dm24s1

Topic 07 : Regression1

Part 01 : Regression - Overview

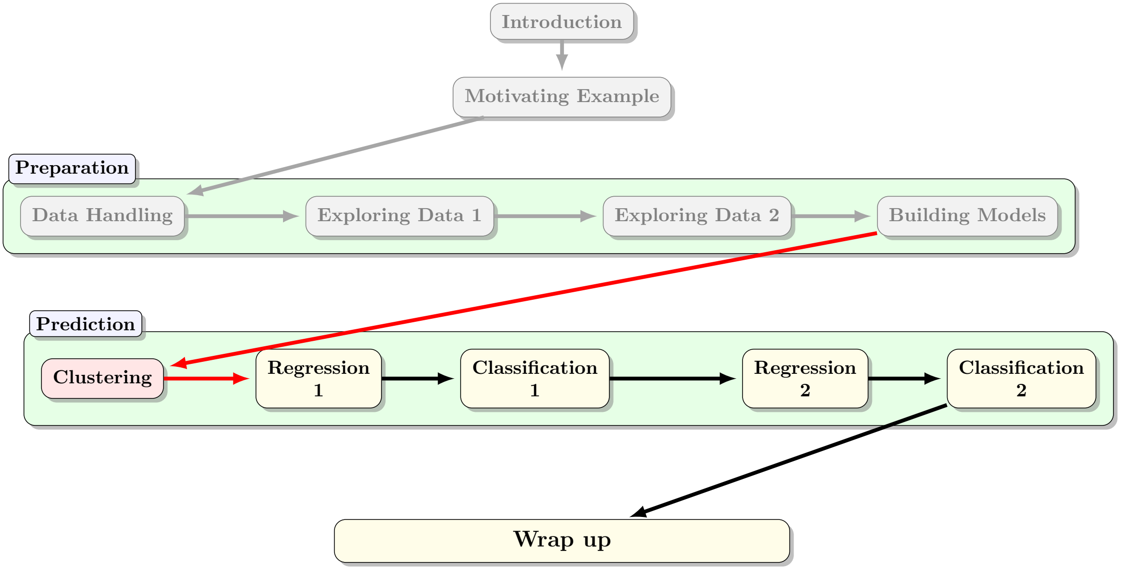
Dr Bernard Butler
Department of Computing and Mathematics, WIT.
(bernard.butler@setu.ie)

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 Diamond sales

Data Mining (Week 7)



Regression - 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.

Simple Linear Regression: Background

- Linear regression was discovered by Gauss and others around 1800. The “name” came later!
- With small data sets, calculations can be done by hand, but they are tedious and error-prone.
- The goal is simple: Given a training set of (x, y) data where y is assumed to have a linear relationship with x
  - Find the line that is the “best fit” to that data
  - Use the specification of that line to *predict* y for the test x values
- Note that the “linear relationship” of y upon x is just one of the underlying assumptions
- In practice, the data does not have an exact linear relationship, but it should be “close enough”—but what does that mean?

Review: Linear combinations (scalar product)

Definition 1 (Linear Combination of two vectors)

Given two vectors $\mathbf{a}$ and $\mathbf{b}$, each with n elements, the *linear combination* (c) of $\mathbf{a}$ and $\mathbf{b}$ is

$$c \equiv a_1 b_1 + a_2 b_2 + \ldots + a_n b_n = \sum_{i=1}^{n} a_i b_i \equiv |\mathbf{a}||\mathbf{b}| \cos(\mathbf{a}, \mathbf{b})$$

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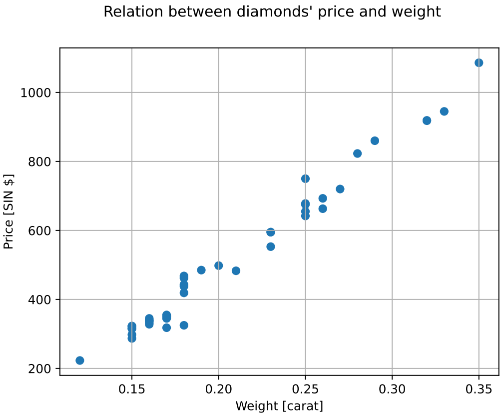
- Linear combinations are used for prediction from linear (regression) models.

