dm24s1

Topic 09 : Regression2

Part 01 : Overview

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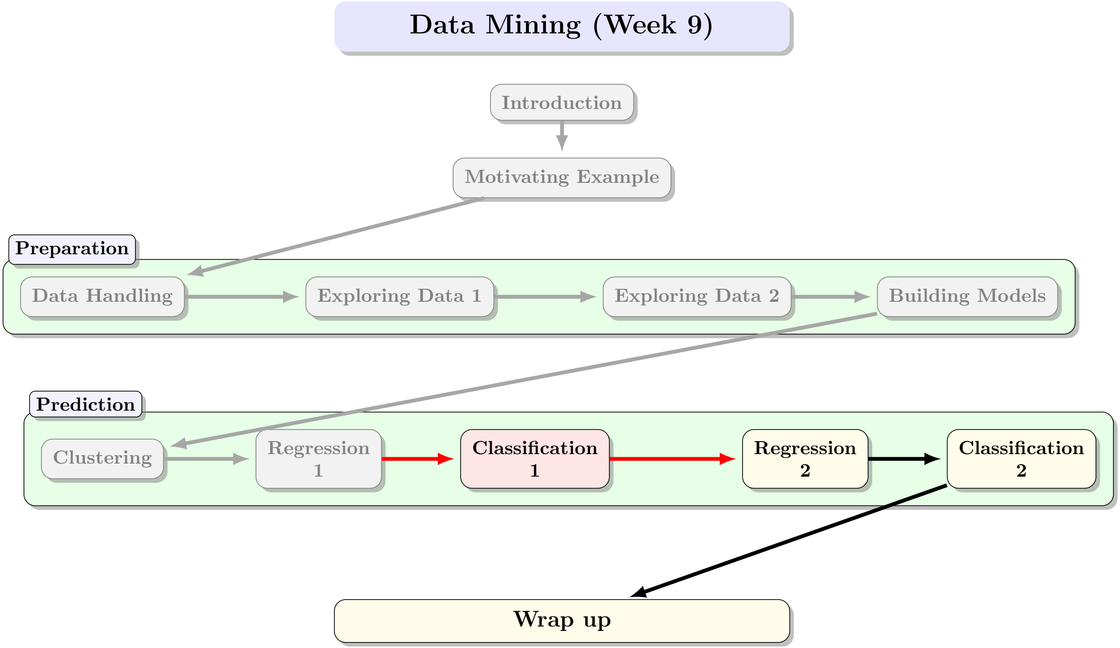
Autumn Semester, 2024

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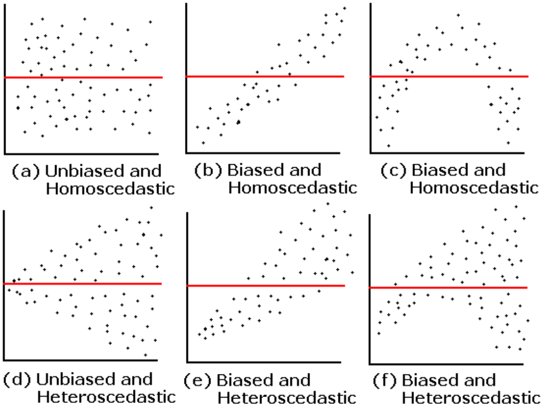
> These assumptions can be used constructively, when model building, or as checks, when validating models.

Bias and variance in regression



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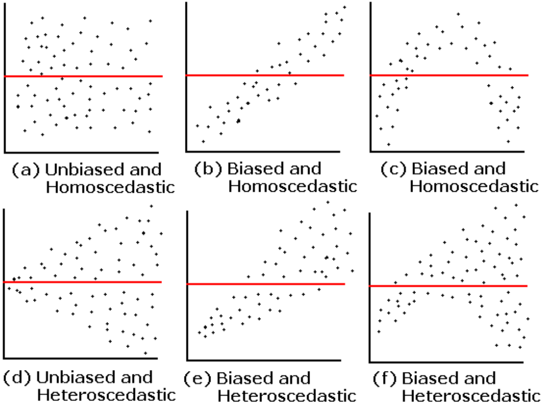

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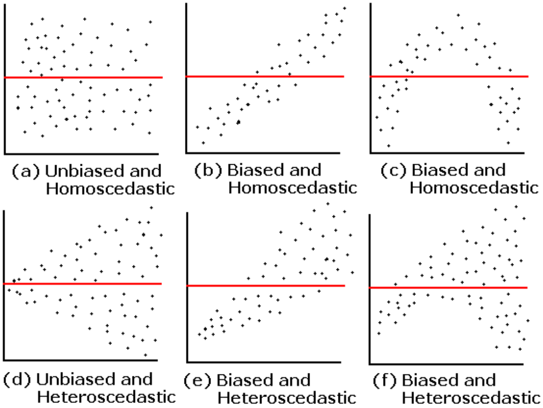

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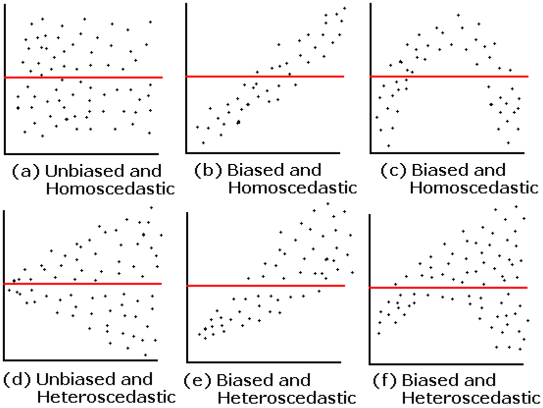

