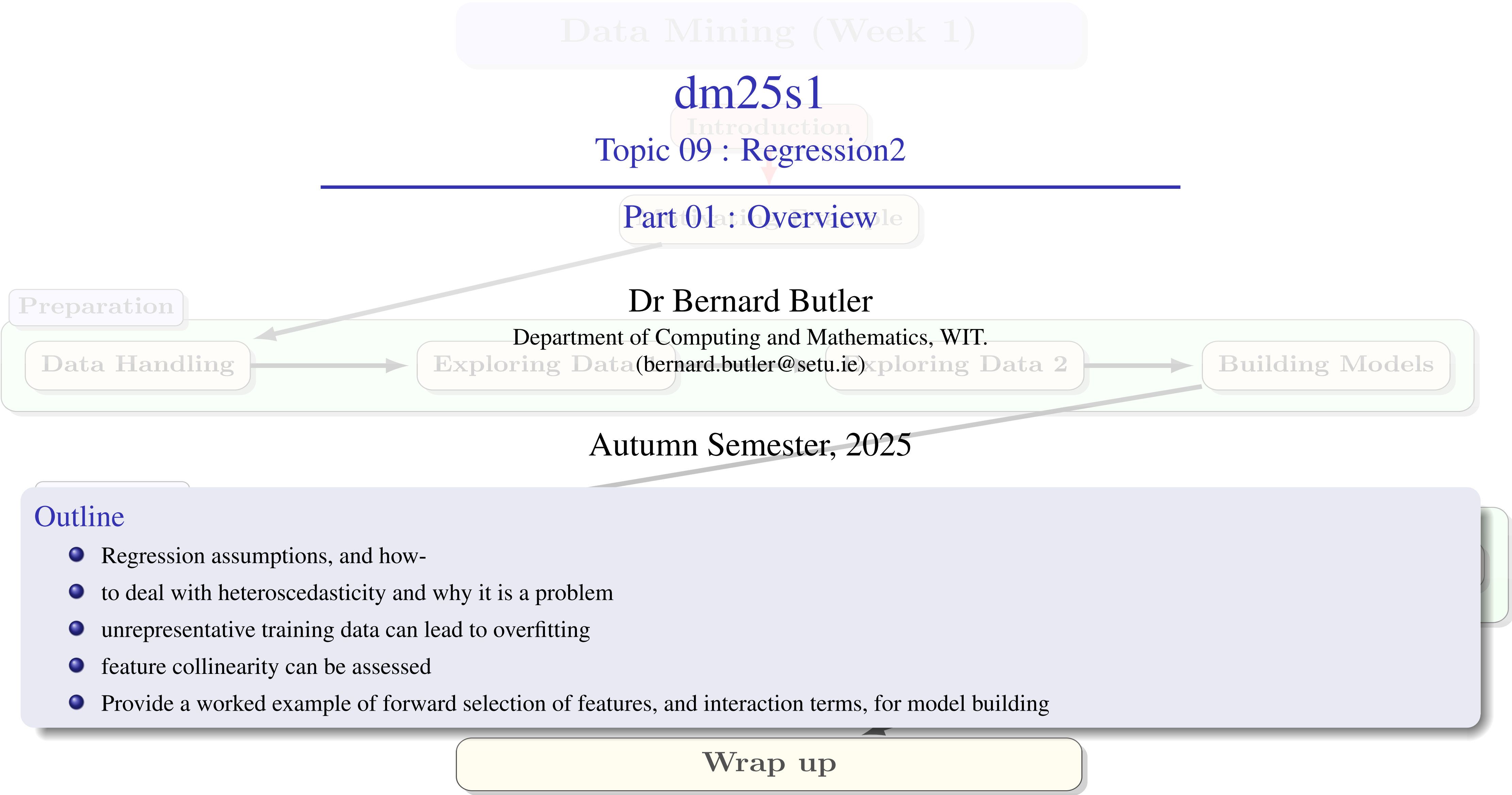

dm25s1

Topic 09 : Regression2

Part 01 : Overview

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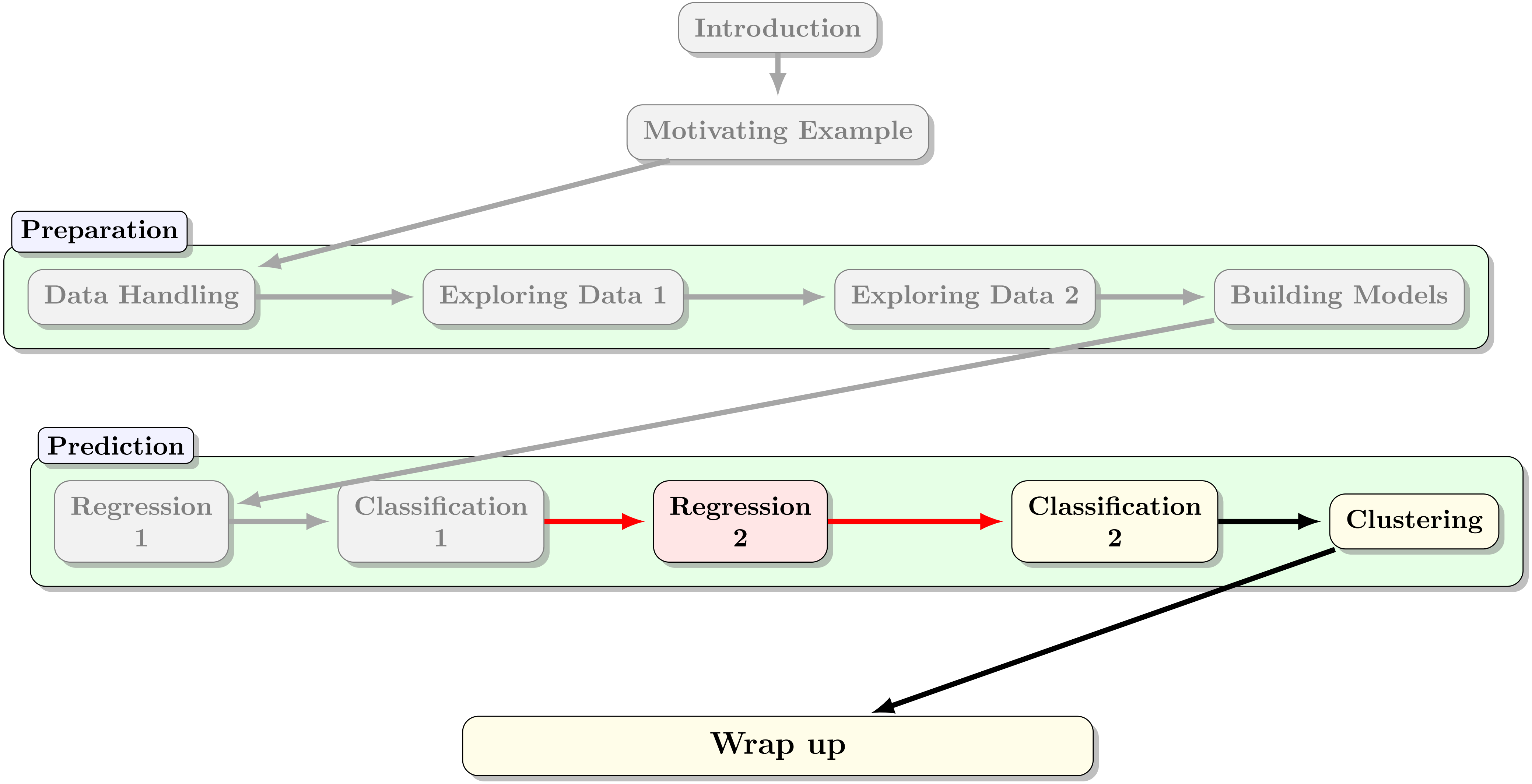
Outline

- 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)



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Motivating Example

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Data Handling

Exploring Data 1

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Building Models

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Classification 2

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This Week’s Aim

This week’s aim is to continue the introduction to linear regression, focusing more on how to deal with problems with more challenging datasets.

- Examine some extensions to the simplest case of linear regression.
- We introduce two new concepts: dimensionality reduction and regularisation
- 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.