Motivating example: Diamond data



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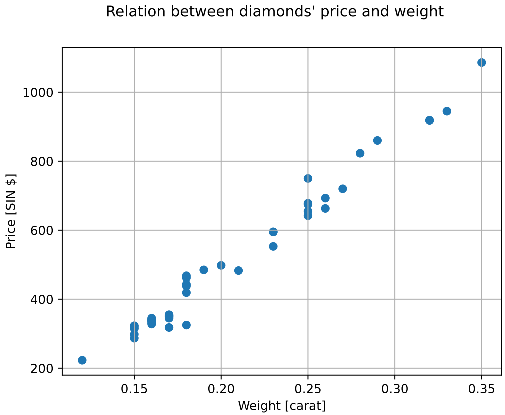

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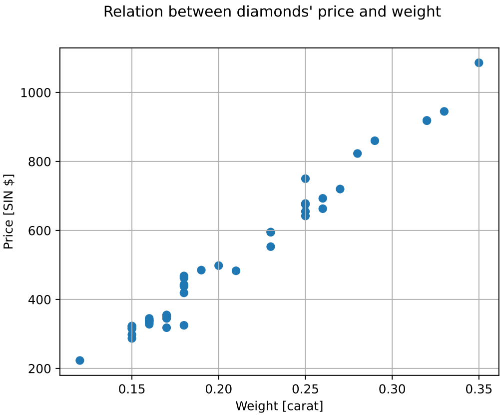
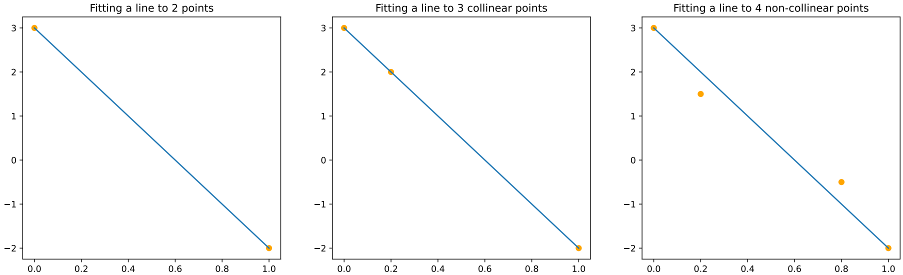


Diamond Prices by Weight

- Given the data on the left, can we use it to predict the price of a diamond that weighs 0.22 carat?
- NB - we have not seen a diamond with that weight before in the data
- Can you think of at least 4 other factors that might affect the price?

Simple Linear Regression: Geometric Intuition

- Given data $\{x_i, y_i\}$ where $i = 2, 3, \ldots, n$ and β_0, β_1 as the (unknown, but to be determined) *intercept* and *slope* of the regression line for this data.



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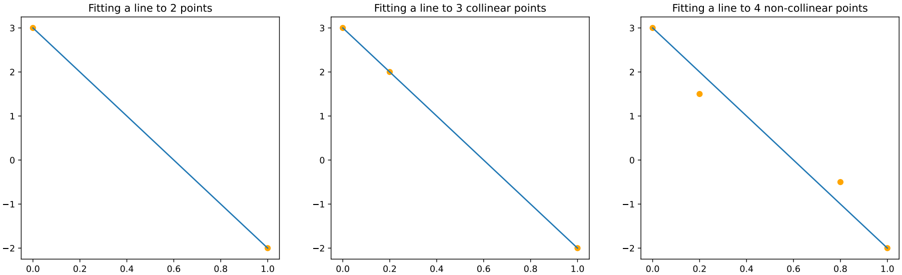

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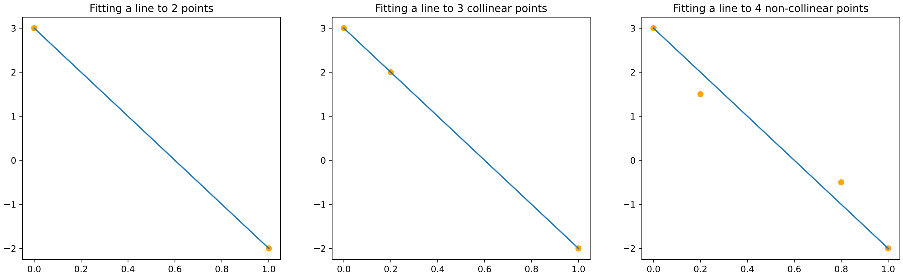

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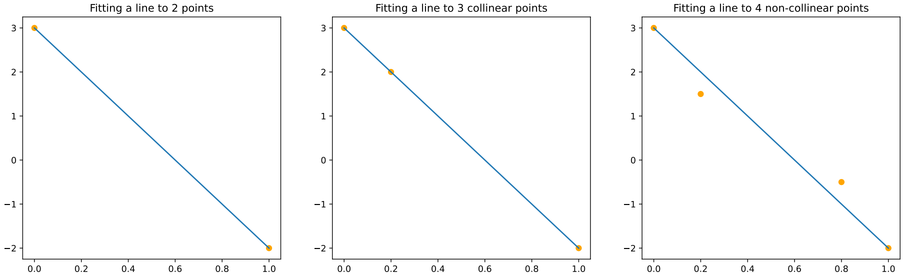

