dm25s1

Topic 09 : Regression2

Part 01 : Overview

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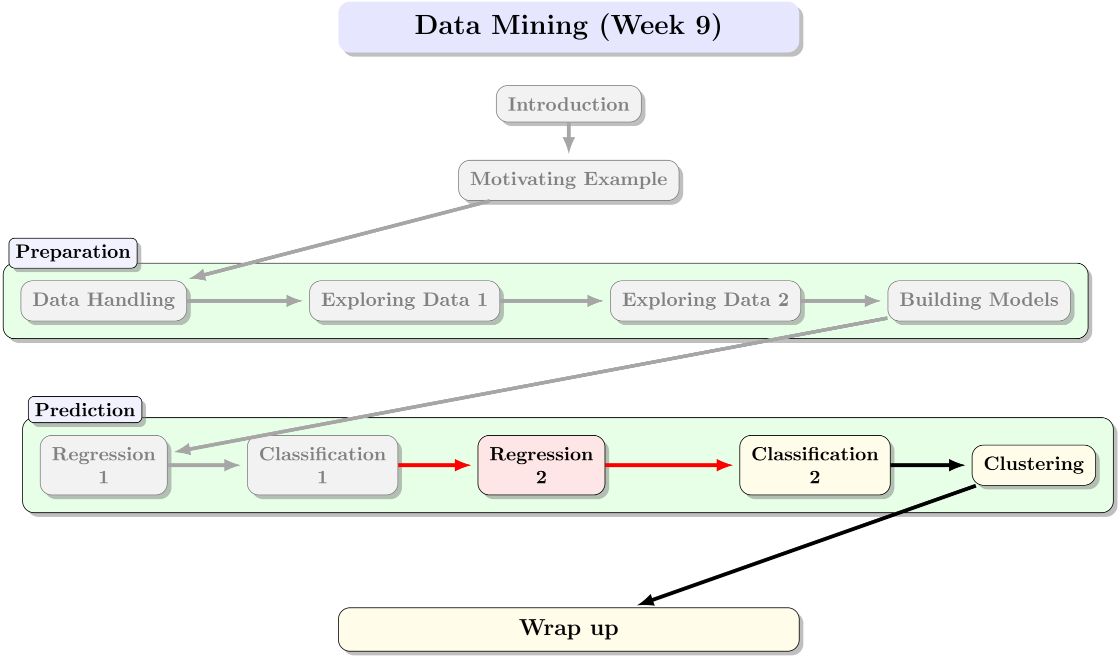
Outline

- Regression assumptions, and how-
- to deal with heteroscedasticity and why it is a problem
- unrepresentative training data can lead to overfitting
- feature collinearity can be assessed
- Provide a worked example of forward selection of features, and interaction terms, for model building



Data Mining (Week 9)
Introduction
Motivating Example
Preparation
Data Handling
Exploring Data 1
Exploring Data 2
Building Models
Prediction
Regression 1
Classification 1
Regression 2
Classification 2
Clustering
Wrap up

Outline

1. Introduction 3

2. Regression1 review 5

3. Case Study 1: Generated 9

4. Case Study 3: Advertising 14

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  - 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.

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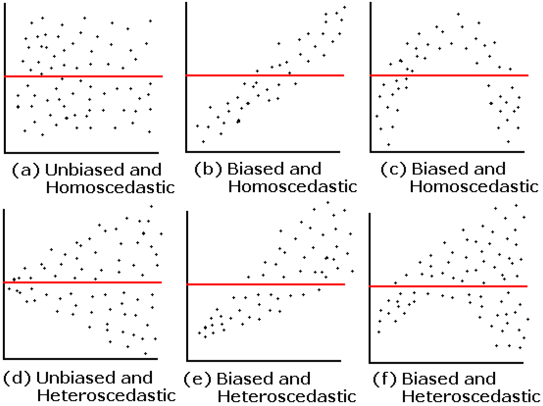

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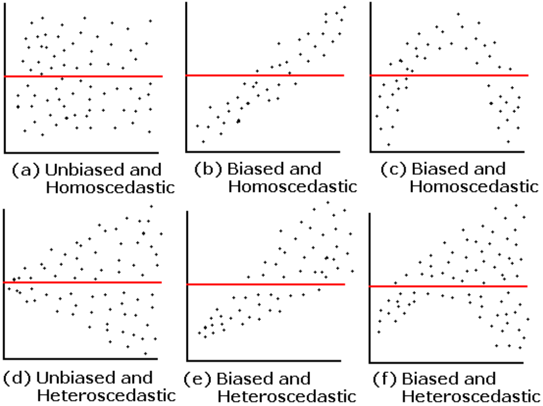