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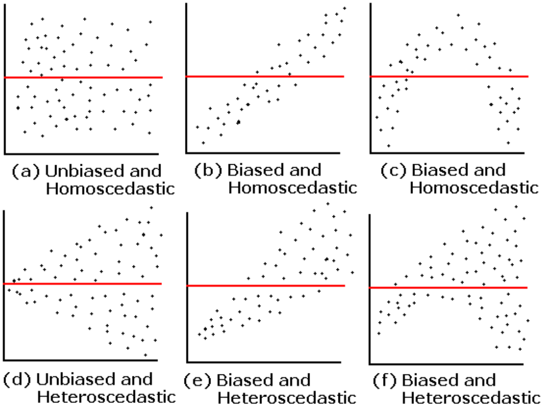

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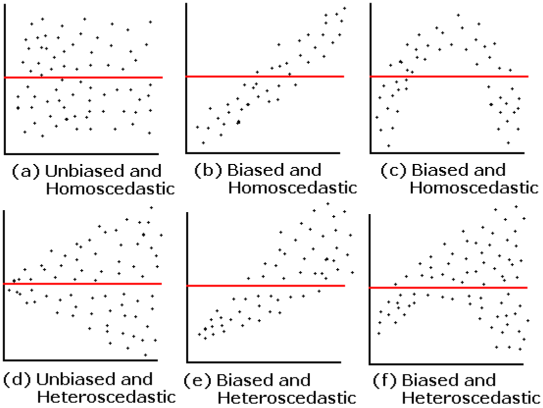

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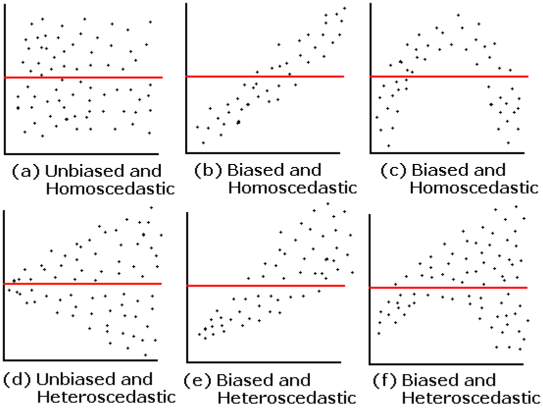

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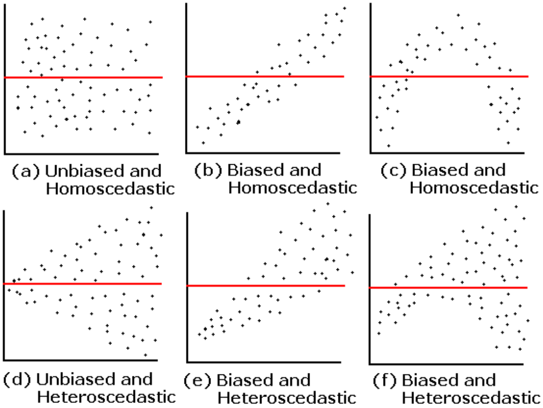

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  - Using scikit-learn: add the argument `sample_weight = someWeights`, e.g., `model.fit(Xtrain, yTrain, sample_weight=someWeights)`.
  - Using statsmodels: use the weighted version of least squares: `WLS(y, X, someWeights)` not `OLS(y, X)`

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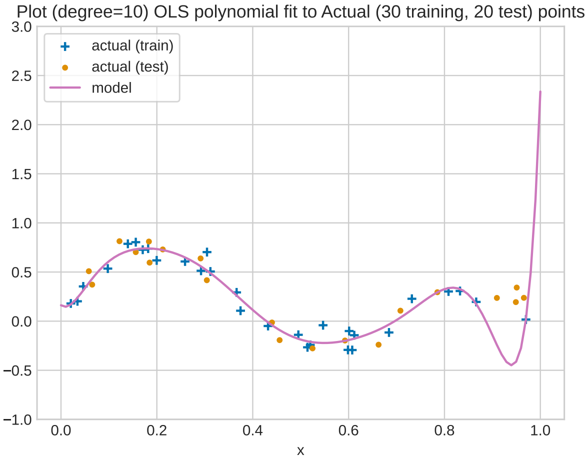

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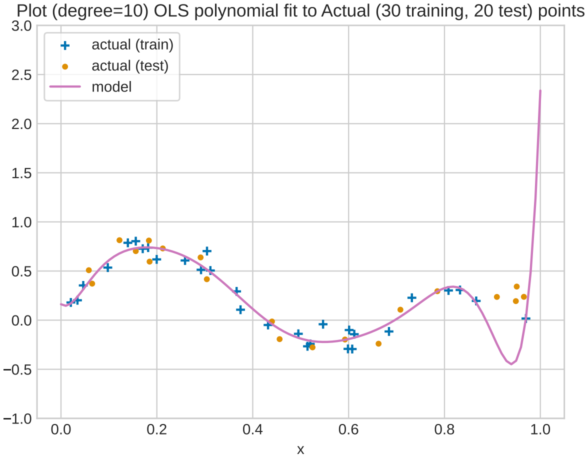

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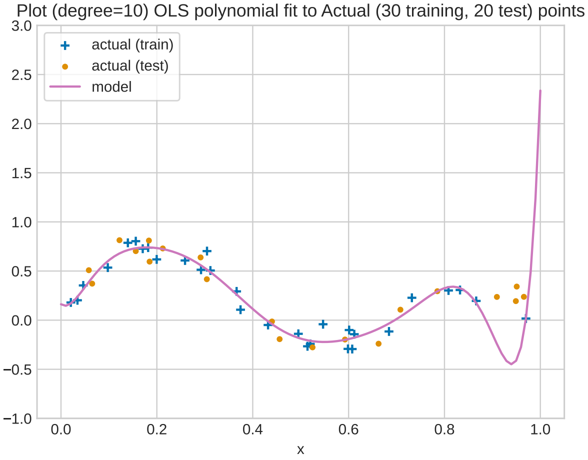

