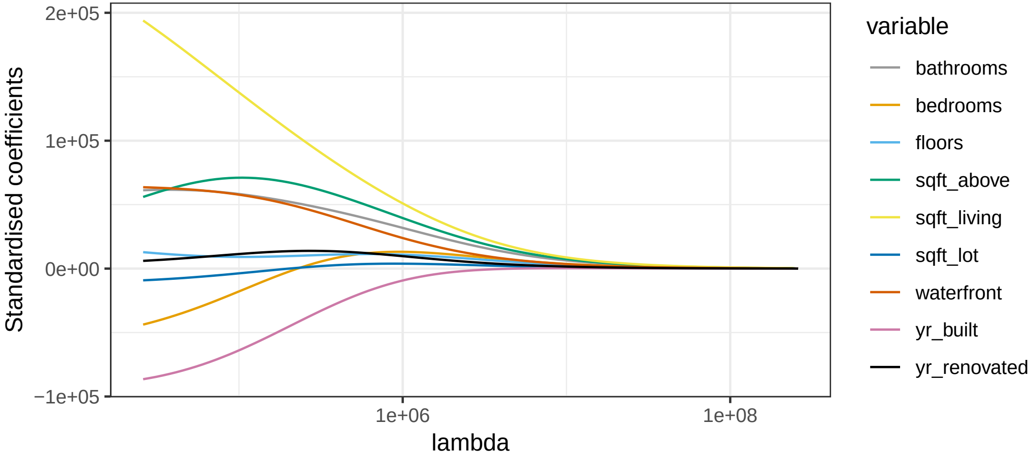
- Note that β_0's estimate is not penalised: Coefficient estimates are heavily scale-variant
- Need to standardise all predictors so their sample variance is 1:

$$x'_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}}$$

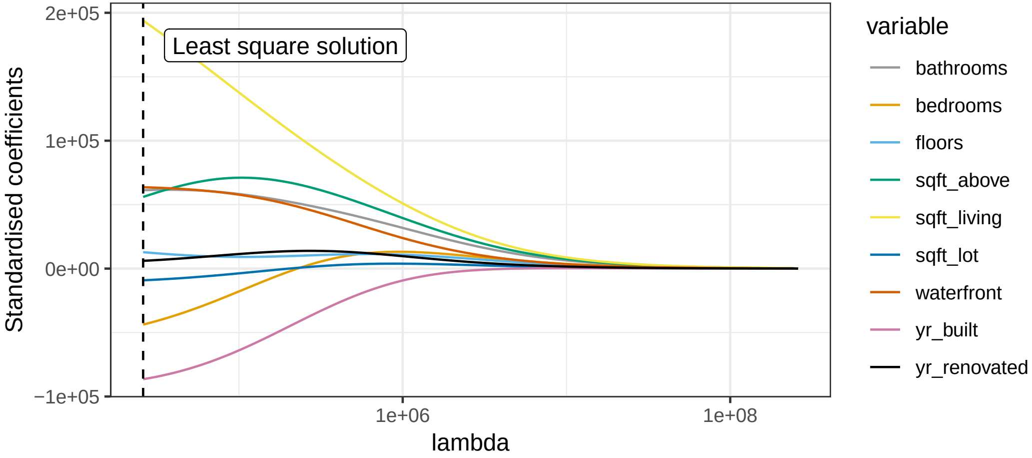
Tuning Parameter λ

- Different λ will give different estimates. Use cross-validation to find the best λ
- Lower λ leads to more flexible errors: lower bias but higher variance
- But λ can be changed: flexibility can be modified to get a model minimising MSE