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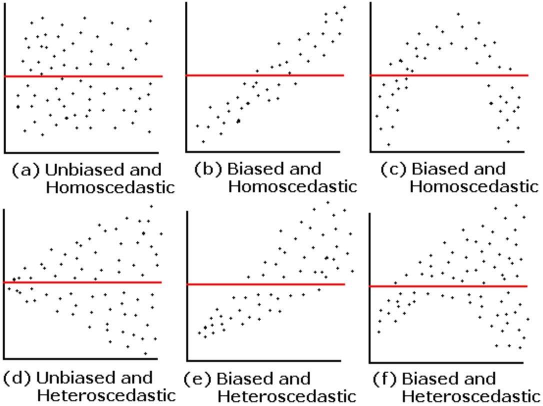

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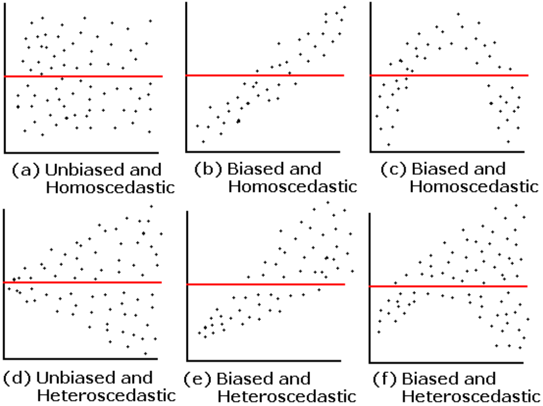

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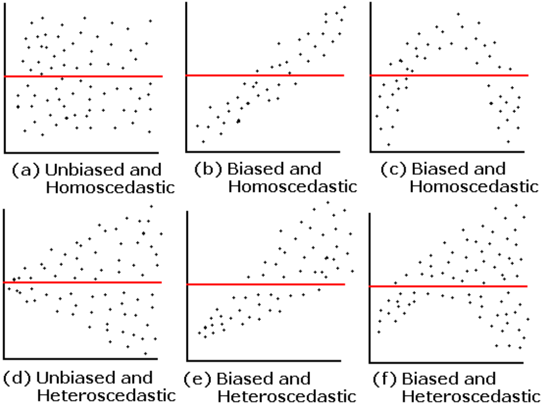

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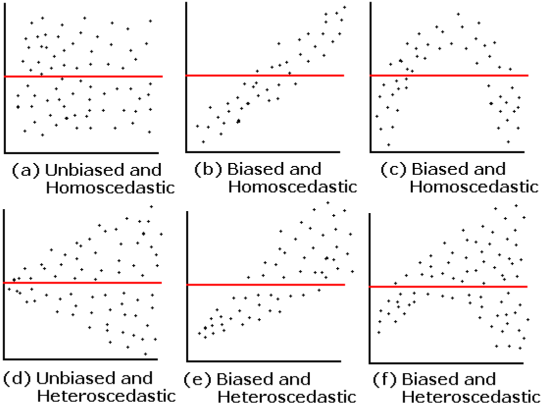

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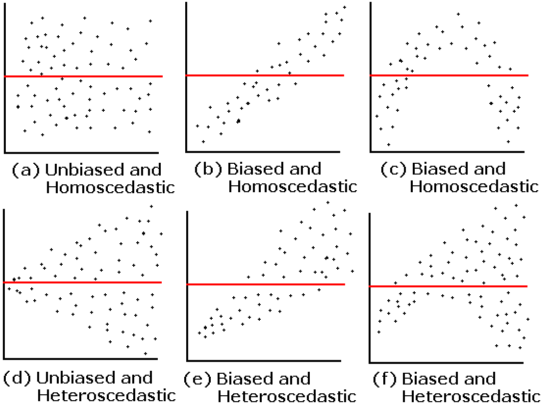