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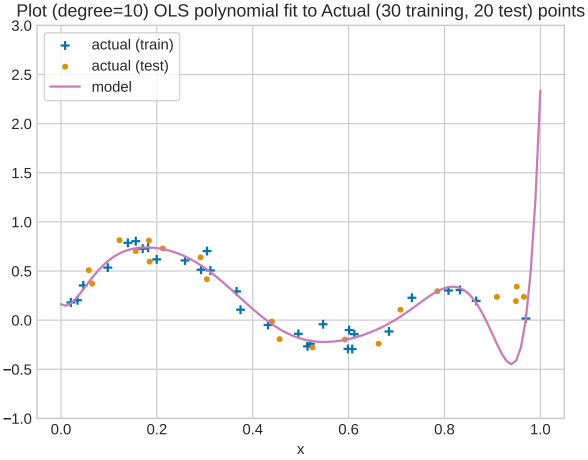
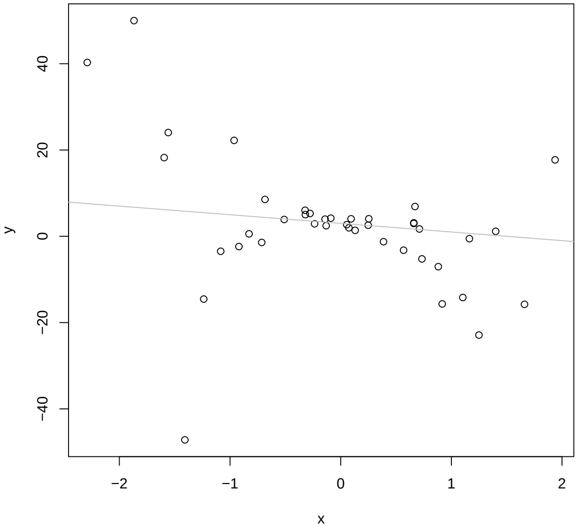


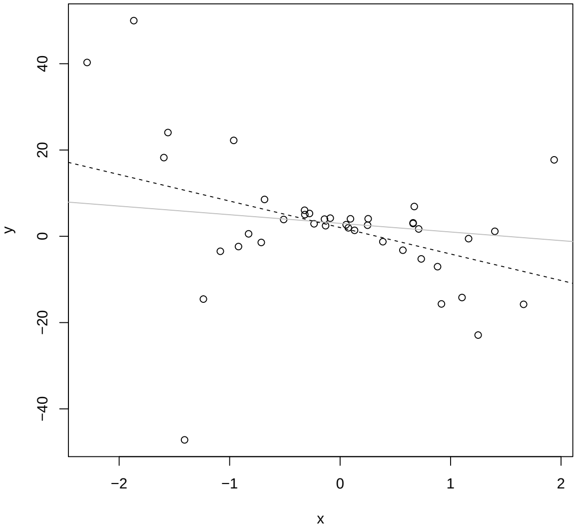
1. Data is quite noisy
2. Training data has gaps near the edges
3. Model may be overfitting

Case Study 1: Heteroscedasticity - Step 1



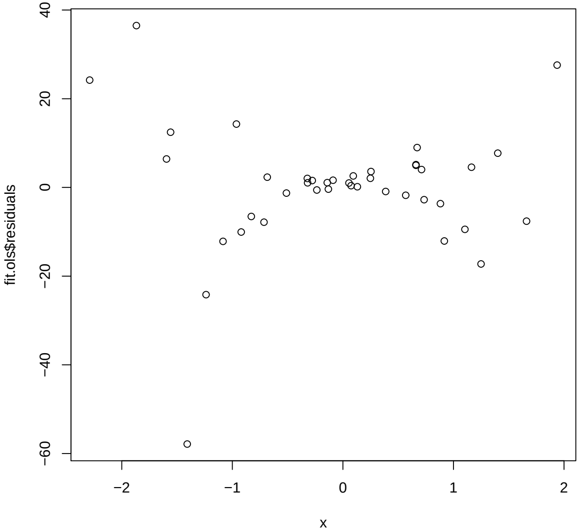
I generated 41 x, y points based on $y = 3 - 2x$, but with added errors that increase away from $x = 0$. The plot shows the line with $\beta = (3, -2)$ in grey.

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 ϵ_{OLS} increase rapidly away from 0, as expected (since this was how the data was generated).

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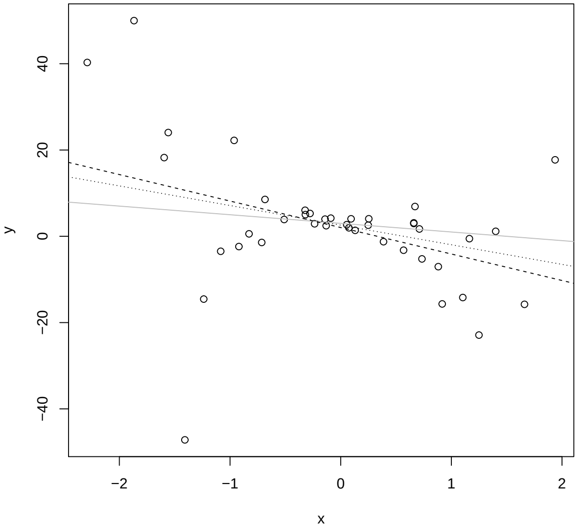

By inspecting the previous residual plot I estimated a weighting function so that the residuals would be "more constant". When this was used to scale the residuals, the resulting Weighted Least Squares estimates were $\beta \approx (2.6, -4.5)$ (shown as a dotted line) and hence closer to the "true"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

