

# dm24s1

## Topic 09 : Regression2

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### Part 01 : Overview

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Autumn Semester, 2024

#### Outline

- Regression as a means of minimising sum of the squared errors
- Regression assumptions - what they mean, how they can be used for validation and model building
- Case studies from Advertising and Credit Balance prediction

# Data Mining (Week 9)

Introduction



Motivating Example

## Preparation

Data Handling



Exploring Data 1



Exploring Data 2



Building Models

## Prediction

Clustering



Regression  
1



Classification  
1



Regression  
2



Classification  
2

Wrap up



# Overview — Summary

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1. Introduction
2. Regression1 review
3. Case Study 1: Generated
4. Case Study 3: Advertising
5. Case Study 4: Credit Balances
6. Multivariate Analysis
7. Review and Summary
8. Resources

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- To provide context we will use the following datasets:
  - Generated data (various)
  - Advertising dataset: predicting widgets sold based on spending in different advertising channels
  - Credit dataset: predicting credit balance using income, status, etc.

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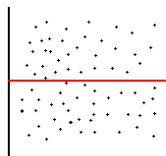
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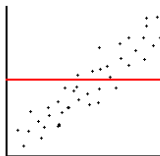
These assumptions can be used constructively, when model building, or as checks, when validating models.

# Bias and variance in regression

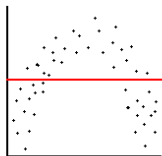
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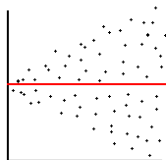
(a) Unbiased and Homoscedastic



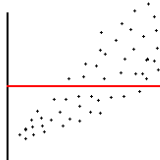
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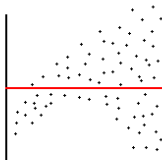
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(d) Unbiased and Heteroscedastic



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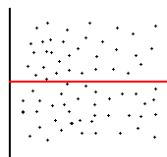
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Source: <https://bit.ly/3vC9zK7>

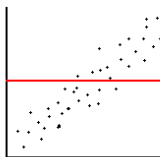


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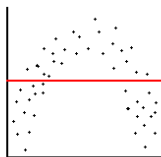
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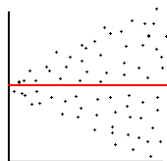
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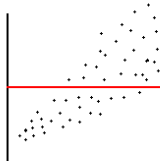
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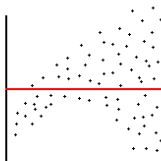
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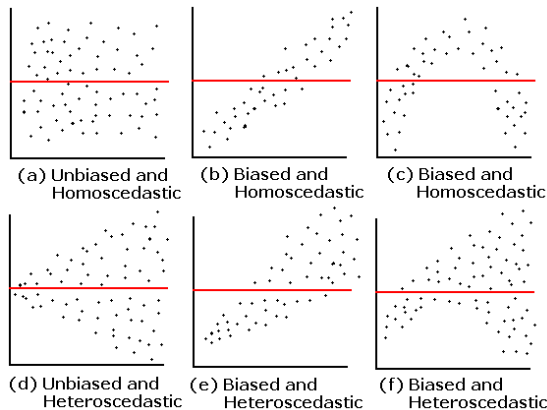
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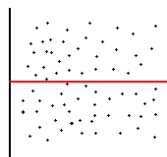
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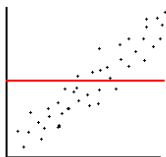
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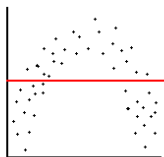
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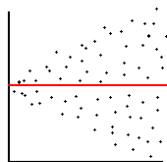
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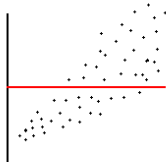
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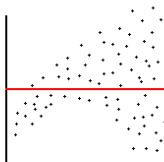
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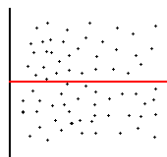


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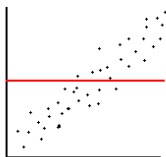
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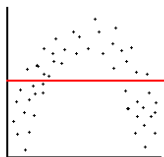
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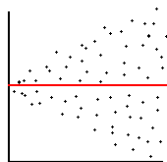
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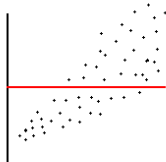
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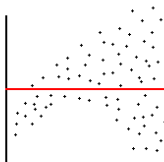
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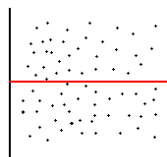


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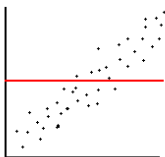
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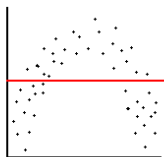
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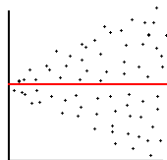
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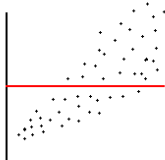
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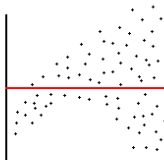
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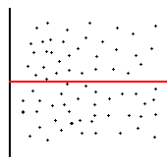


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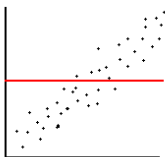
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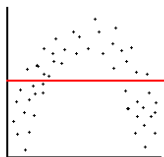
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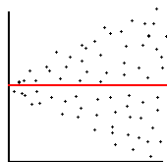
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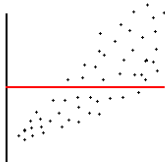
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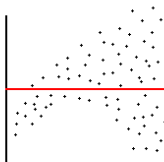
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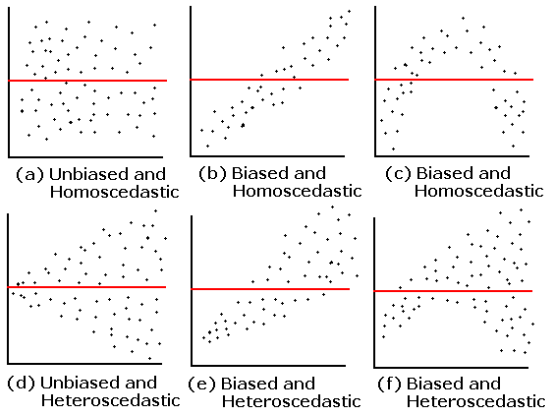


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  - Using scikit-learn: add the argument `sample_weight = someWeights`, e.g., `model.fit(Xtrain, yTrain, sample_weight=someWeights)`.