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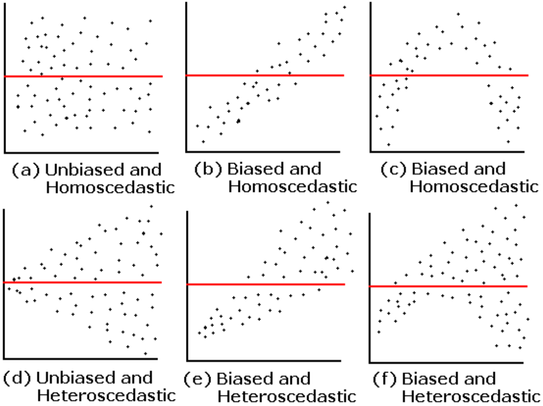

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  - Using scikit-learn: add the argument `sample_weight = someWeights`, e.g., `model.fit(Xtrain, yTrain, sample_weight=someWeights)`.
  - Using statsmodels: use the weighted version of least squares: `WLS(y, X, someWeights)` not `OLS(y, X)`

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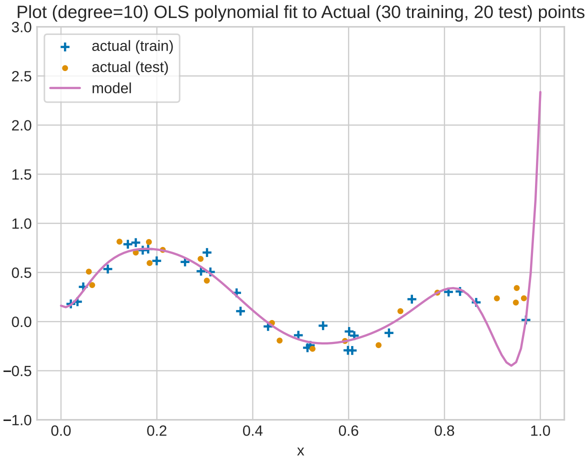

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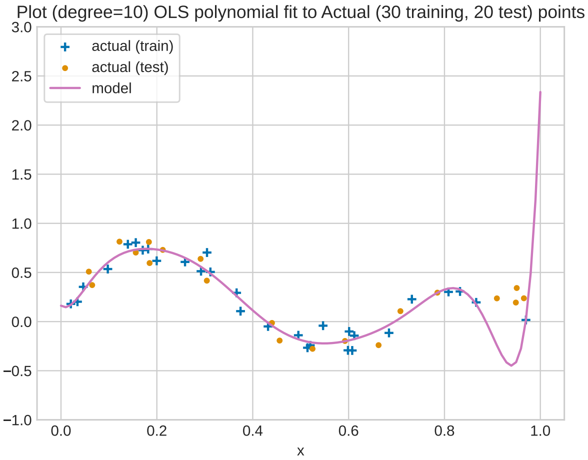

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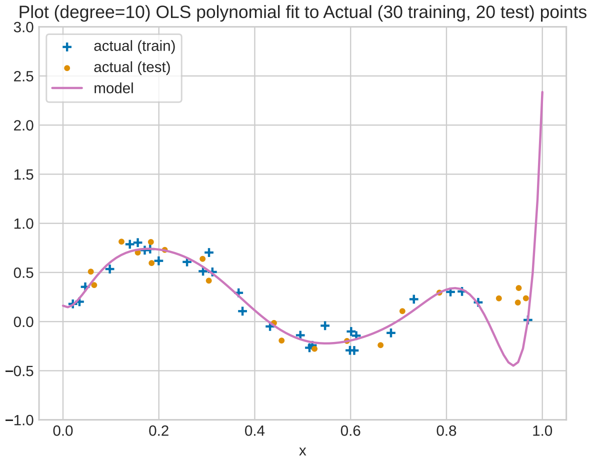

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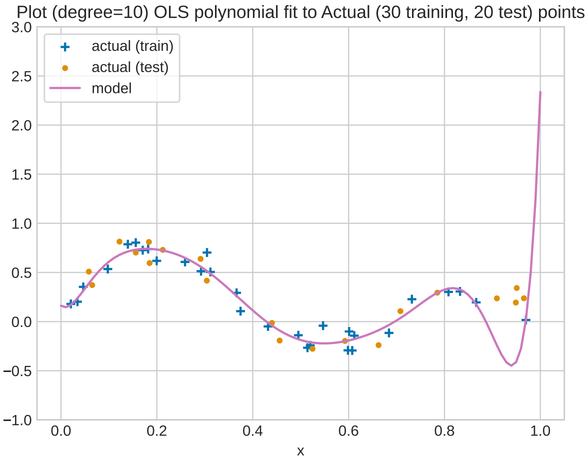