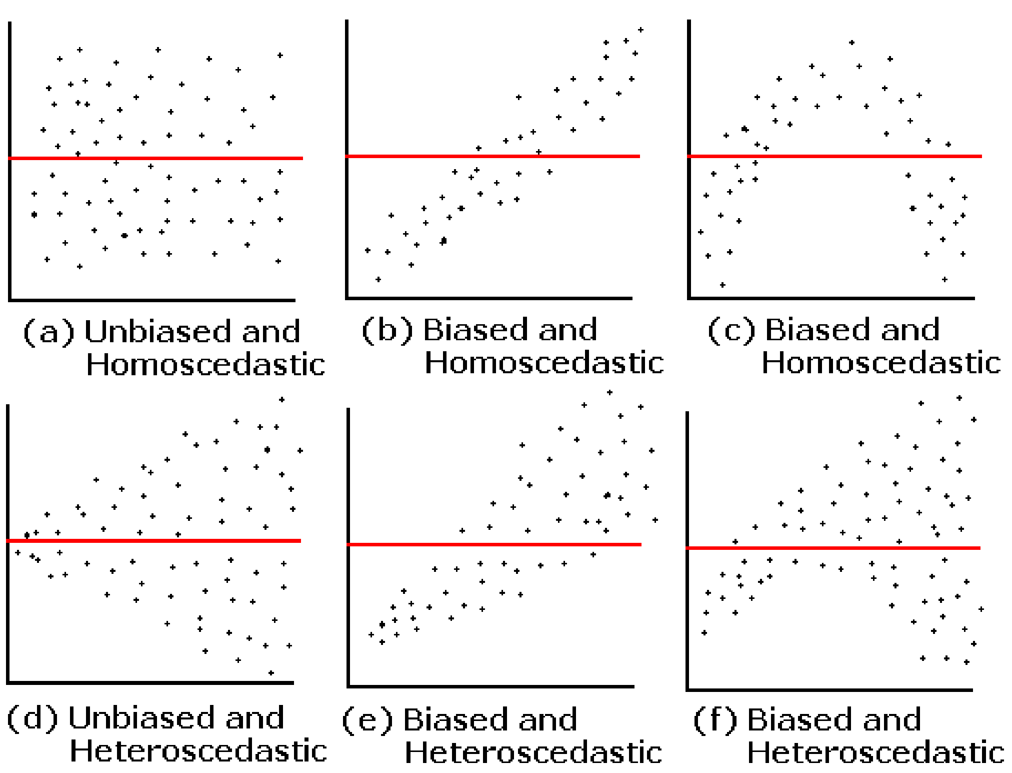
Assumptions required for the linear model to be meaningful

Definition 1 (Linear Regression Assumptions)

1. The underlying relationship between the predictors and the response is linear in the regression parameters $\boldsymbol{\beta}$.
2. The residual errors $\boldsymbol{\epsilon}$ are drawn from a (multivariate) Normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\sigma}^2)$ where $\boldsymbol{\mu} = \mathbf{0}$.
3. The predictors are not pairwise collinear, i.e., each pair of predictors β_{j_1} and β_{j_2} (associated with columns $X(:, j_1)$ and $X(:, j_2)$) have low correlation (equivalently, the inner product of $X(:, j_1)$ and $X(:, j_2)$ is far from zero).
4. There is no auto-correlation in $\boldsymbol{y}$: each observation is independent of its "neighbours".
5. The errors are *homoscedastic* (i.e., Var($\boldsymbol{\epsilon}$) is constant over the range of $\boldsymbol{x}$ or $\boldsymbol{y}$).