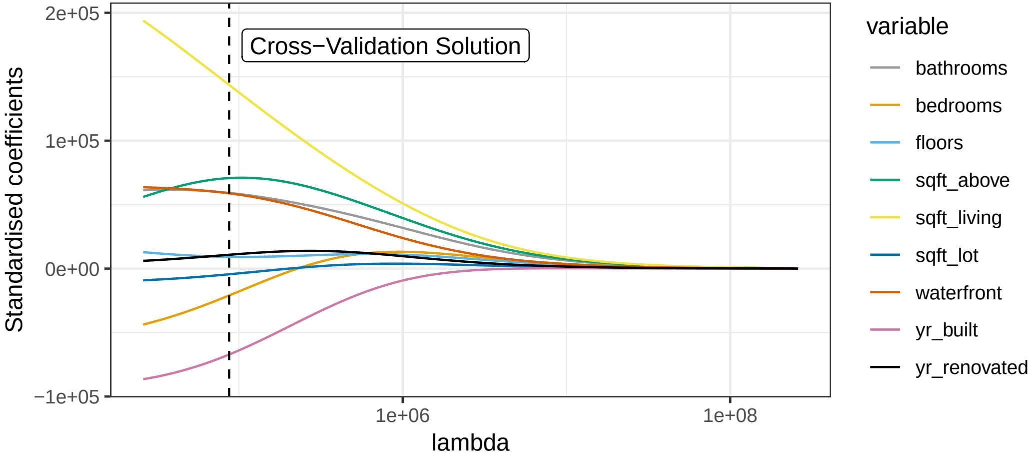
Ridge Solutions paths: The house data



Ridge Solutions paths: The house data



Ridge Solutions paths: The house data

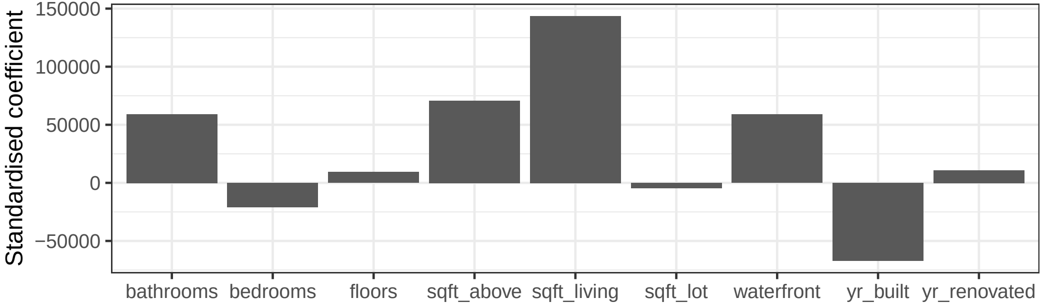


Ridge Cross-Validation Solution: The house data

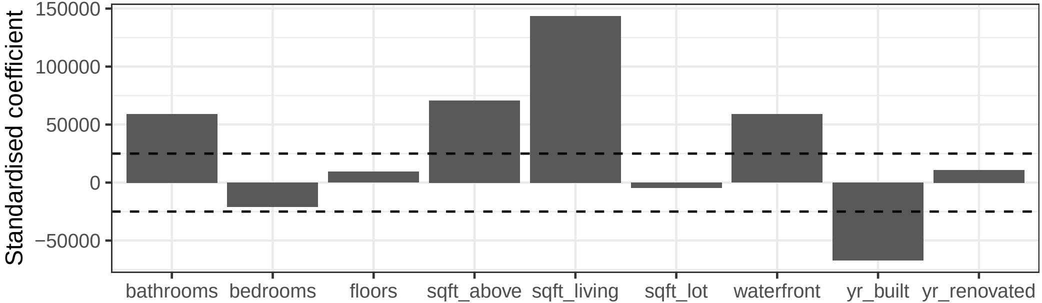
Variable	Estimate
(Intercept)	4461371.36
bedrooms	-23152.81
bathrooms	76655.13
sqft_living	155.79
sqft_lot	-0.11
floors	17043.10
yr_built	-2290.26
yr_renovated	27.11
waterfront	675263.65
sqft_above	85.58

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

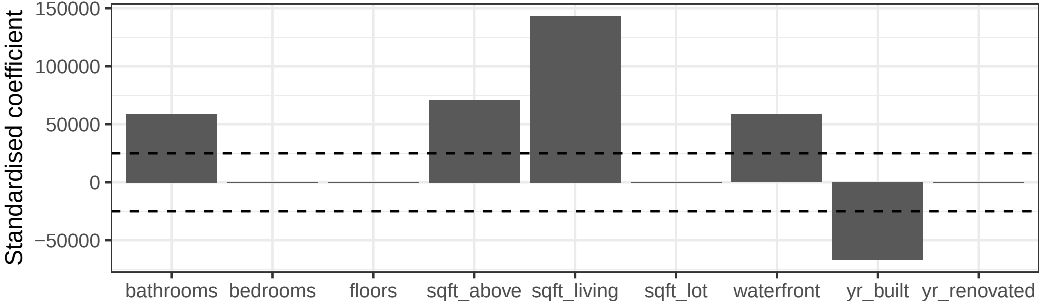
Thresholding ridge coefficients?



Thresholding ridge coefficients?



Thresholding ridge coefficients?