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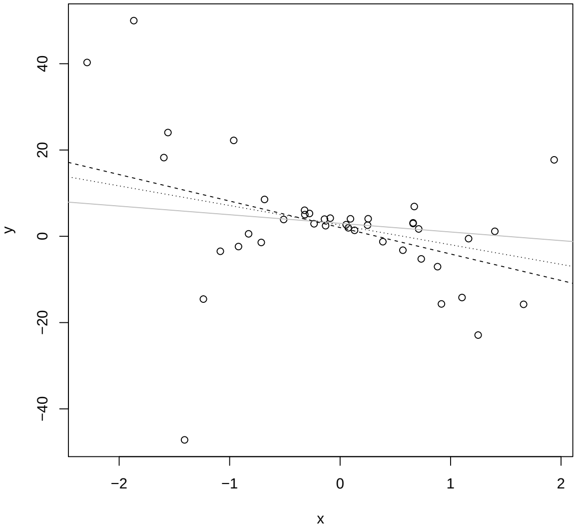

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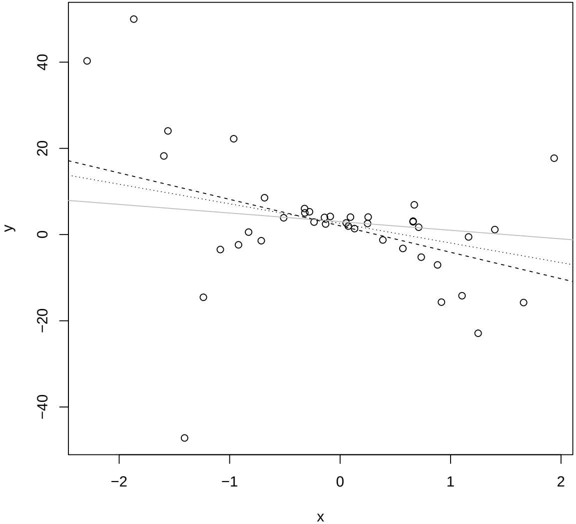

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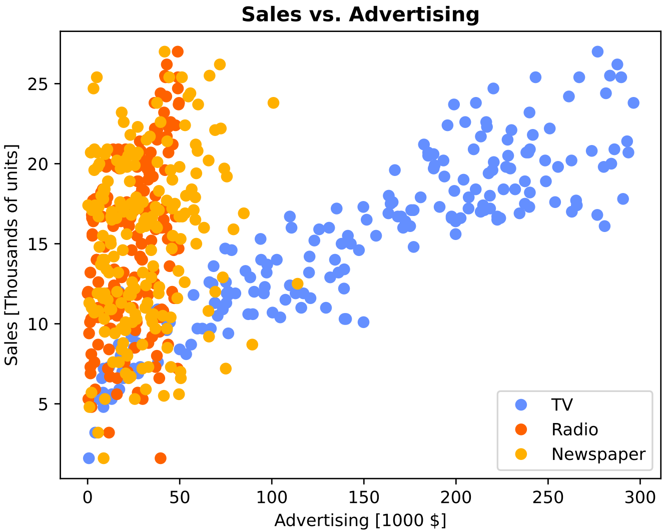
Case Study 3: Advertising: Data and Hypotheses

	TV	Radio	Newspaper	Sales
0	230.1	37.8	69.2	22.1
1	44.5	39.3	45.1	10.4
2	17.2	45.9	69.3	12.0
3	151.5	41.3	58.5	16.5
4	180.8	10.8	58.4	17.9

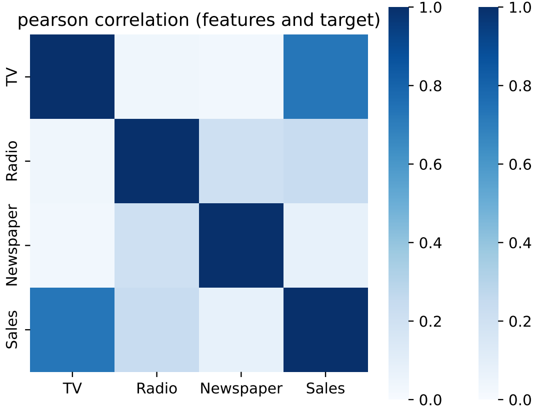
In this data set, the sales figure captures thousands of widgets of a particular type wss sold in a year. Newspaper, Radio and TV represent the annual spend per widget type on the associated advertising channel. The hypothesis is that spend on advertising is a good predictor of sales performance. Since marketing budgets are limited, where should the adverts be placed for maximum sales? Alternatively, how should marketing funds be distributed across the 3 channels to achieve a specified sales performance, while keeping the total spend as low as possible?

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?

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The sklearn way

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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

Example 2 (Forward Selection for Advertising Data)

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

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

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Forward selection in action, with and without the interaction term

Main features only

	feature	test_neg_mean_squared_error	test_r2
0	TV	(-7.324310374422005, -3.9369810322191725)	(0.7603440777107349, 0.8390841989031752)
1	Radio	(-4.718440611471557, -1.8510139478354648)	(0.8456097326980663, 0.9322678692463672)
2	Newspaper	(-4.720392592253671, -1.8510521207093056)	(0.8455458626911012, 0.9317779087301497)

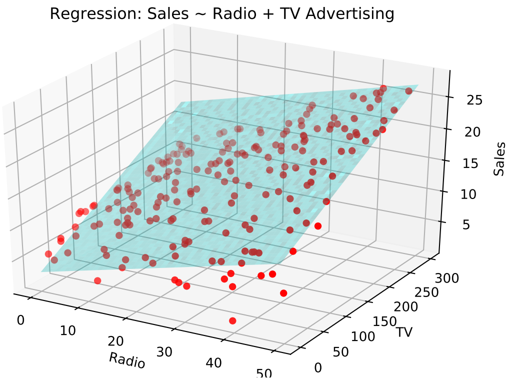
MSE(TV) $\approx$ 5.5; MSE(TV + Radio) $\approx$ 3.5; MSE(TV + Radio + Newspaper) $\approx$ 3.5 $\approx$ MSE(TV + Radio). Adding Newspaper does not reduce MSE.