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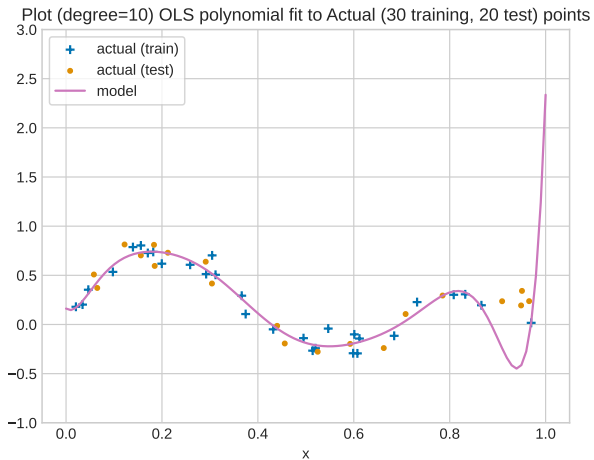
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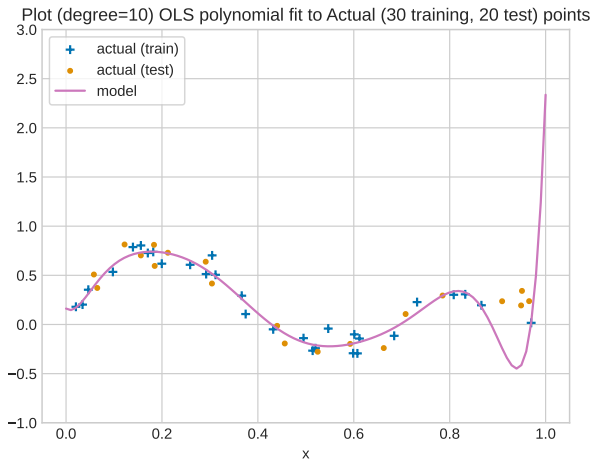
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  - Using scikit-learn: add the argument `sample_weight = someWeights`, e.g., `model.fit(Xtrain, yTrain, sample_weight=someWeights)`.
  - Using statsmodels: use the weighted version of least squares: `WLS(y, X, someWeights)` not `OLS(y, X)`

# What's happening here???



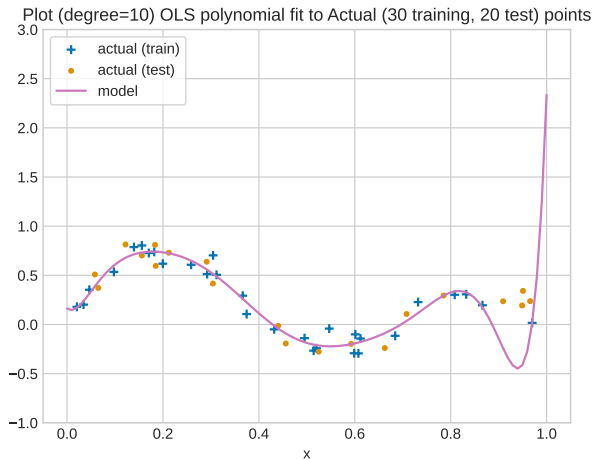


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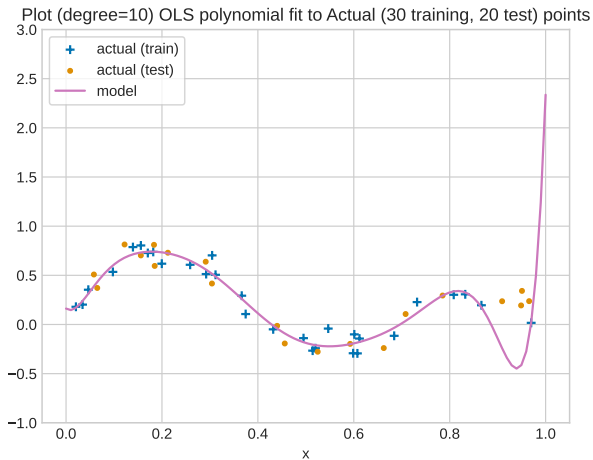
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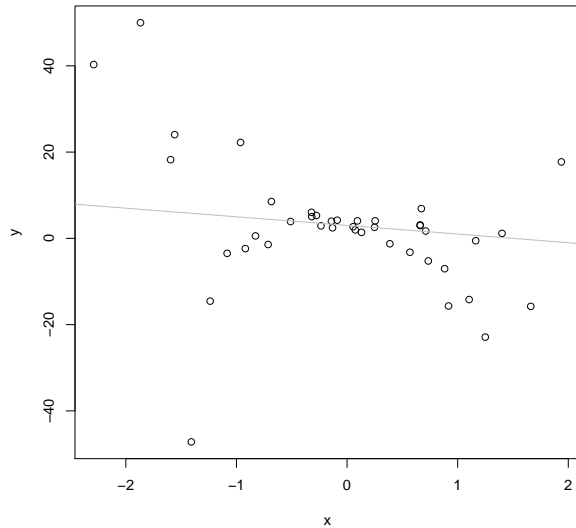
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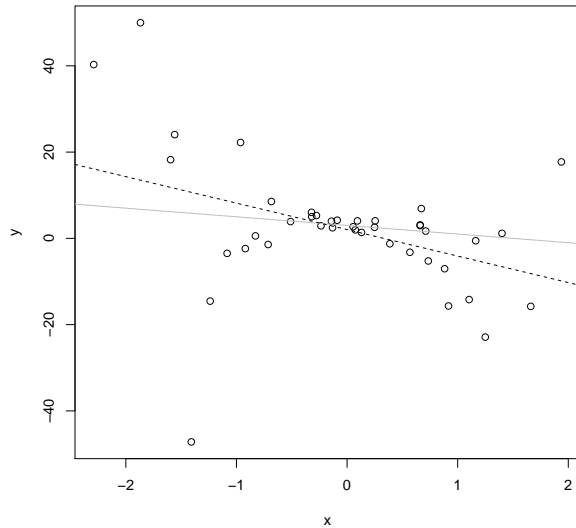
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- 3 Model may be overfitting

# Case Study 1: Heteroscedasticity - Step 1



I generated 41  $x, y$  points based on  $y = 3 - 2x$ , but with added errors that increase away from  $x = 0$ . The plot shows the line with  $\beta = (3, -2)$  in grey.