Feature selection via regularisation

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

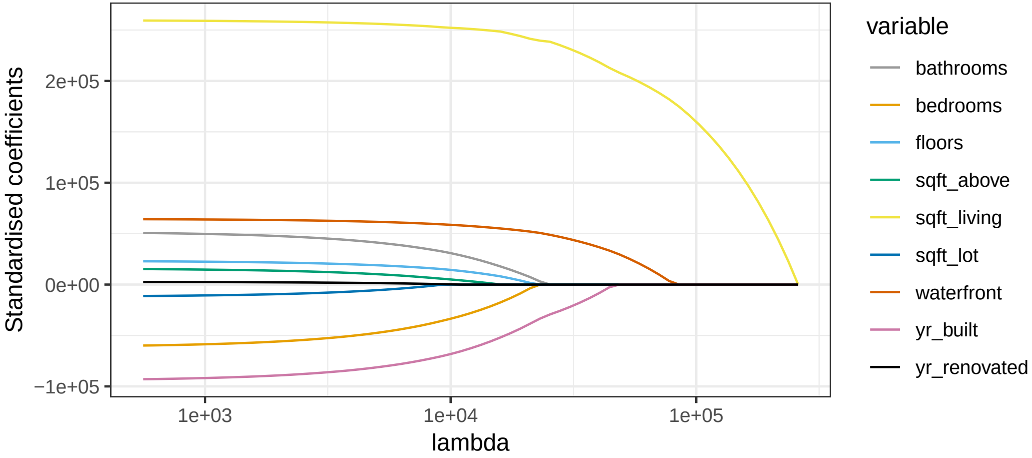
Lasso regression

Minimise on β:

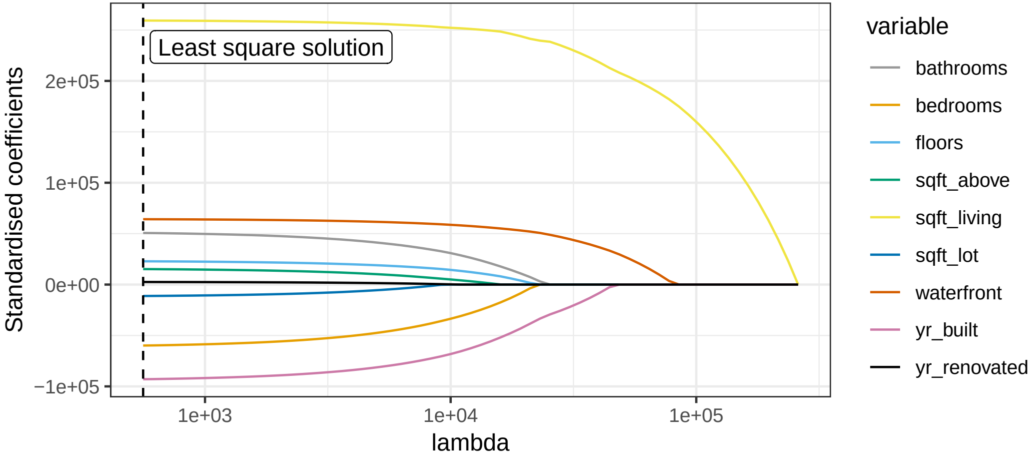
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = RSS + \lambda\sum_{j=1}^{p}|\beta_j|$$