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

Bias and variance in regression



(a) Unbiased and Homoscedastic

(b) Biased and Homoscedastic

(c) Biased and Homoscedastic

(d) Unbiased and Heteroscedastic

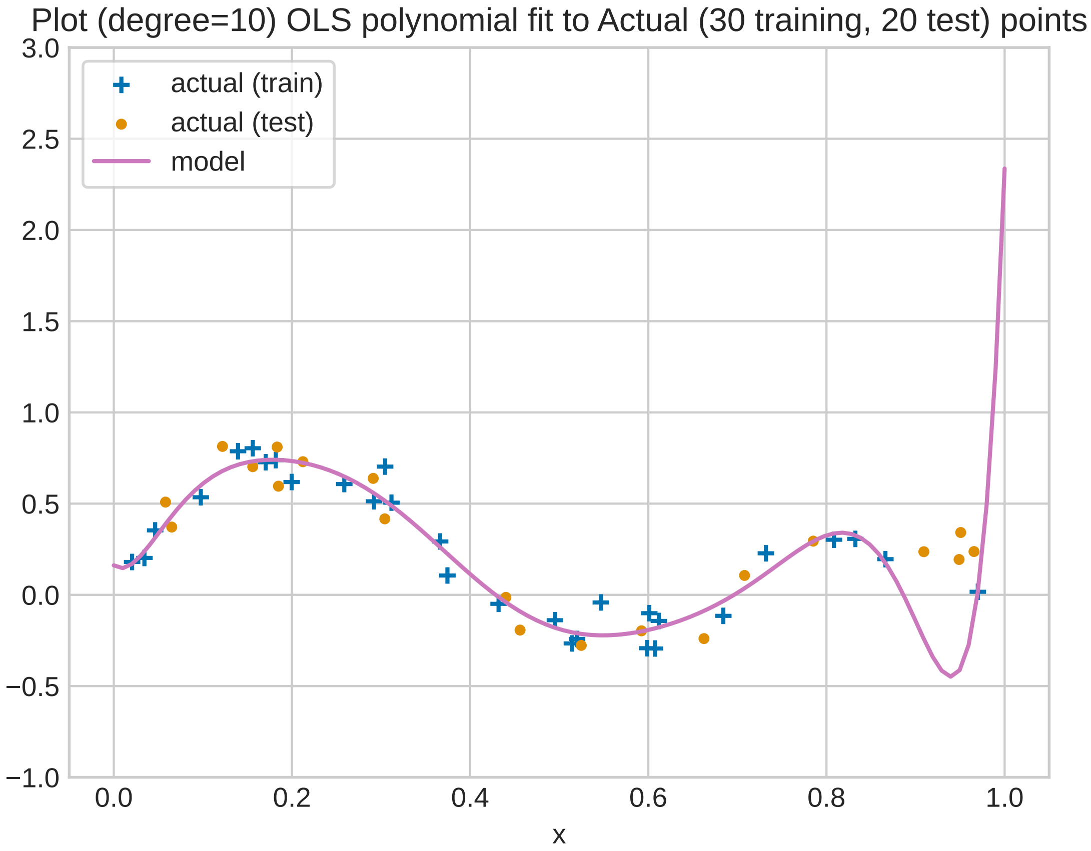
(e) Biased and Heteroscedastic

(f) Biased and Heteroscedastic

Source: `https://bit.ly/3vC9zK7`

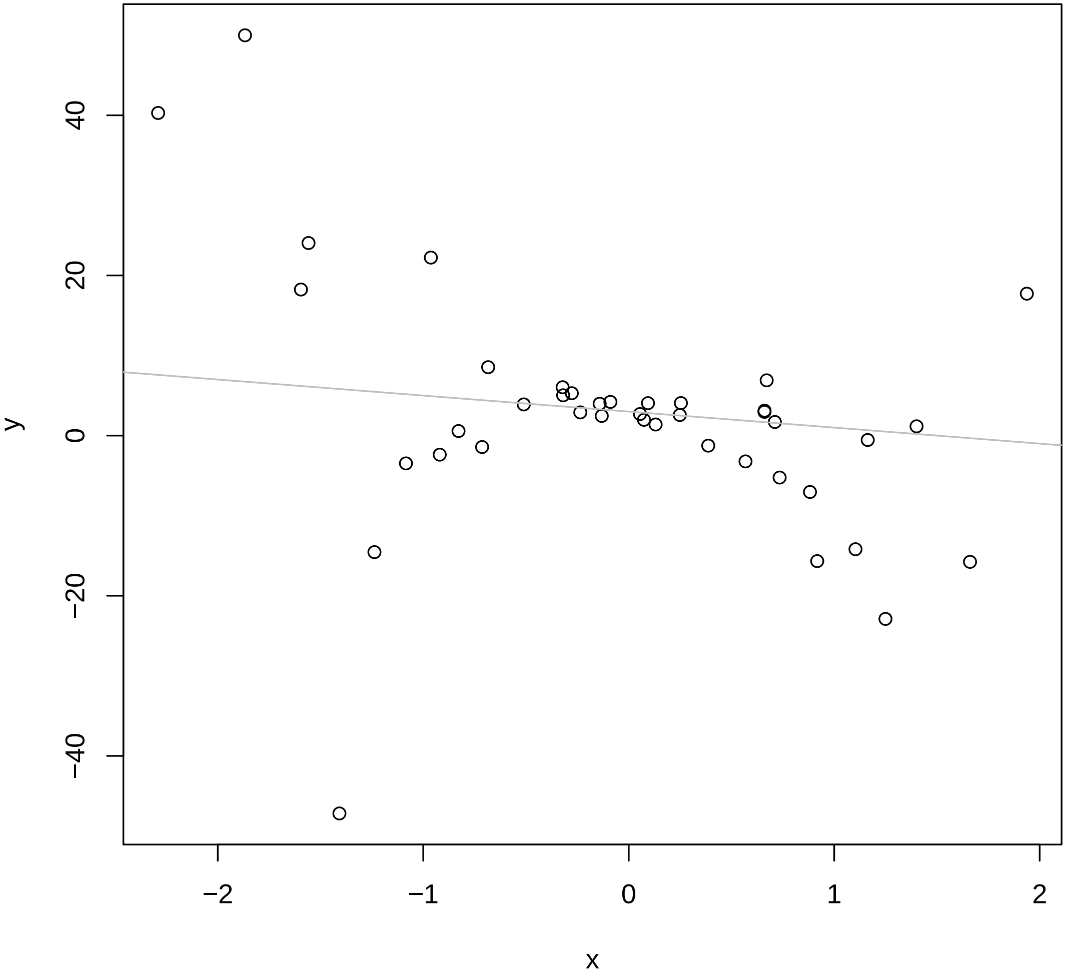
- Bias is caused by underfitting.
- Fix bias by adding suitable predictors.