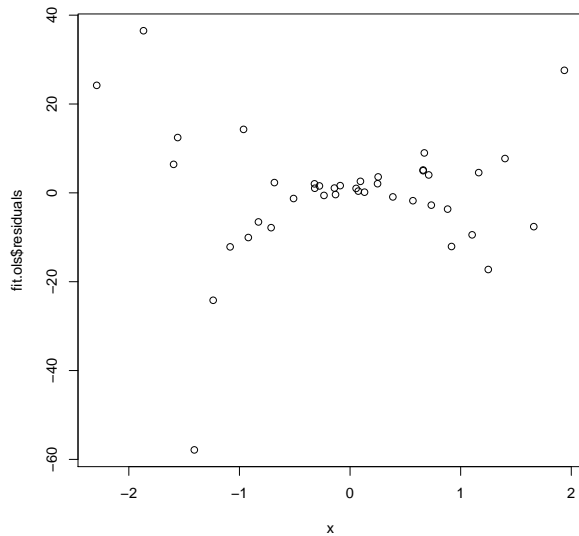
## Case Study 1: Heteroscedasticity - Step 2



In this plot I added the OLS fit as a dashed line. Note that the parameters of the fit are quite different:

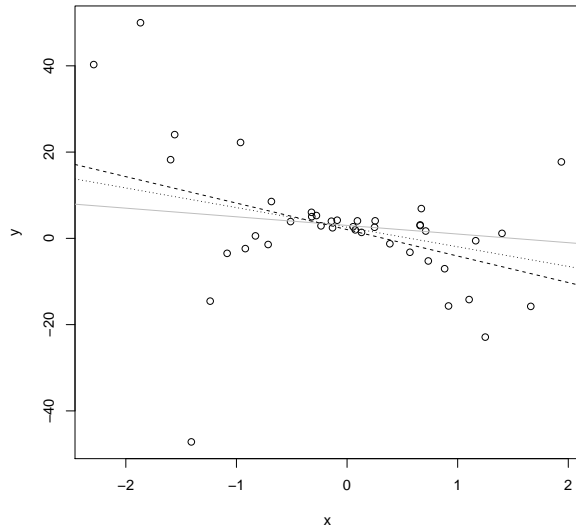
$$\beta_{OLS} \approx (2, -6).$$

## Case Study 1: Heteroscedasticity - Step 3



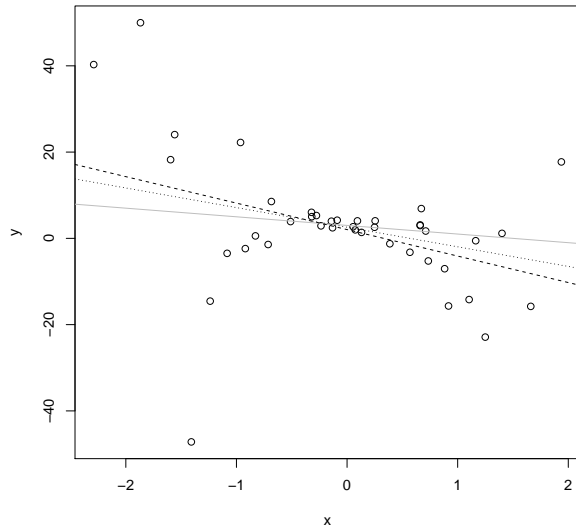
This plot shows how the OLS residuals  $\epsilon_{OLS}$  increase rapidly away from 0, as expected (since this was how the data was generated).

## Case Study 1: Heteroscedasticity - Step 4



By inspecting the previous residual plot I estimated a weighting function so that the residuals would be “more constant”. When this was used to scale the residuals, the resulting Weighted Least Squares estimates were  $\beta \approx (2.6, -4.5)$  (shown as a dotted line) and hence closer to the “true”  $\beta$ .

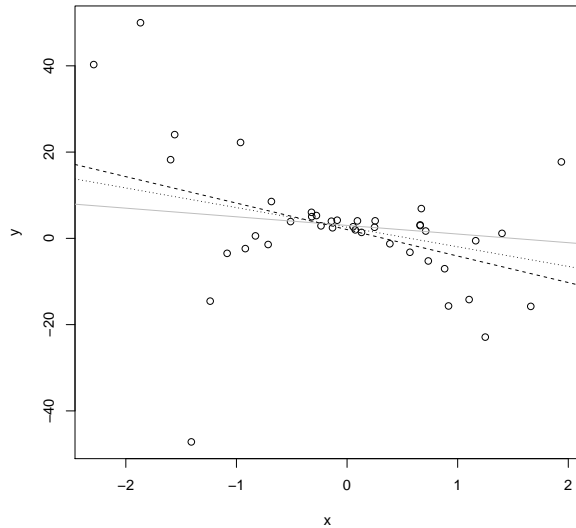
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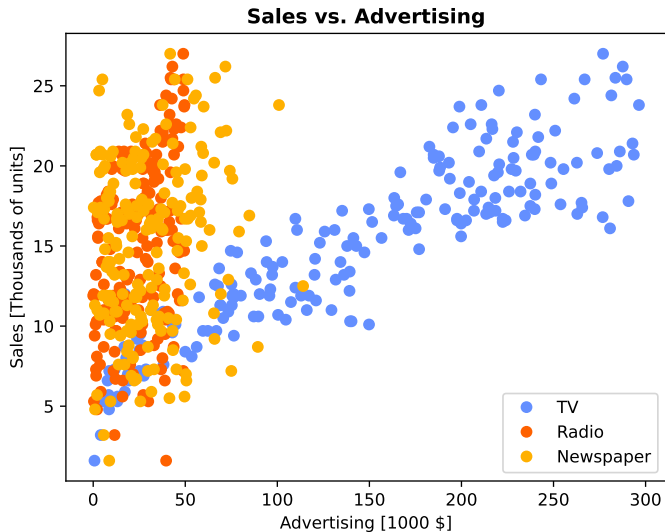
## Case Study 3: Advertising: Data and Hypotheses