Main features with TV:Radio interaction term

	feature	test_neg_mean_squared_error	test_r2
0	TV	(-7.324310374422005, -3.9369810322191725)	(0.7603440777107349, 0.8390841989031752)
1	TV:Radio	(-3.695048288640372, -1.8479935191656147)	(0.8790957564264389, 0.9377953274242408)
2	Radio	(-3.929784758825856, -1.751389612982792)	(0.8714150353235093, 0.9410470781968057)
3	Newspaper	(-3.9387465036567293, -1.7715653928145365)	(0.8711218015427203, 0.940367948229423)

MSE(TV) $\approx$ 5.5; MSE(TV + TV:Radio) $\approx$ 2.8; MSE(TV + TV:Radio + Radio) $\approx$ 2.8 $\approx$ MSE(TV + TV:Radio). Adding Radio and Newspaper does not reduce MSE.

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

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
1	14.891	3606	283	2	34	11	Male	No	Yes	Caucasian	333
2	106.025	6645	483	3	82	15	Female	Yes	Yes	Asian	903
3	104.593	7075	514	4	71	11	Male	No	No	Asian	580
4	148.924	9504	681	3	36	11	Female	No	No	Asian	964
5	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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- Take-away: look for inconsistent subsets in the data, remove them if possible

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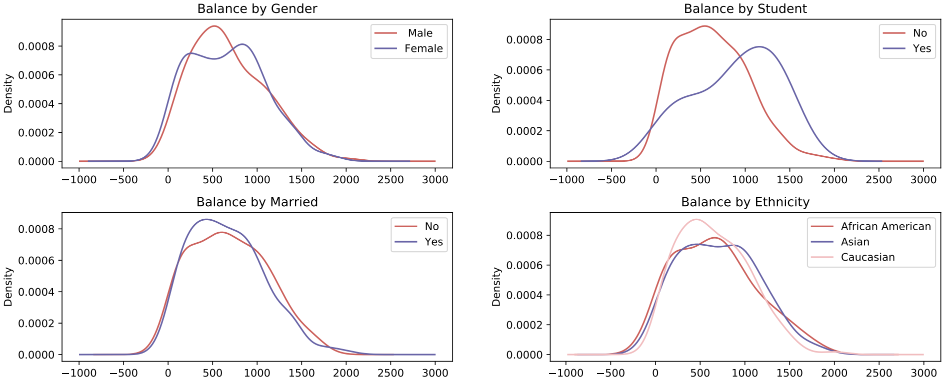
- Take-away: remove correlated attributes, because they increase the standard error (hence variance) and make the solver’s job much more difficult

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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3. Use *regularisation*, to "penalise" large model coefficients (solve a related problem with a different loss function)

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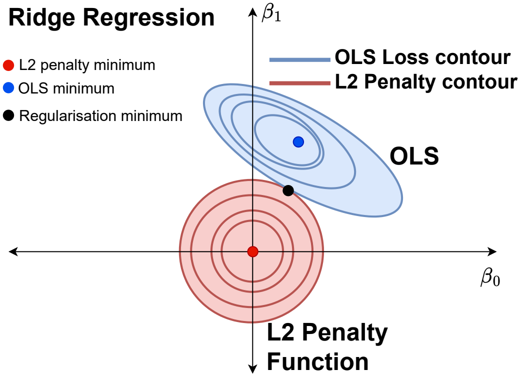
  - if too large: tries less to match the data, increases the bias
  - if too small: tries too hard to match the data so $\beta \to \infty$ and increases the variance

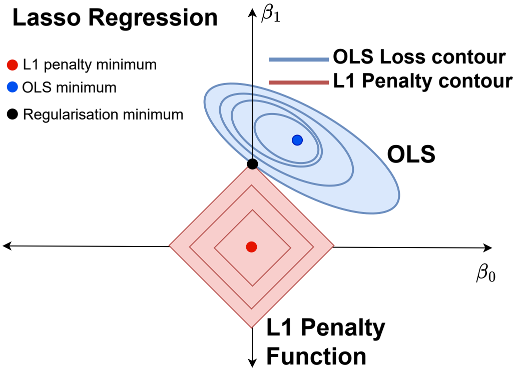
Ridge vs Lasso Regression

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.

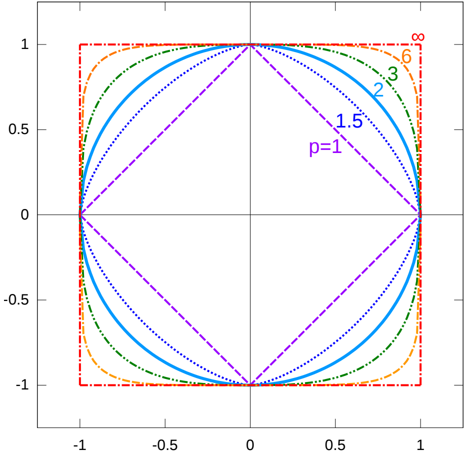
Ridge Regression



Lasso Regression



Sidebar - vector norms and their unit balls in 2D



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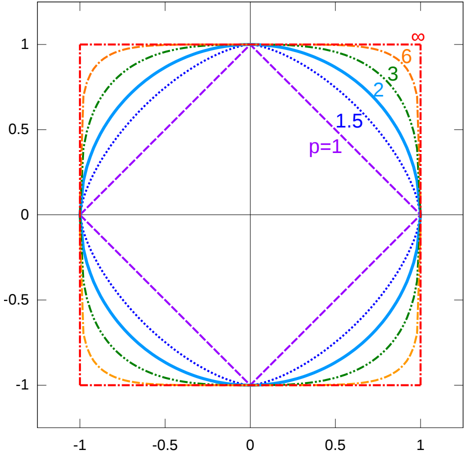

What about unit balls with $0 < p < 1$?