- Overfitting causes large variance.
- If variance changes over the range, some errors get undue attention.
- Fix this by weighting the errors so the weighted errors satisfy $w_i e_i \approx w_j e_j, \forall i, j$.
- In practice, $w_i \approx \frac{1}{\widehat{\mathrm{Var}}(e_i)}$.
  - 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???



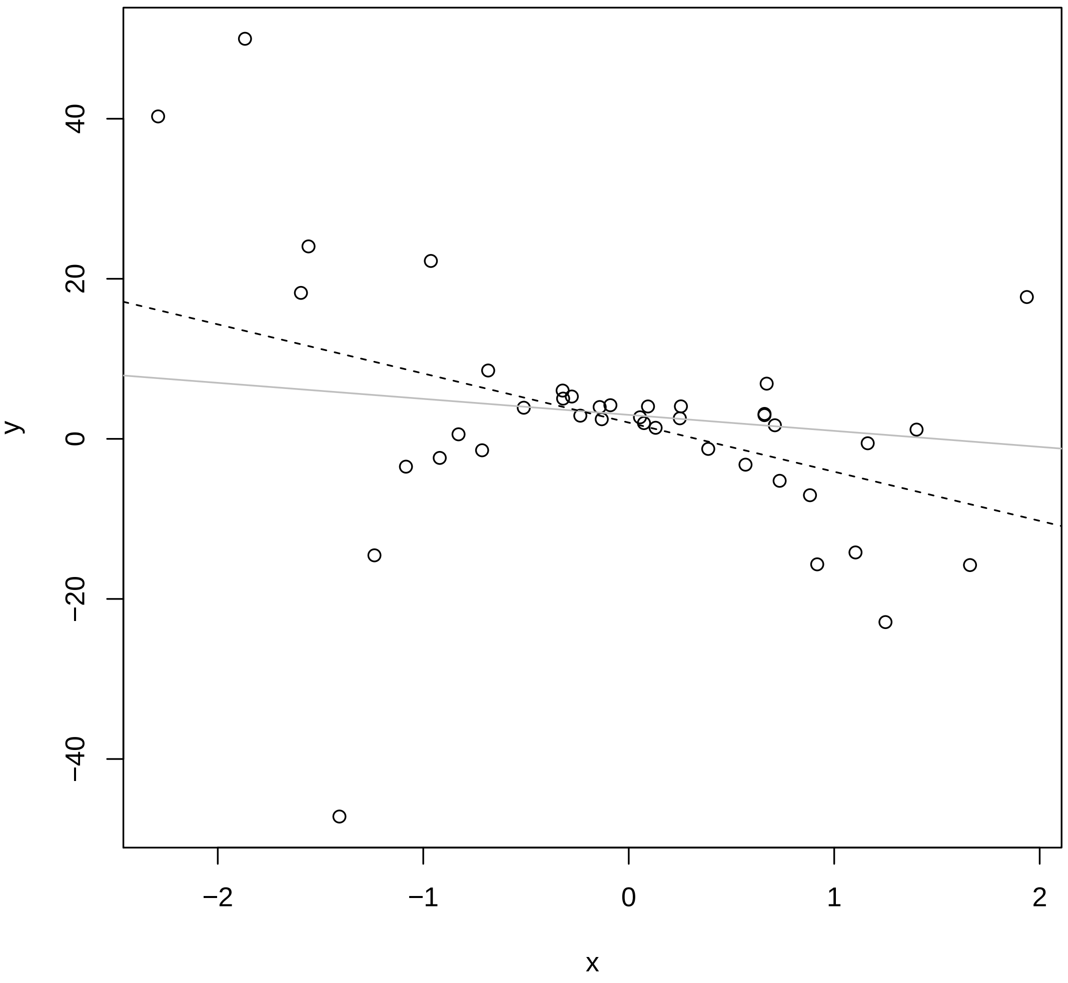
1. Data is quite noisy
2. Training data has gaps near the edges
3. Model may be overfitting