### TV Radio Newspaper Sales

<b>0</b>	230.1	37.8	69.2	22.1
<b>1</b>	44.5	39.3	45.1	10.4
<b>2</b>	17.2	45.9	69.3	12.0
<b>3</b>	151.5	41.3	58.5	16.5
<b>4</b>	180.8	10.8	58.4	17.9

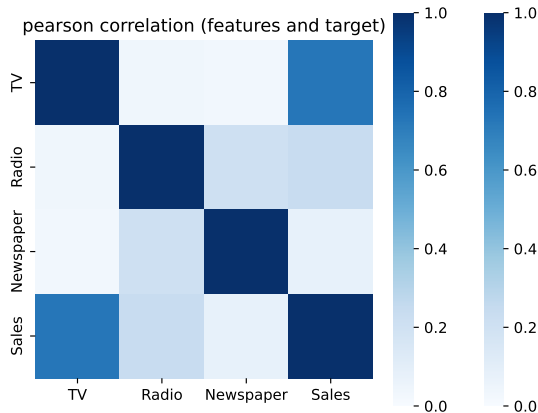
In this data set, the sales figure captures thousands of widgets of a particular type wss sold in a year. Newspaper, Radio and TV represent the annual spend per widget type on the associated advertising channel. The hypothesis is that spend on advertising is a good predictor of sales performance. Since marketing budgets are limited, where should the adverts be placed for maximum sales?

## Case Study 3: Advertising: Looking at the data



**Which of the advertising channels appear to have a linear relationship with Sales?**

## Case Study 3: Advertising: Collinearity?



Correlation matrix can indicate which attributes should participate in the model as predictors.

A good predictor should have a high correlation with the dependent variable (Sales in this case) and should have low correlation with other candidate predictors.

**What are expected to be good predictors for this data?**

## Sidebar: specifying models

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- The dataframe contains the observed variables

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Both statsmodels and sklearn use the same libraries (scipy, numpy, etc.) underneath.

## Case Study 3: Advertising: Model Building

- Start from a “full model” and prune, versus from an “empty model” and add
- We choose the latter, as it is often easier to avoid overfitting

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Define: model score: mean-square-error on the test set for a given model.

- 1 Fit “Sales  $\sim$  Newspaper”, “Sales  $\sim$  Radio”, “Sales  $\sim$  TV” and calculate their loss values.

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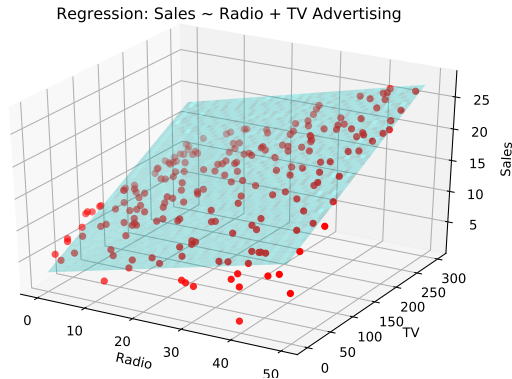
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- 4 Fit “Sales  $\sim$  TV + Radio + Newspaper”. Its loss is the same ( $\text{MSE}(\text{TV} + \text{Radio}) \approx \text{MSE}(\text{TV} + \text{Radio} + \text{Newspaper})$ ), so we favour the existing simpler two-term model (Occam’s Razor: other things being equal, choose the simplest model.).

*So our preferred model is “Sales  $\sim$  TV + Radio”.*

## Case Study 3: Advertising: Viewing the Model



Since this two-term model ignores the contribution of the newspaper channel, the Newspaper spend as a contribution to Sales is just another component of the unmodelled (and apparently random) contribution to Sales.

However, the result is a model where the model “explains” 90% of the variance of the data, which is high for an observational study. **Why? Can we do better?**



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- Spending on Newspaper advertising should be discontinued as its contribution to Sales is insignificant (indistinguishable from random noise).

## Case Study 4: Credit balances - overview

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### Introducing

- the sklearn approach to regression (we used statsmodels with the Diamonds and Advertising data)
- non-numeric explanatory variables like gender and ethnicity
- more advanced regression modelling, e.g., handling correlated variables

## Case Study 4: Credit balances - introduction

	Income	Limit	Rating	Cards	Age	Education	Gender	Student	Married	Ethnicity	Balance
<b>1</b>	14.891	3606	283	2	34	11	Male	No	Yes	Caucasian	333
<b>2</b>	106.025	6645	483	3	82	15	Female	Yes	Yes	Asian	903
<b>3</b>	104.593	7075	514	4	71	11	Male	No	No	Asian	580
<b>4</b>	148.924	9504	681	3	36	11	Female	No	No	Asian	964
<b>5</b>	55.882	4897	357	2	68	16	Male	No	Yes	Caucasian	331

Note the presence of some categorical attributes (Gender, Student, Married, Ethnicity). These can participate in linear regression models to predict a numeric response, but must be coded first. For example, Gender can become an indicator (0,1)-valued variable of the form IsFemale. Ethnicity has 3 levels and is replaced by  $3-1=2$  indicator variables.