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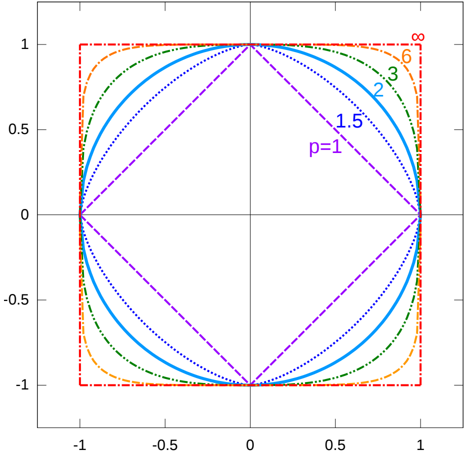

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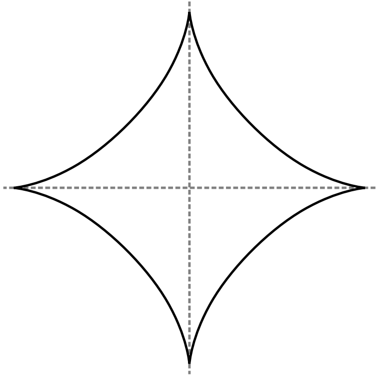

Unit ball, $p = \frac{2}{3}$

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Case Study 4: Credit balances - Regularisation - Searching for λ

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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 μ_1 and μ_2, respectively, σ_{12} is a measure of the 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 $\sigma_{ij}, i = 1, \ldots, n; j = 1, \ldots, n$. 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 pf 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.

Feature reduction

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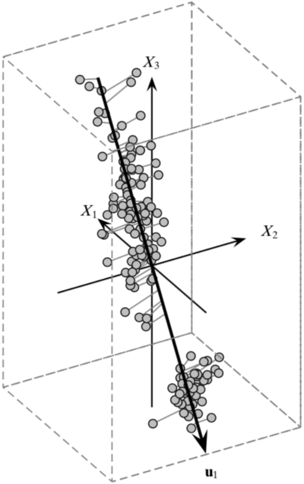
- The best known of these techniques is *Principal Components Analysis* (PCA).

PCA visualisation

Mapping to 1 Principal Component



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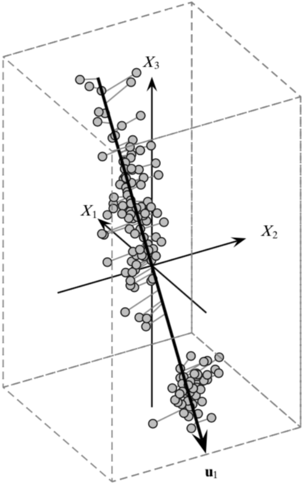

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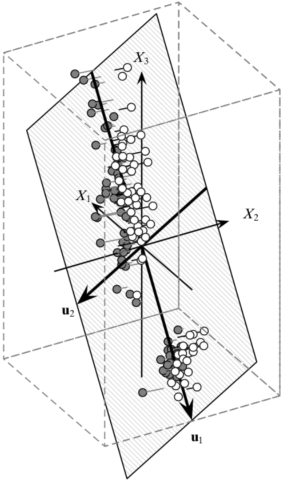

Mapping correlated X_1, X_2, X_3 to uncorrelated u_1, u_2

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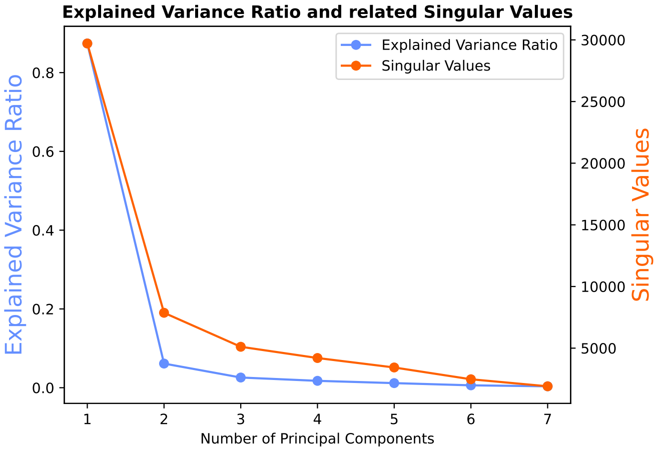
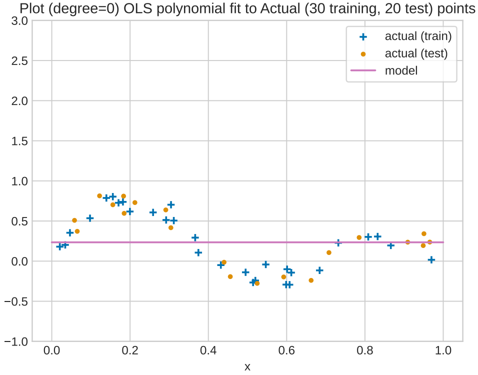
- However, it is helpful to interpret the results in terms of the original attributes.