Case Study 1: Heteroscedasticity - Step 1



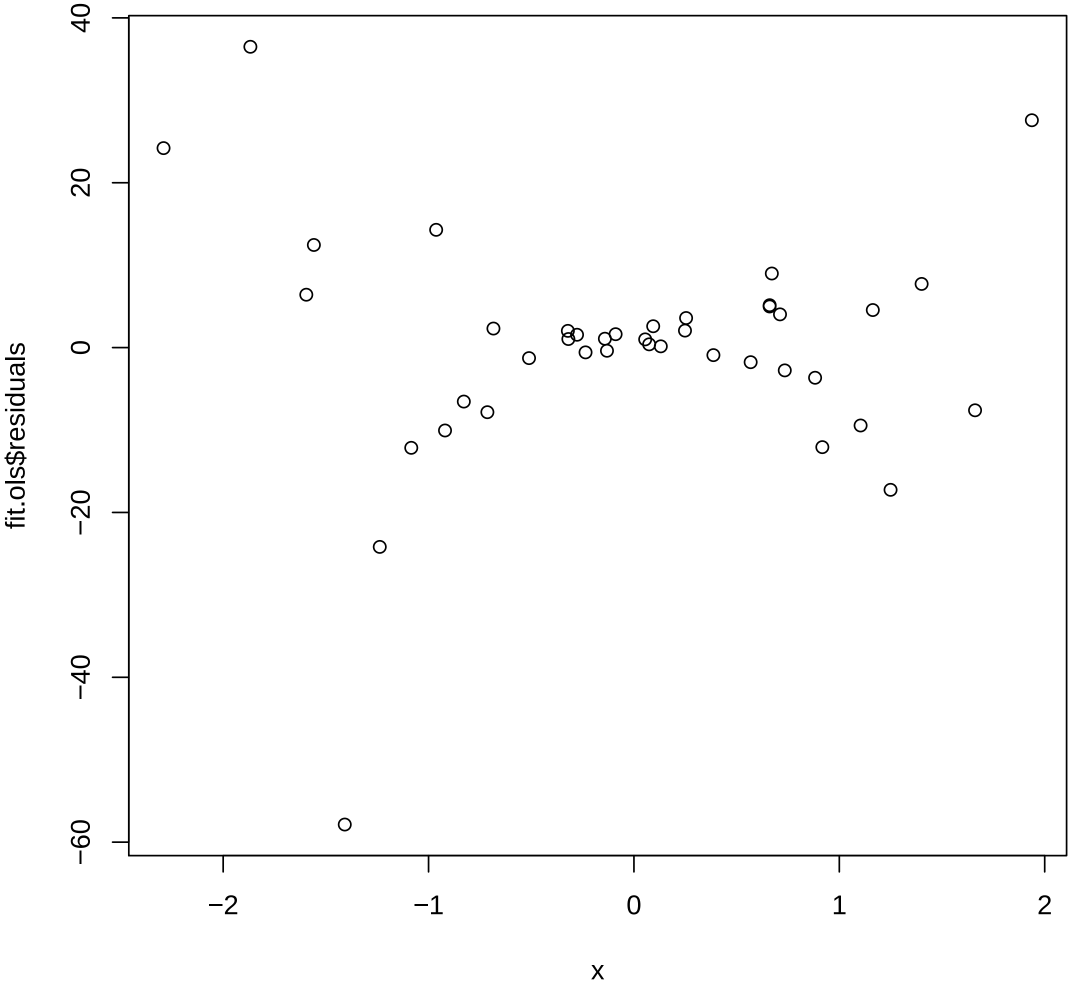
I generated 41 x, y points based on $y = 3 - 2x$, but with added errors that increase away from $x = 0$. The plot shows the line with $\boldsymbol{\beta} = (3, -2)$ in grey.