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- Removing data relating to the first cohort meant that the remaining data looked more cohesive and also made linear regression easier
- Take-away: look for inconsistent subsets in the data, remove them if possible

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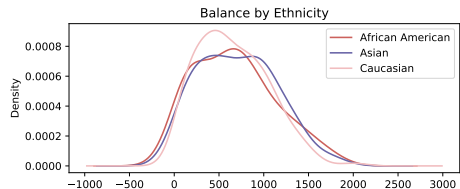
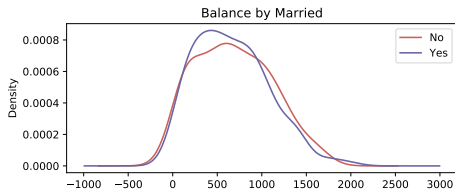
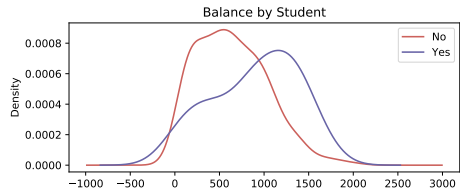
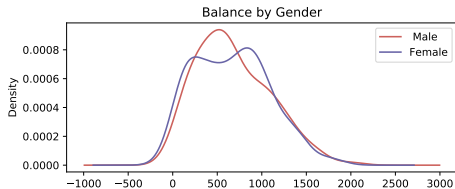
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- Take-away: remove correlated attributes, because they increase the standard error (hence variance) and make the solver’s job much more difficult

# Case Study 4: Credit balances - Contribution of Categorical Variables



**Which of these categorical attributes has a significant effect on Balance?**

## Case Study 4: Credit balances - Model building

- Using forward selection as before, the best model was found to be “Balance  $\sim$  poly(Income,2) + Rating + Age + Student + Income:Rating”
- Could also use Backward Elimination to prune from a complex model
- For this data, high correlations between features can cause difficulties - we need techniques to handle this

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---

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- ➌ Use *regularisation*, to “penalise” large model coefficients (solve a related problem with a different loss function)

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- if too large: tries less to match the data, increases the bias
  - if too small: tries too hard to match the data so  $\beta \rightarrow \infty$  and increases the variance

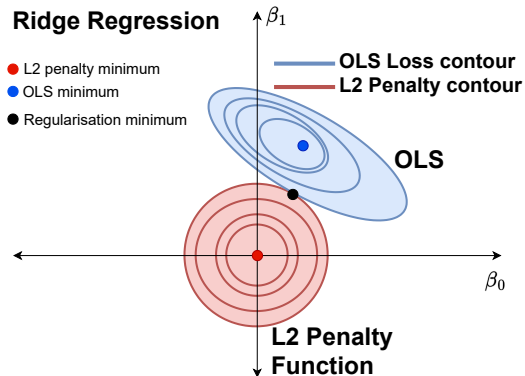


# Ridge vs Lasso Regression

Because lasso regression favours the “corners” in parameter space, it tends to set some parameter values to 0 (essentially dropping the associated features). This has the added benefit of making the model smaller and easier to interpret.

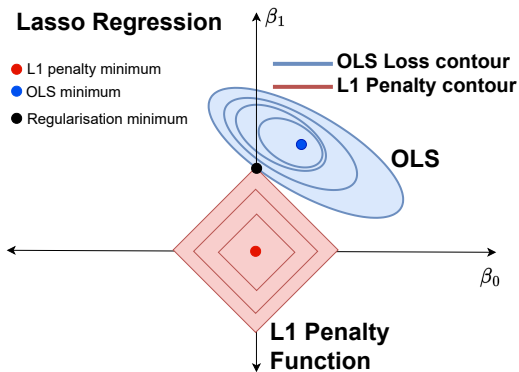
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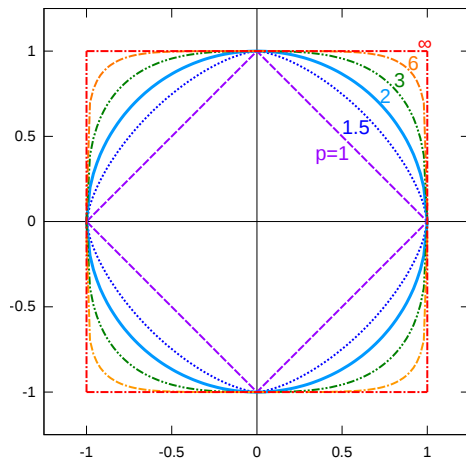


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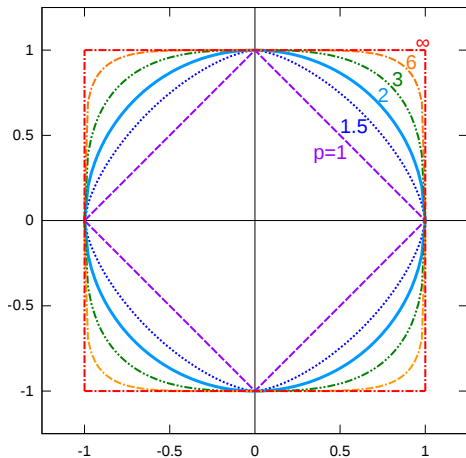


# Sidebar - vector norms and their unit balls in 2D



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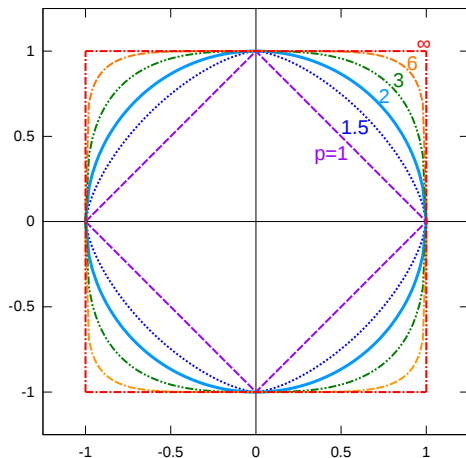
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What about unit balls with  $0 < p < 1$ ?

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# Sidebar - vector norms and their unit balls in 2D



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Unit ball,  $p = \frac{2}{3}$

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## Case Study 4: Credit balances - Regularisation - Searching for $\lambda$

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Ridge regression downweights certain terms but does not set them to zero. However, it can be more performant, because it keeps some contribution from each feature.