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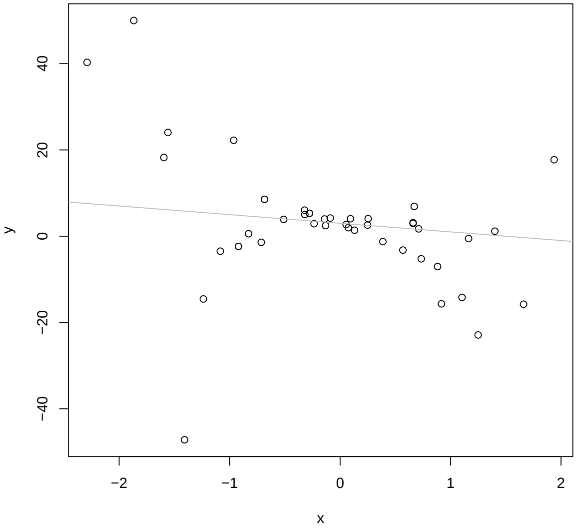
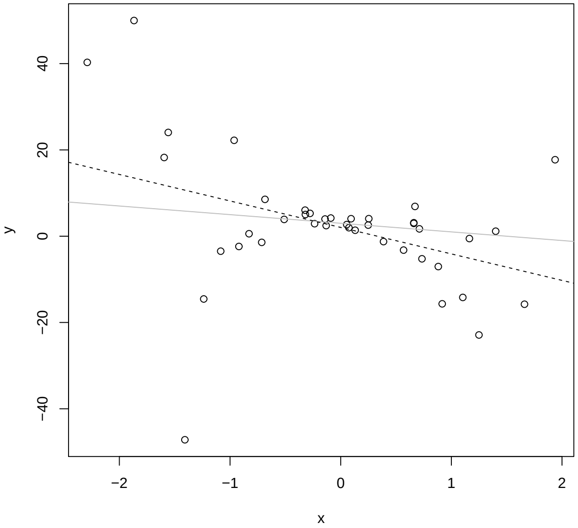
Case Study 1: Heteroscedasticity - Step 1



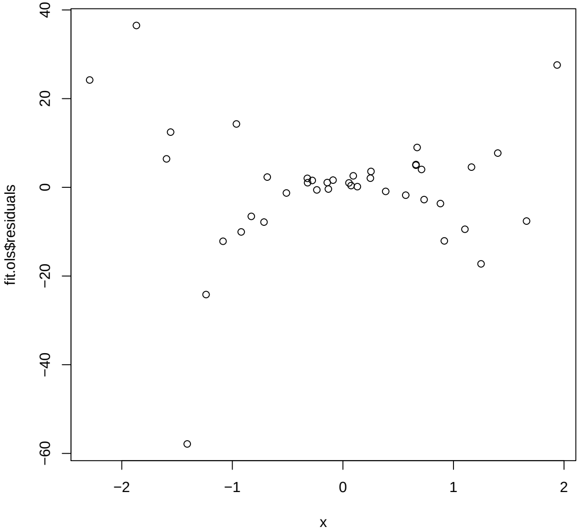
I generated 41 x, y points based on $y = 3 - 2x$, but with added errors that increase away from $x = 0$. The plot shows the line with $\beta = (3, -2)$ in grey.

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: $\beta_{OLS} \approx (2, -6)$, equivalent to $y = 2 - 6x$.

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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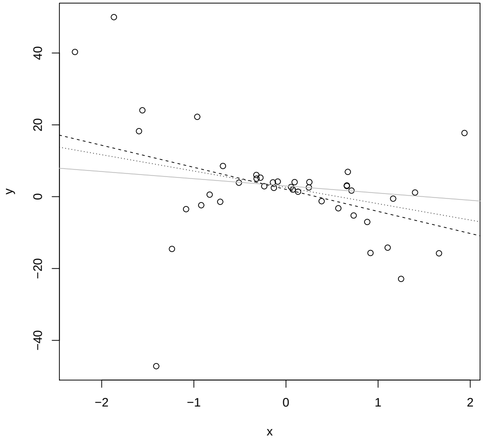