Case Study 1: Heteroscedasticity - Step 2



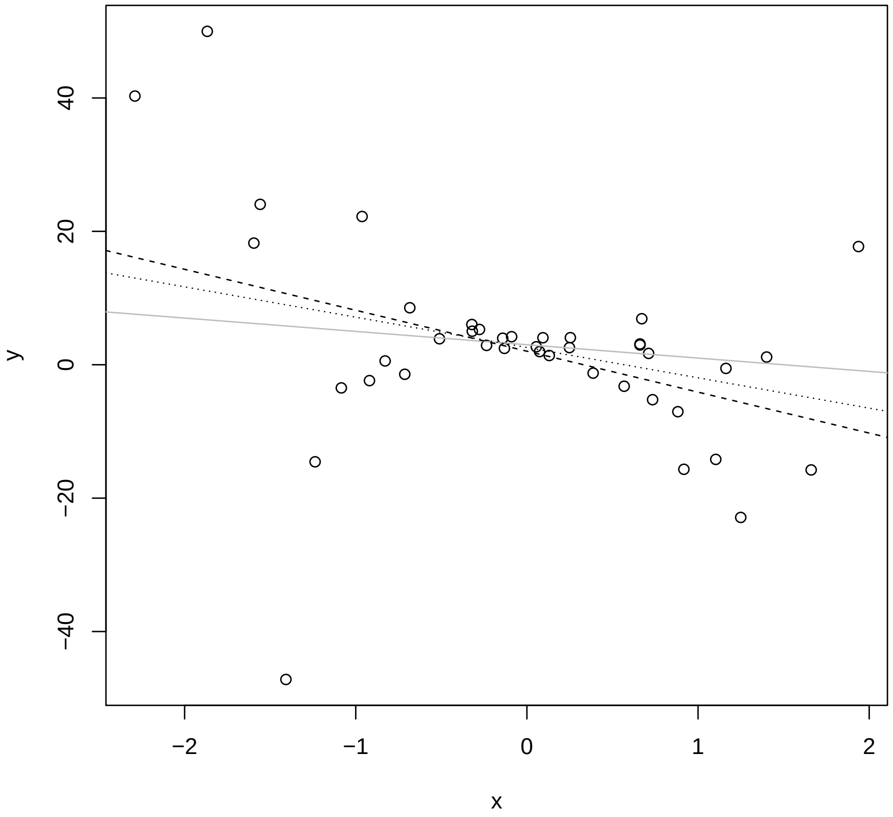
In this plot I added the OLS fit as a dashed line. Note that the parameters of the fit are quite different: $\beta_{OLS} \approx (2, -6)$, equivalent to $y = 2 - 6x$.

Case Study 1: Heteroscedasticity - Step 3



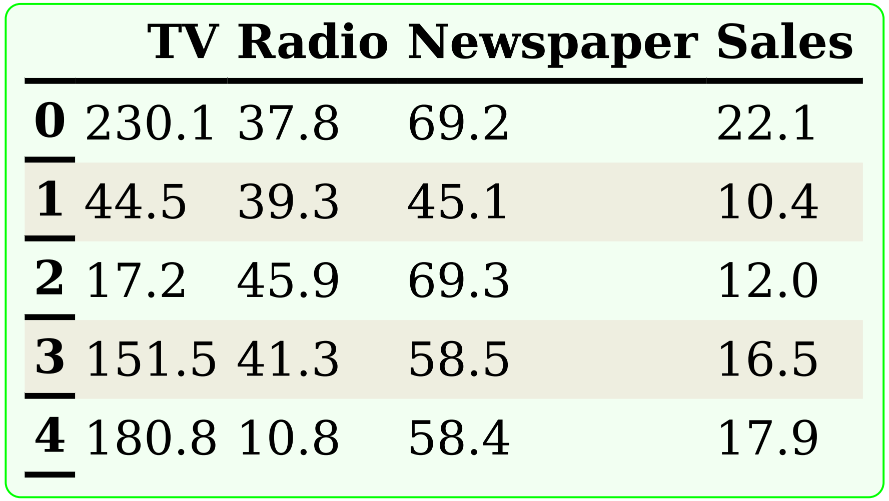
This plot shows how the OLS residuals ϵ_{OLS} increase rapidly away from 0, as expected (since this was how the data was generated).

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 $\boldsymbol{\beta} \approx (2.6, -4.5)$ (shown as a dotted line) and hence closer to the “true” $\beta = (3, -2)$.
- So we were only partially successful at stripping away the noise and recovering the original line.
- **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.

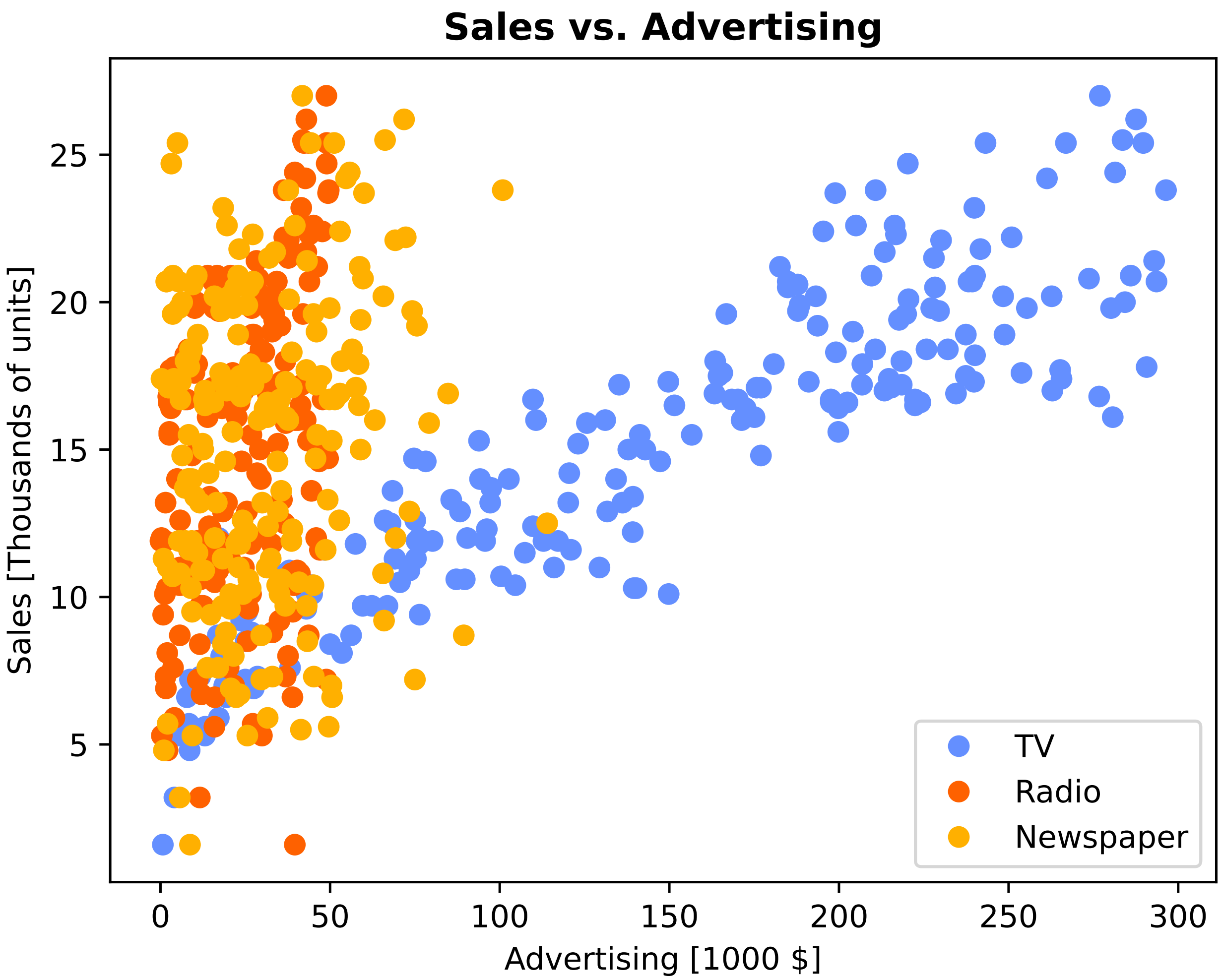
Case Study 3: Advertising: Data and Hypotheses