# Recall: Attribute independence in Multivariate Data

## Definition 3 (Covariance)

$\sigma_{12} = E[(X_1 - \mu_1)(X_2 - \mu_2)]$ . In words, for two attributes  $X_1$  and  $X_2$ , with means  $\mu_1$  and  $\mu_2$ , respectively,  $\sigma_{12}$  is a measure of the linear dependence between them. If they are independent, we can show that  $\sigma_{12} = 0$ .

## Definition 4 ((Variance-)Covariance Matrix)

When there are  $n$  numeric attributes, there are  $n \times n$  pairs of covariances  $\sigma_{ij}, i = 1, \dots, n; j = 1, \dots, n$ . The resulting covariance matrix is symmetric and diagonally dominant. This matrix captures the covariance structure of the set of  $n$  attributes  $\{X_i\}$ .

Sometimes it is convenient to work with the correlation matrix, which is a scaled version of the covariance matrix, with elements  $\rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$ , which is scaled so that all the diagonal elements are 1 and the off diagonal elements satisfy  $-1 < \rho_{ij} < 1$ . If two attributes are highly correlated, adding the second into the model does not increase the explanatory power of the model. Therefore, it pays to determine the covariance matrix from the data before building any models.

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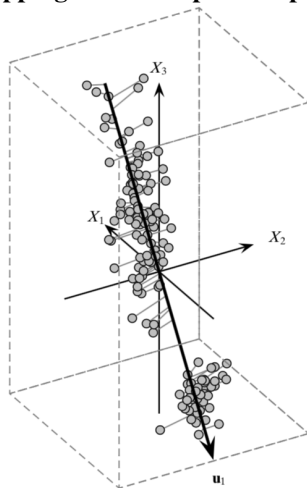
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- The best known of these techniques is *Principal Components Analysis* (PCA).

# PCA visualisation

## Mapping to 1 Principal Component

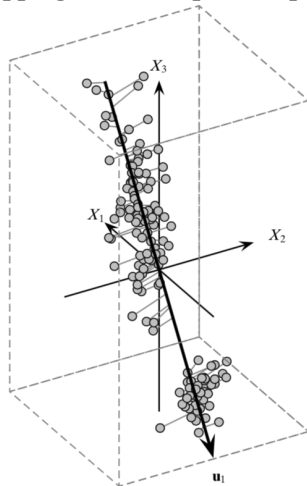


Mapping correlated  $X_1, X_2, X_3$  to uncorrelated  $u_1$



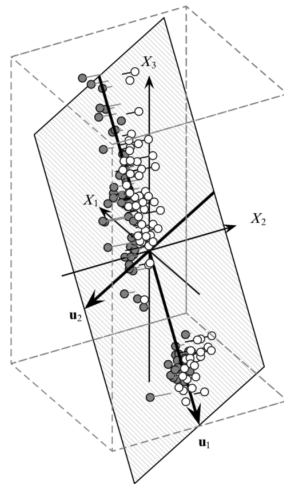
# PCA visualisation

## Mapping to 1 Principal Component



Mapping correlated  $X_1, X_2, X_3$  to uncorrelated  $u_1$

## Mapping to 2 Principal Components



Mapping correlated  $X_1, X_2, X_3$  to uncorrelated  $u_1, u_2$

# PCA interpretation

- Although the data has dimension  $d = 3$ , it is possible to find the line (on the left;  $d = 1$ ) and plane (on the right,  $d = 2$ ) which retain most of the variance of the data after it has been projected onto this lower dimensional subspace.

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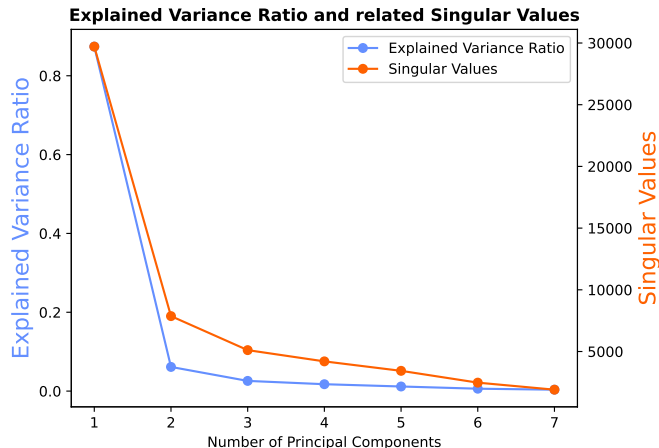
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- However, it is helpful to interpret the results in terms of the original attributes.

# PCA example

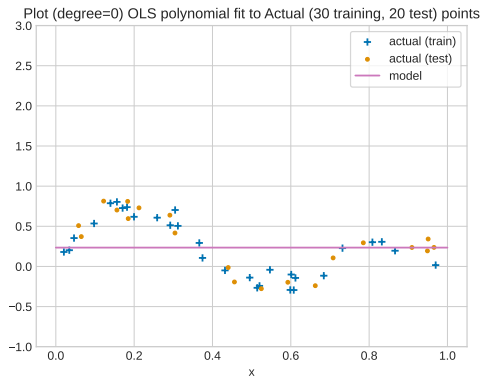


The plot shows that the first 3 **singular values** (associated with principal components  $u_1, u_2, u_3$ ) capture the bulk of the variance in the training set. Therefore, three attributes, which are transformations of the other 7, are sufficient. You could interpret those attributes as representing the measles outbreaks in three archetypal English cities. . .

This [youtube video](#) describes PCA concepts well.