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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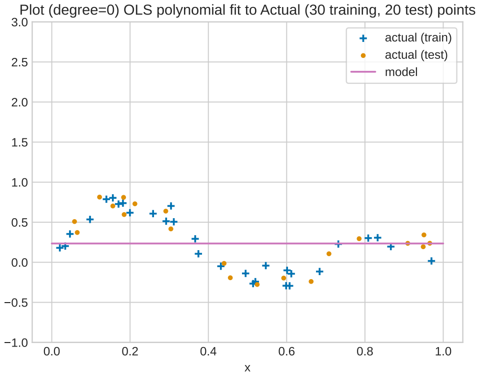

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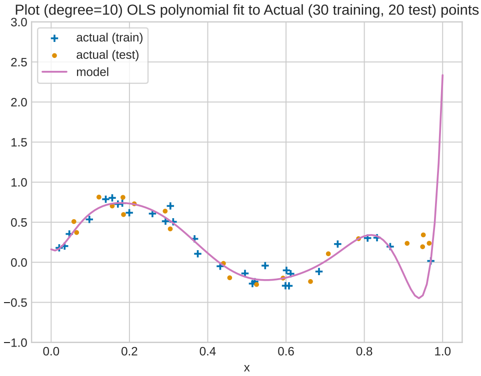
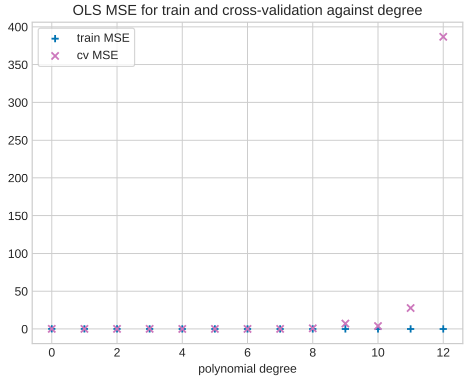


Degree 10 (up to x^{10}) fit: low bias, high variance

Diagnosis - OLS



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

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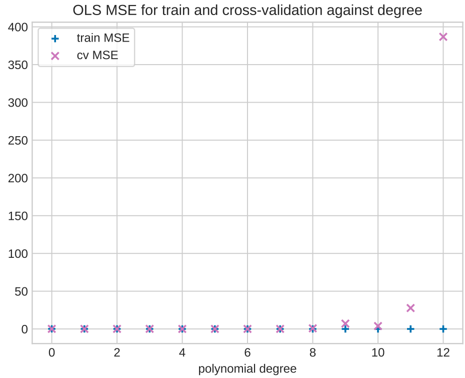

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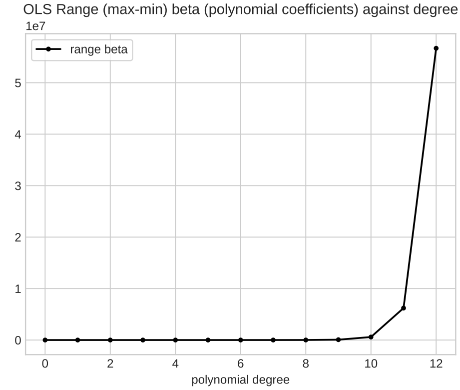

Polynomial coefficient range (max-min) increases dramatically with degree due to overfitting.

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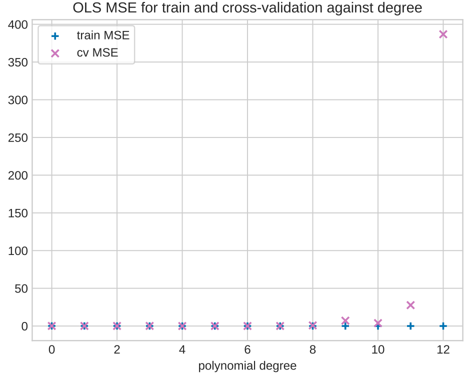

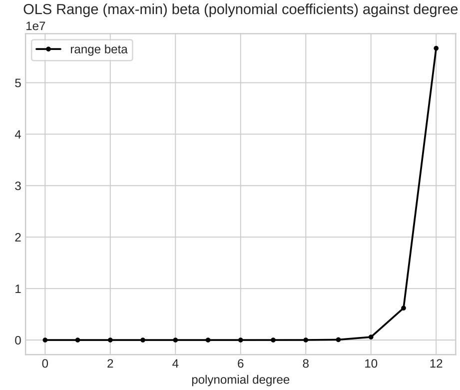

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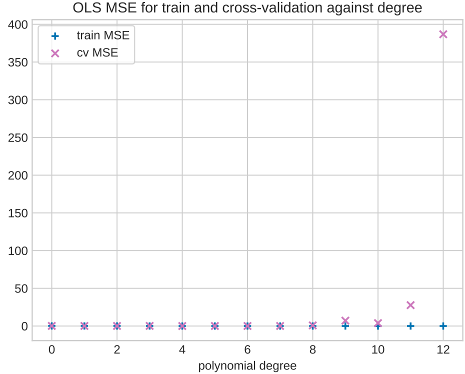

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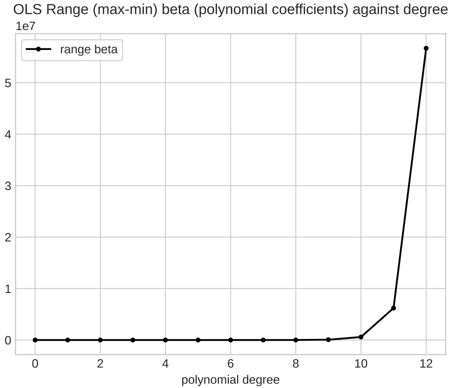