	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

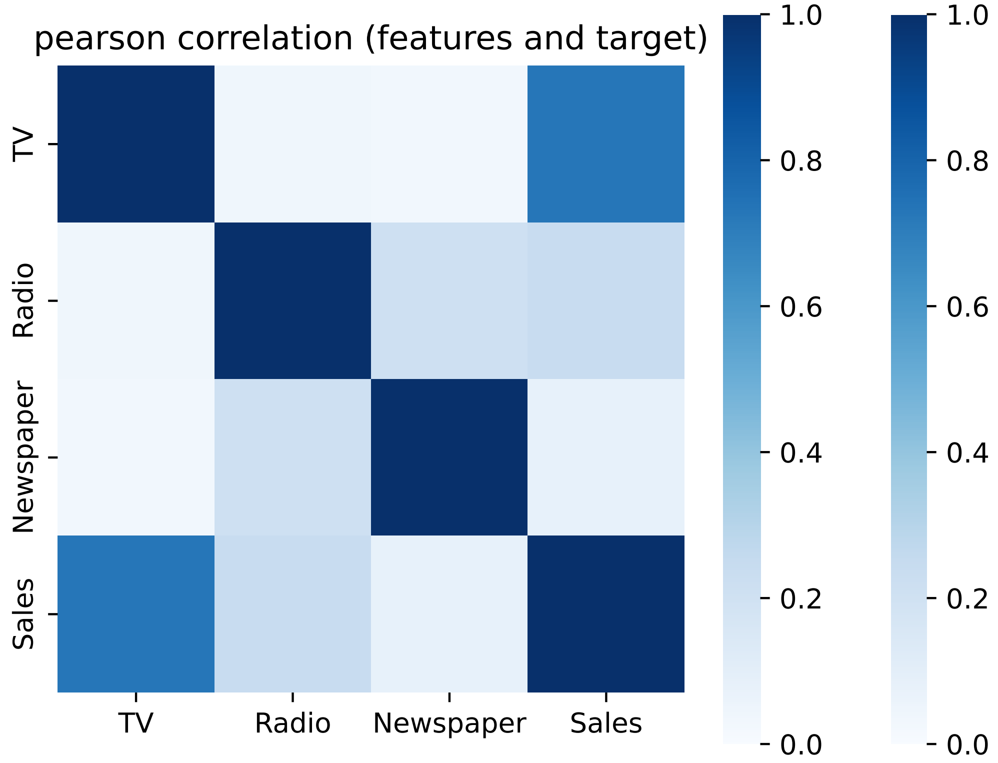
- In this data set, the sales figure captures how many thousands of widgets of a particular type were sold in a year.
- Newspaper, Radio and TV represent the annual spend per widget type on the associated advertising channel.
- The hypothesis is that spend on advertising is a good predictor of sales 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?

Case Study 3: Advertising: Collinearity?



- Correlation matrix can indicate which features should participate in the model as predictors.
- A good predictor should have a high correlation with the target (Sales in this case) and should have low correlation with other candidate predictors.
- **What are expected to be good predictors for this data?**
  - Sales (the target) is placed in the last row (or column).
  - TV $>$ Radio $>$ Newspaper, with moderate correlation between Radio and Newspaper.

Sidebar: specifying models

The statsmodels way

- The dataframe contains the observed variables
- The model is specified separately
- Easier to change the model when experimenting

The sklearn way

- The dataframe contains the (computed) features
- The model is defined implicitly
- Standard interface across all sklearn

- 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.