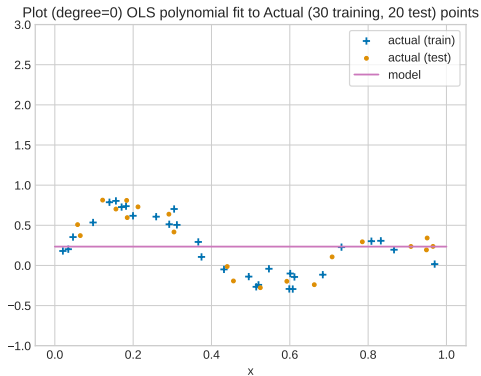


# Returning to the problematic example

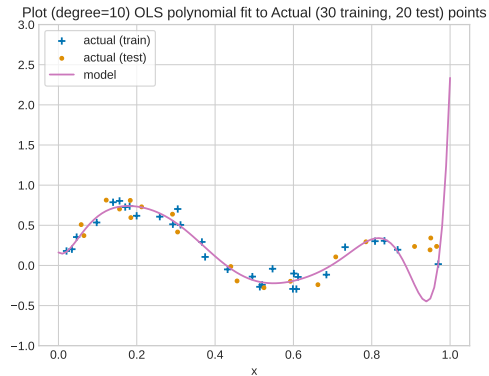


*Degree 0 (constant) fit: high bias, low variance*

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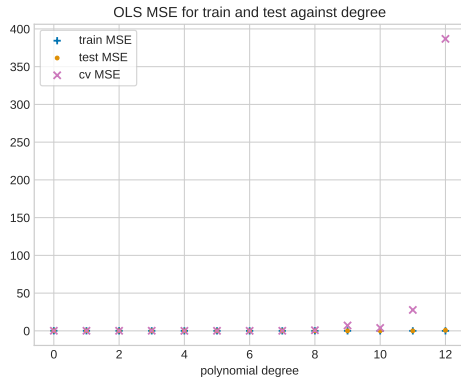


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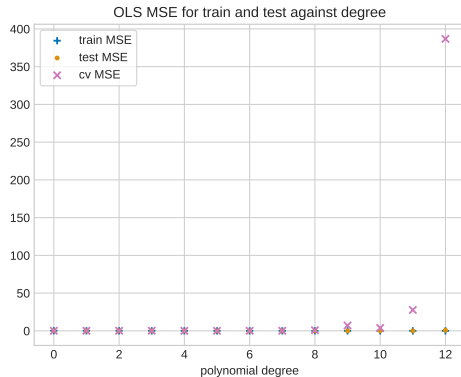
*Degree 10 (up to  $x^{10}$ ) fit: low bias, high variance*

# Diagnosis - OLS

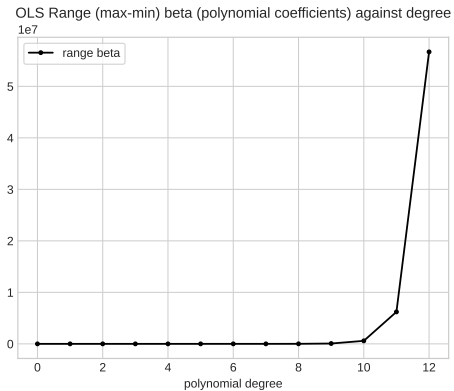


*Train MSE decreases with degree, Test MSE decreases, then increases*

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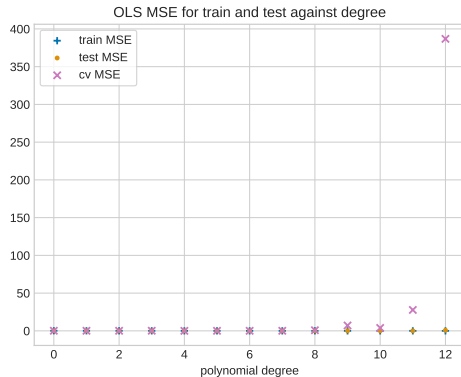


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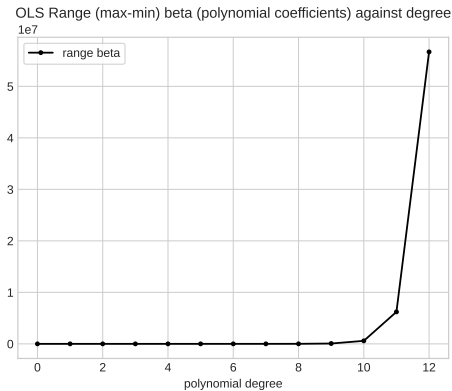
*Polynomial coefficient range (max-min) increases dramatically with degree due to overfitting.*

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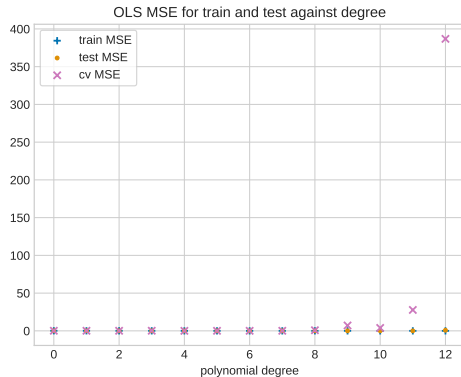
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Is there any way we can use high-degree polynomials?



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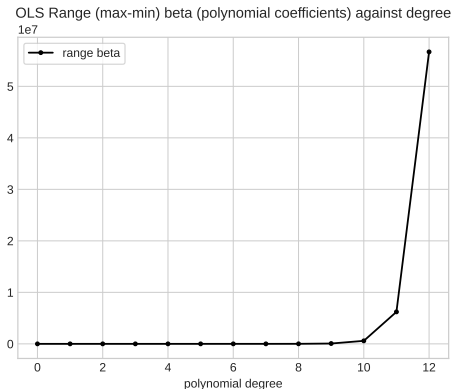
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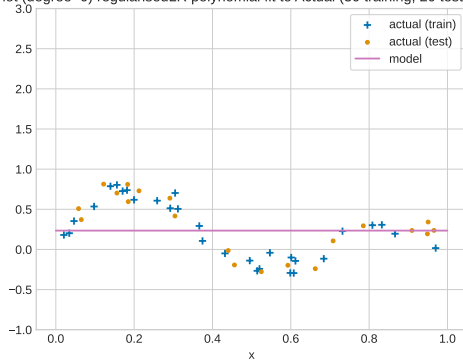
Yes, if we add regularisation...