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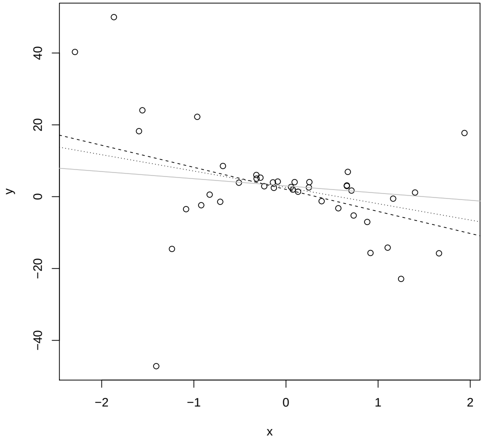

- By inspecting the previous residual plot I estimated a weighting function so that the residuals would be "more constant". When this was used to scale the residuals, the resulting Weighted Least Squares estimates were $\beta \approx (2.6, -4.5)$ (shown as a dotted line) and hence closer to the "true" $\beta = (3, -2)$.

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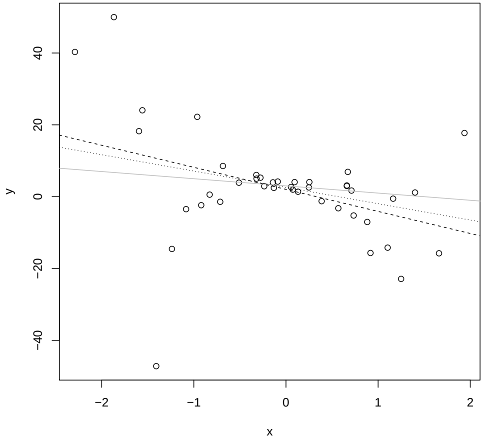

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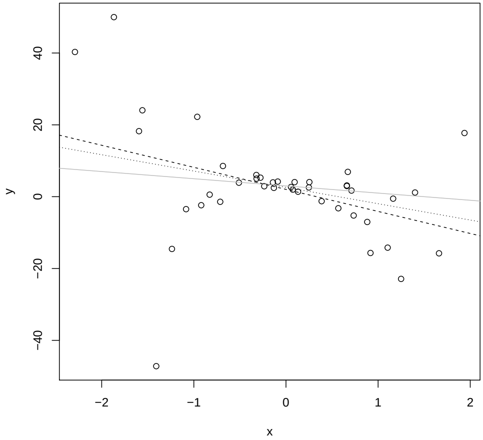

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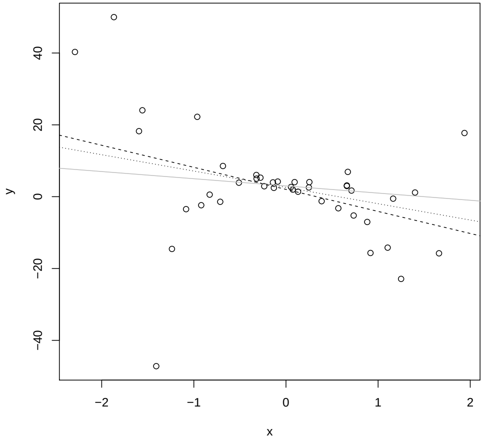

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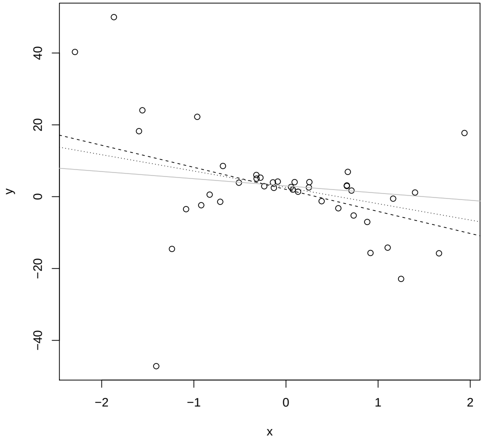

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- **Can you see a problem with finding the weights?**
- If the weights are computed from the errors, they depend on the fit, hence on the weights!!
- *Iteratively Reweighted Least Squares* has been proposed to optimise regression models.