- 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

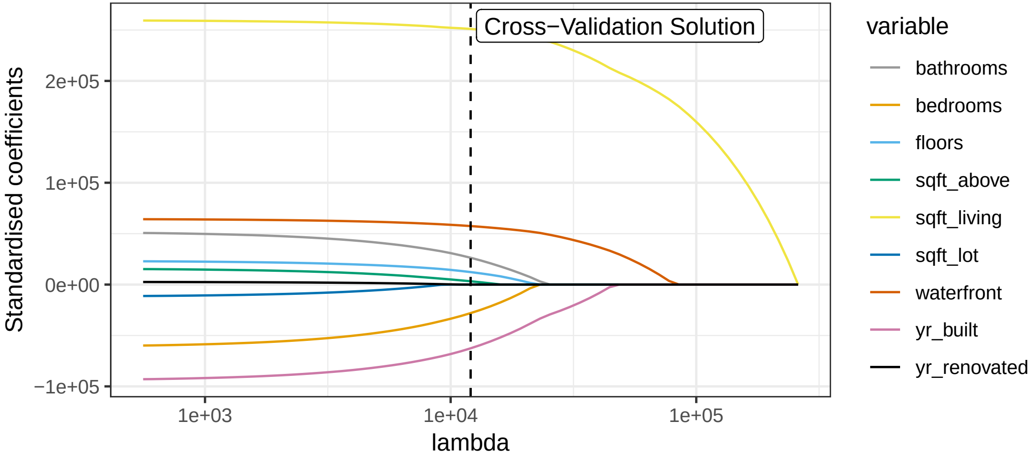
Lasso Solutions paths: The house data



Lasso Solutions paths: The house data



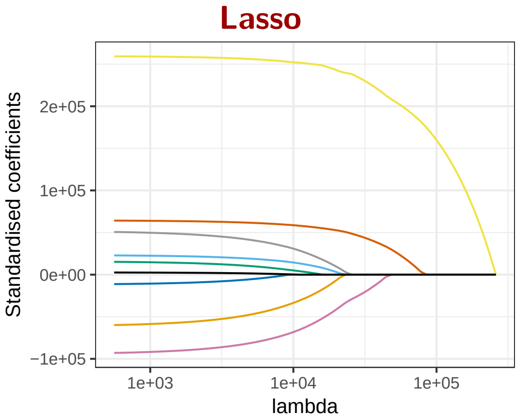
Lasso Solutions paths: The house data

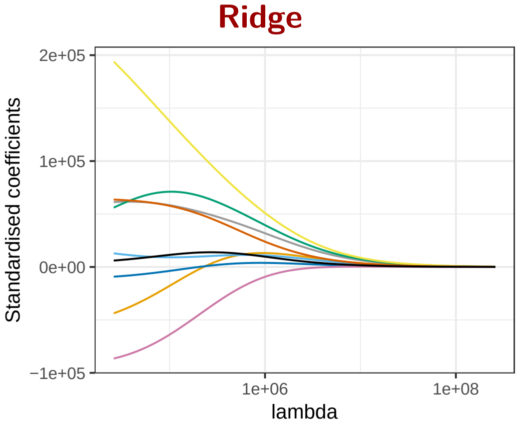


Lasso Cross-Validation Solution: The house data

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





Alternate formulation

Ridge regression: minimise MSE subject to

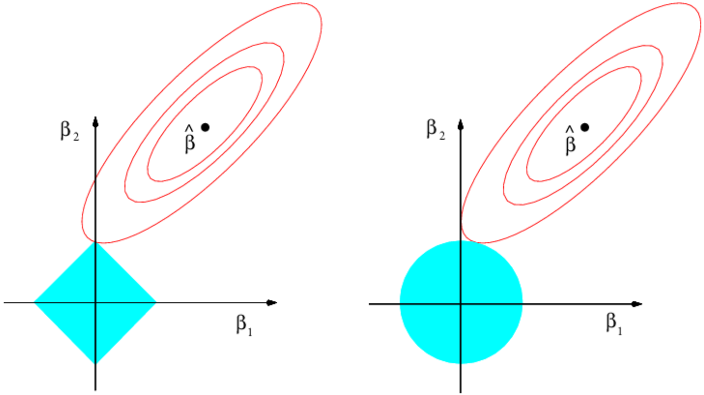
$$\sum_{j=1}^{n} \beta_j^2 \leq s$$

Lasso regression: minimise MSE subject to

$$\sum_{j=1}^{n} |\beta_j| \leq s$$

- Each method is assigns a "budget" to "spend" on the coefficient estimates
- The size of the "budget" is based on λ (ridge and lasso)
- This is like Lagrange multipliers (actually look up Karush–Kuhn–Tucker (KKT) conditions)

Ridge vs Lasso: Some intuition



Contours of training MSE against the constraint regions for ridge & lasso.

Lasso leads to a pointier solution space: more likely to set parameters to zero.

Extensions

Ridge & lasso for GLMs

- Ridge and lasso can be applied to any GLM, the penalties are added to the negative log-likelihood

Elastic net penalty

$$\lambda\left[\alpha\sum_{j=1}^{p}|\beta_j| + (1-\alpha)\sum_{j=1}^{p}\beta_j^2\right]$$

- $\alpha = 1$ is lasso, $\alpha = 0$ is ridge
- $0 < \alpha < 1$ is elastic net, a compromise between ridge and lasso

Elastic net in `R`

- `glmnet` package
- `alpha` parameter controls the mix of ridge and lasso
- `lambda` parameter controls the strength of the penalty
- `cv.glmnet` function performs cross-validation to find the best λ

Session 2A - Resampling, cross-validation and regularisation - Summary

We have discussed key concepts in statistical/machine Learning

- Model selection
  - Bias-variance trade-off
  - Training MSE vs. Test MSE
  - Cross-Validation
- Regularisation
  - Ridge regression
  - Lasso regression
  - Elastic net
- During lab, participant may follow the notebook Seattle House Prices