*Polynomial coefficient range (max-min) increases dramatically with degree due to overfitting.*

# Same data, same features, with regularisation this time

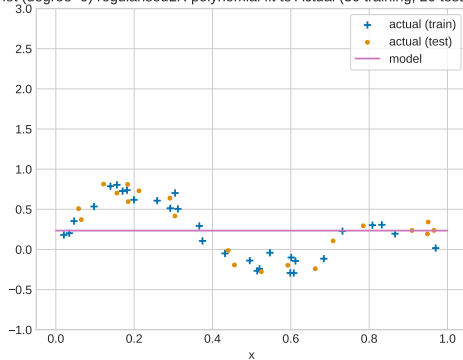
Plot (degree=0) regularisedLR polynomial fit to Actual (30 training, 20 test) points



*Degree 0 (constant) fit,  $\lambda \approx 0$ : no change*

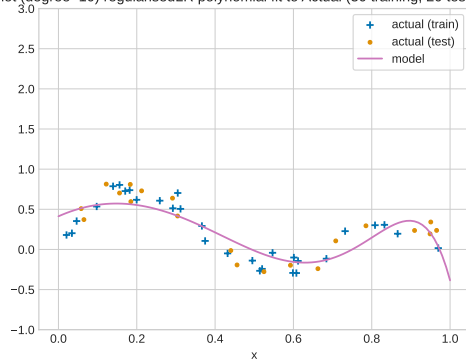
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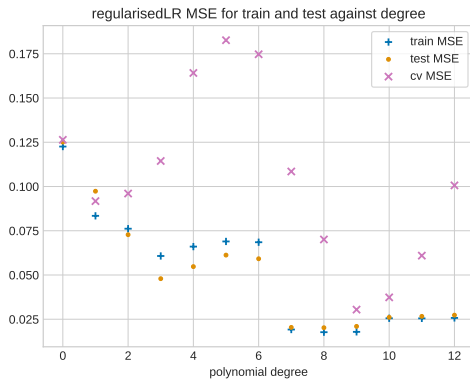
Plot (degree=10) regularisedLR polynomial fit to Actual (30 training, 20 test) points



*Degree 10 (up to  $x^{10}$ ) fit: stabilised polynomial*

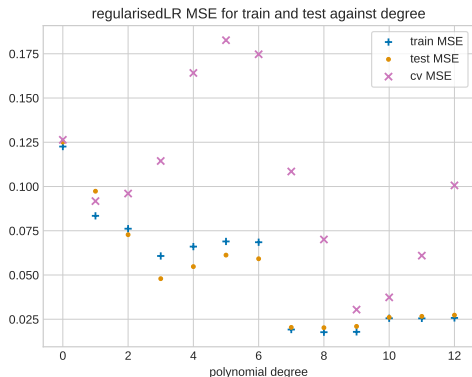


# Diagnosis - Regularised Linear Regression

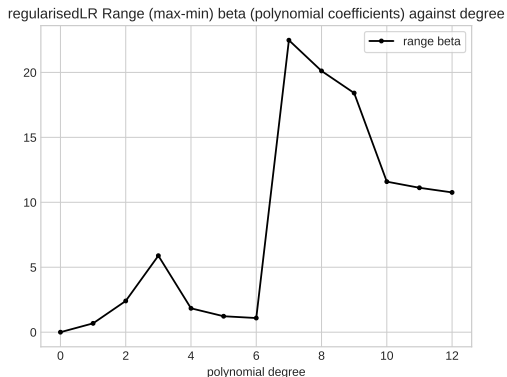


*MSE behaviour is affected by choice of  $\lambda$ , but degree 8 or 9 looks good*

# Diagnosis - Regularised Linear Regression

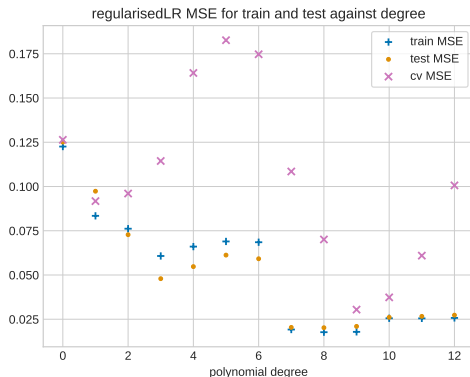


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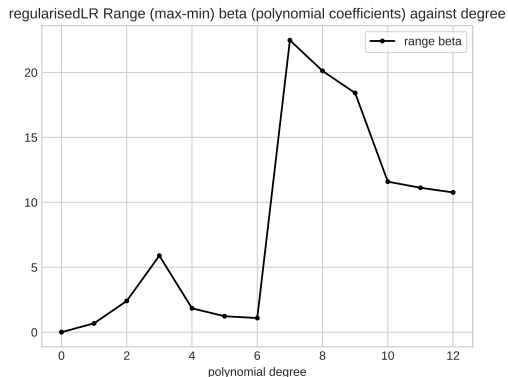


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# Diagnosis - Regularised Linear Regression



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So regularisation can control overfitting and/or high correlation between features

# Review and summary

- Linear regression is one of the foundations of data mining
- It has two phases, of which the first (learning) is generally the most challenging
- It has many variants, so is quite flexible, but flexibility can be abused!
- Careful validation and model building is essential for success - it is an extension of the exploratory work done earlier in the process
- In machine learning, prediction error is the main focus, but you need to be aware of other considerations such as
  - ① model parsimony (keep them as small as possible!): faster at both training and evaluation time
  - ② the bias-variance dilemma: avoid overfitting and underfitting - remember, your model needs to generalise well from the training to the test set
  - ③ model interpretability: some models are easier to understand because the terms in the model represent concepts from the domain the data is from

## Some Additional Resources

- Book: Introduction to Statistical Learning with R (2013) by James, Gareth and Witten, Daniela and Hastie, Trevor and Tibshirani, Robert.

*I strongly recommend that you read Chapter 3 of the book, as it is very well written and available online for free.*

- Kaggle notebooks relating to the datasets addressed this week. There are many, but searching Kaggle should provide nice examples of data mining in action.
- I wrote a report on linear regression that has been added to moodle.