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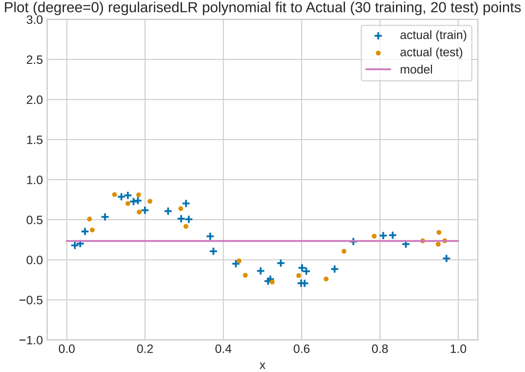
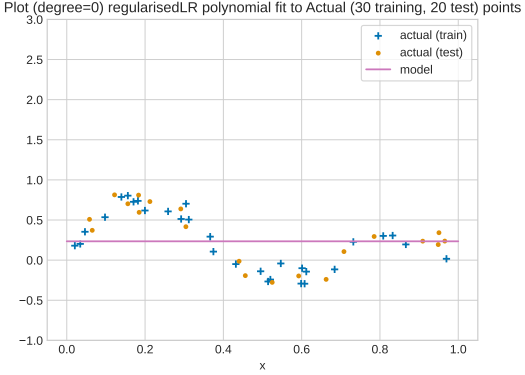
> Yes, if we add regularisation. . .

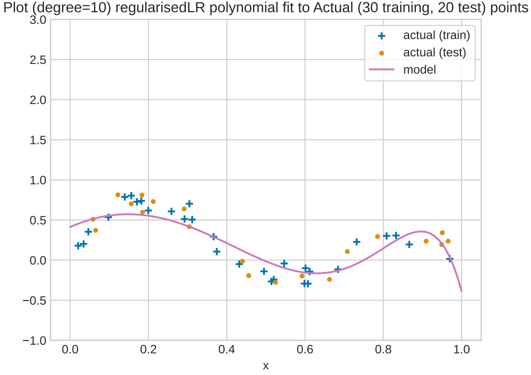
Same data, same features, with regularisation this time



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

Same data, same features, with regularisation this time

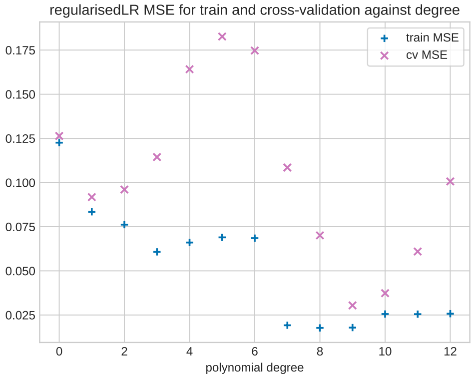




Degree 0 (constant) fit, $\lambda \approx 0$*: no change*

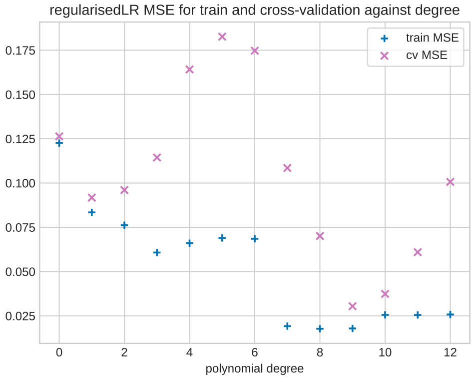
Degree 10 (up to x^{10}*) fit: stabilised polynomial*

Diagnosis - Regularised Linear Regression

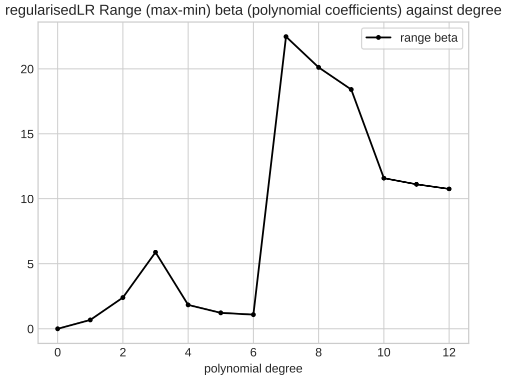


MSE behaviour is affected by choice of λ*, but degree 8 or 9 looks good*

Diagnosis - Regularised Linear Regression

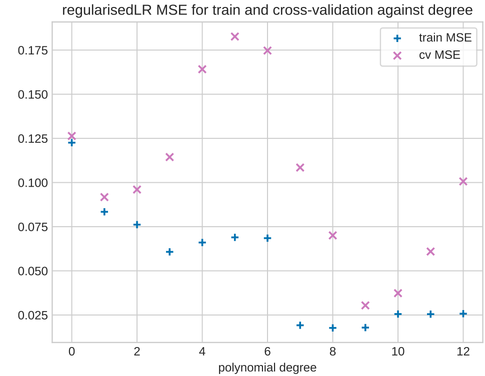


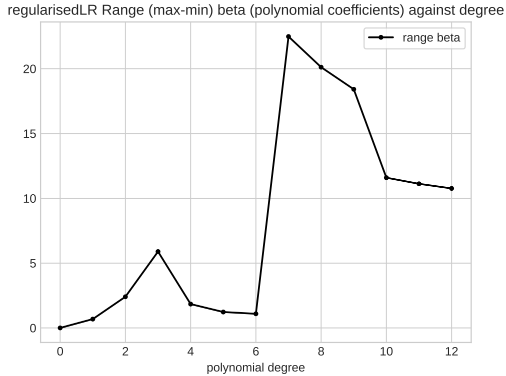
MSE behaviour is affected by choice of λ, but degree 8 or 9 looks good



Polynomial coefficient range (max-min) is controlled - no evidence of overfitting.

Diagnosis - Regularised Linear Regression





MSE behaviour is affected by choice of λ, but degree 8 or 9 looks good

Polynomial coefficient range (max-min) is controlled - no evidence of overfitting.

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.