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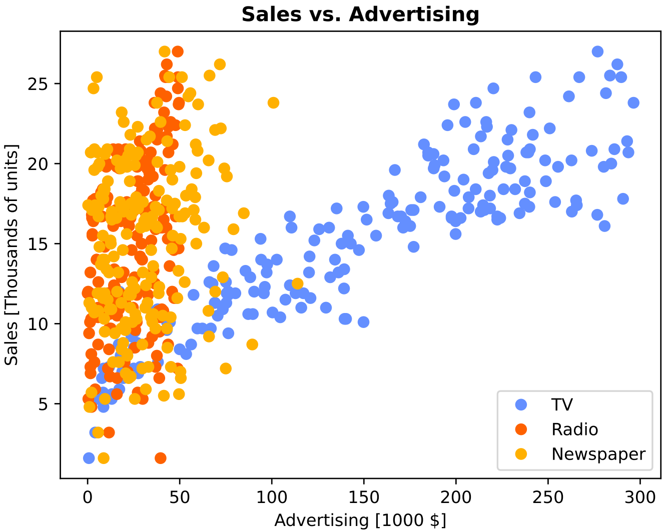
Case Study 3: Advertising: Data and Hypotheses

	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 how many thousands of widgets of a particular type were 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?

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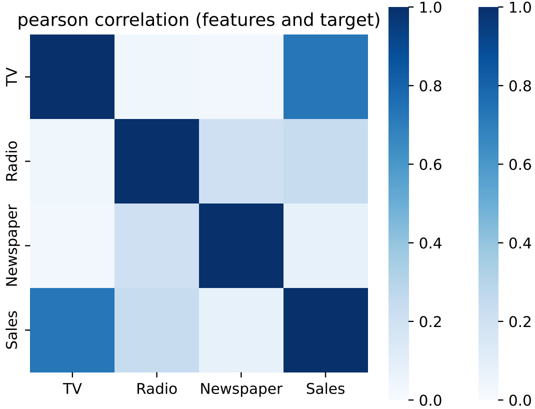

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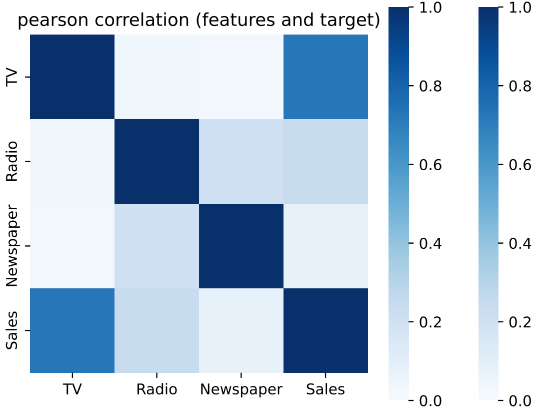

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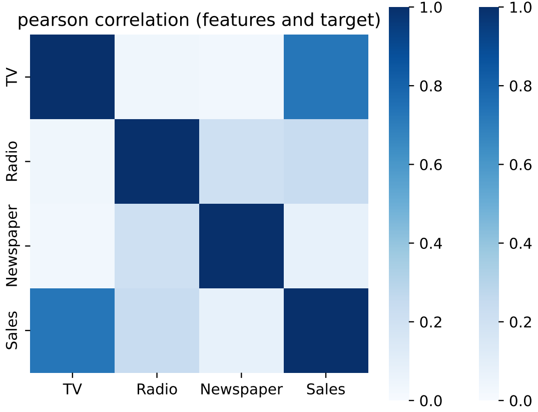

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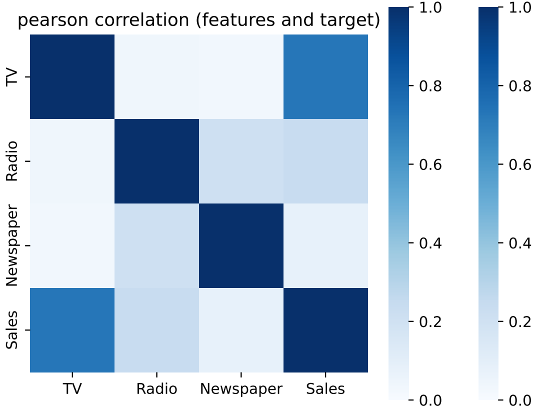

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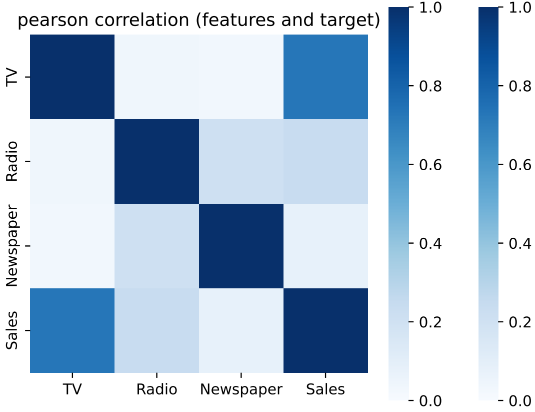

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  - TV $>$ Radio $>$ Newspaper, with moderate correlation between Radio and Newspaper.