Case Study 3: Advertising: Model Building (“stats” way)

- 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)

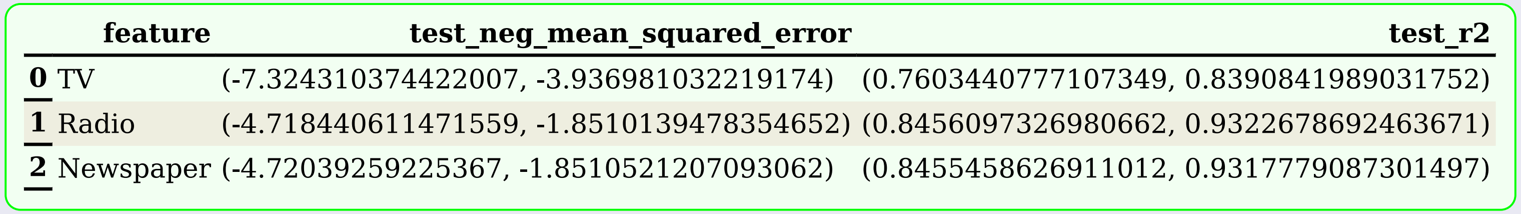
Define: model score: mean-square-error on the test set for a given model.

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

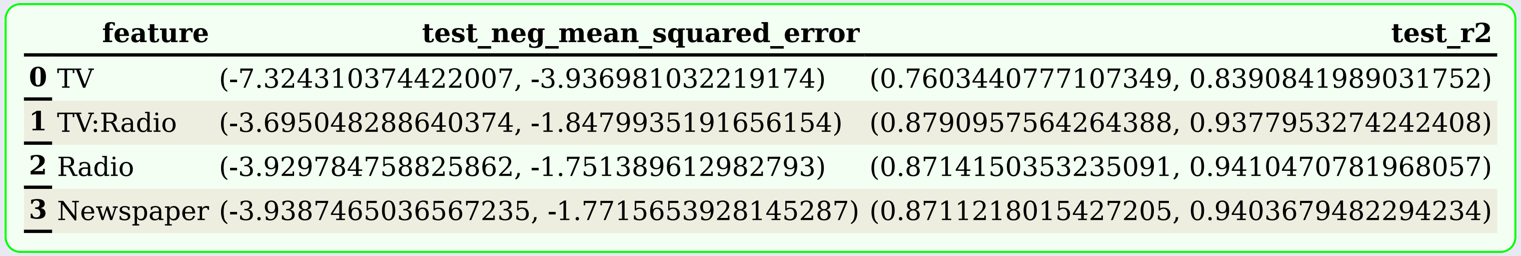
Main features only



	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) ≈ 5.5; MSE(TV + Radio) ≈ 3.5; MSE(TV + Radio + Newspaper) ≈ 3.5 ≈ MSE(TV + Radio). Adding Newspaper does not reduce MSE.

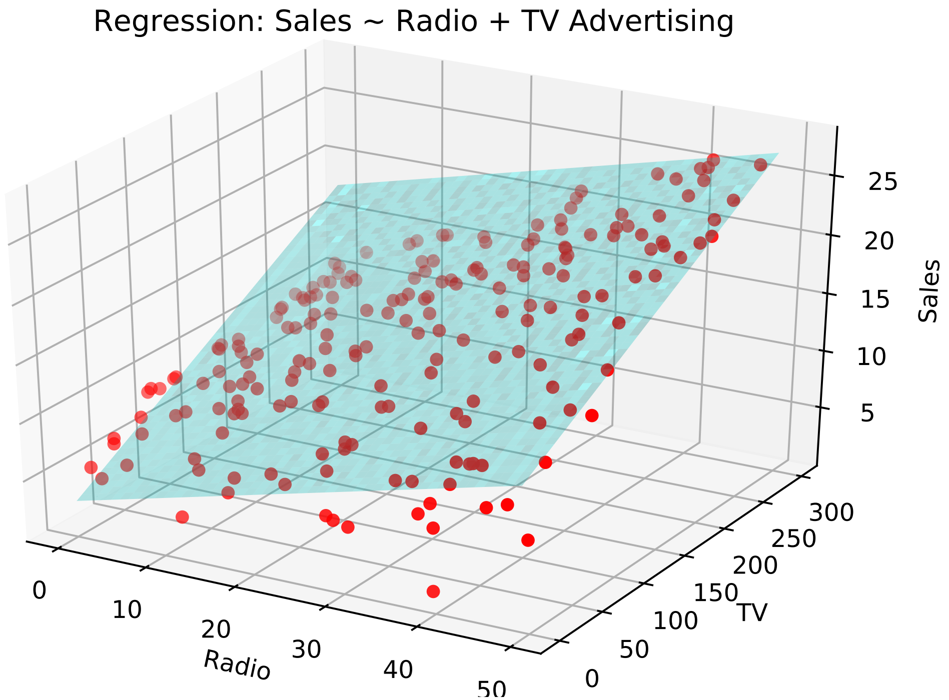
Main features with TV:Radio interaction term



	feature	test_neg_mean_squared_error	test_r2
0	TV	(-7.324310374422007, -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) ≈ 5.5; MSE(TV + TV:Radio) ≈ 2.8; MSE(TV + TV:Radio + Radio) ≈ 2.8 ≈ 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

- Trying powers greater than 1 of the Radio and TV features did not offer much more.
- However, by adding the TV,Radio interaction so that the model became "Sales $\sim$ TV + TV:Radio" or equivalently "Sales $\sim$ TV * Radio - Radio", the loss decreased significantly, indicating the interaction term is valuable, even more so than the Radio feature.
- All β terms have $t-$statistic significance of approximately 0.001 which is extremely significant.
- $\beta_0 = 6.75$, $\beta_{\text{TV}} = 0.019$, $\beta_{\text{Radio}} = 0.029$ 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 ($\beta_{\text{Radio}} > \beta_{\text{TV}}$).
- Spending on Newspaper advertising should be discontinued as its contribution to Sales is insignificant (indistinguishable from random noise).