Sidebar: specifying models

The statsmodels way

- The dataframe contains the observed variables

The sklearn way

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- statsmodels models are expressed like "Sales $\sim$ TV * Radio + poly(Newspaper,2)". This notation came from the applied statistics community.
- In words: "Sales depends on TV spending, Radio spending, the interaction between TV and Radio spending, Newspaper spending and Newspaper spending squared (5 features from 3 measured features)."
- statsmodels offers its own plotting (like seaborn but not as good). Its model summary is very convenient.
- sklearn exposes more of the details (e.g., choice of algorithm and configuration parameters).
- Both statsmodels and sklearn use the same libraries (scipy, numpy, etc.) underneath.

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Example 2 (Forward Selection for Advertising Data)

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.
2. Choose the best (lowest loss) single-term model ("Sales $\sim$ TV" in this case), with loss MSE(TV).
3. Fit "Sales $\sim$ TV + Newspaper" and "Sales $\sim$ TV + Radio" and choose the lowest loss score, which is "Sales $\sim$ TV + Radio" with loss being MSE(TV + Radio), which is significantly better.
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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Example 2 (Forward Selection for Advertising Data)

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.
2. Choose the best (lowest loss) single-term model ("Sales $\sim$ TV" in this case), with loss MSE(TV).
3. Fit "Sales $\sim$ TV + Newspaper" and "Sales $\sim$ TV + Radio" and choose the lowest loss score, which is "Sales $\sim$ TV + Radio" with loss being MSE(TV + Radio), which is significantly better.
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.).

So our preferred model is "Sales $\sim$ TV + Radio".

Forward selection in action, with and without the interaction term

Main features only

	feature	test_neg_mean_squared_error	test_r2
0	TV	(-7.324310374422007, -3.936981032219174)	(0.7603440777107349, 0.8390841989031752)
1	Radio	(-4.718440611471559, -1.8510139478354652)	(0.8456097326980662, 0.9322678692463671)
2	Newspaper	(-4.72039259225367, -1.8510521207093062)	(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.

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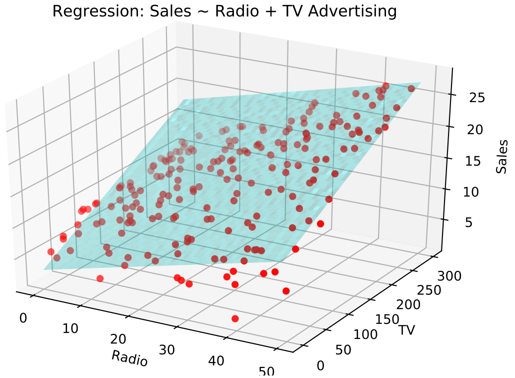
Main features with TV:Radio interaction term

	feature	test_neg_mean_squared_error	test_r2
0	TV	(-7.324310374422007, -3.936981032219174)	(0.7603440777107349, 0.8390841989031752)
1	TV:Radio	(-3.695048288640374, -1.8479935191656154)	(0.8790957564264388, 0.9377953274242408)
2	Radio	(-3.929784758825862, -1.751389612982793)	(0.8714150353235091, 0.9410470781968057)
3	Newspaper	(-3.9387465036567235, -1.7715653928145287)	(0.8711218015427205, 0.9403679482294234)

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 every term is highly significant and the model "explains" 90% of the variance of the data, which is high for an observational study. **Why? Can we do better?**

Case Study 3: Advertising: Interactions; Interpretation

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- $\beta_0 = 6.75$, $\beta_{\text{TV}} = 0.019$, $\beta_{\text{Radio}} = 0.029$ and $\beta_{\text{TV:Radio}} = 0.001$, indicating that there is a favourable relationship between TV and Radio advertising ($\beta_{\text{TV:Radio}} > 0$), and that additional spending on Radio results in more Sales than the same spending on TV ($\beta_{\text{Radio}} > \beta_{\text{TV}}$).

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