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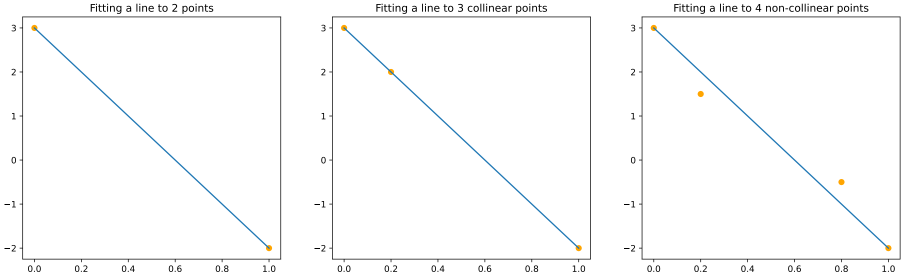
- Otherwise the problem is overdetermined so need a more general formulation to solve for β_0, β_1.



Simple Linear Regression: Formulation

Definition 2 (Matrix formulation)

- General equation is $y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \hat{y}_i + \epsilon_i$ (data = model + error), where $\hat{y}$ is the predicted y for these values of β_0, β_1.

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- Our geometric intuition is that the errors should be "balanced": no benefit to changing intercept (sliding up or down) or slope (tilting the line).

Simple Linear Regression: Normal Equations

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Note that everything on the right is a set of operations on the data.

For more info, and an alternative construction of the Normal equations, see `https://goo.gl/TbLru3`.

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When implemented in software, the Normal equations are not used directly: faster and more numerically accurate algorithms are used instead, but the results are equivalent in exact arithmetic (remember: digital computers perform finite-precision arithmetic and so cannot be exact).

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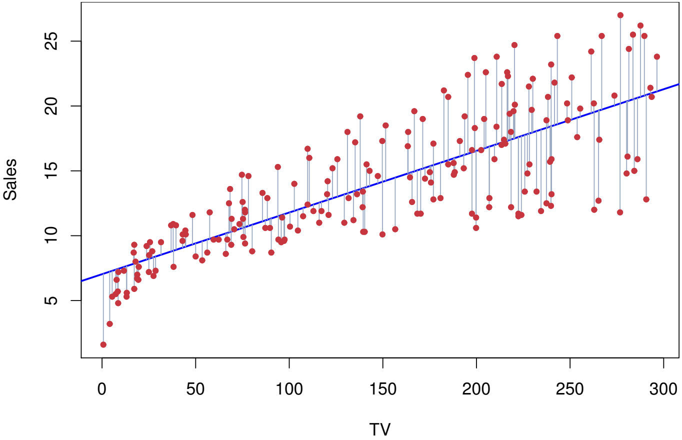
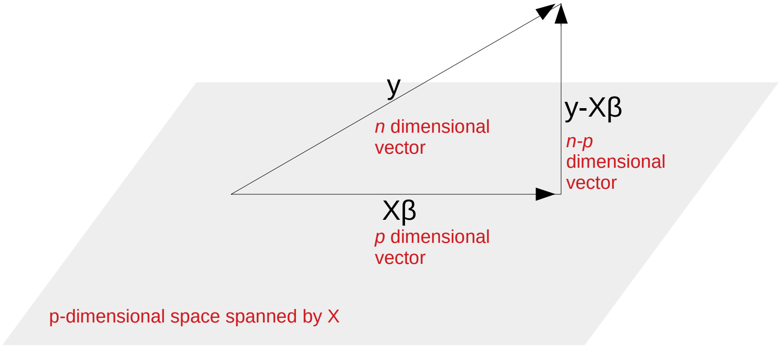
Remember: after *learning* the β parameters using the training data $\{\mathbf{x}_i, y_i\}$, with the model encoded in the feature matrix X, it is then possible to predict $\hat{y}_k$ for "new" (test) $\mathbf{x}_k$ values, using separate *prediction* function calls.

SLR: Residual Plot for the model



Source: ISLR, Fig 3.1: Advertising data with the model "Sales $\sim$ TV".
Note the vertical distance between the red dots (data points) $\mathbf{y}$ and the corresponding $\hat{\mathbf{y}}$ on the regression line, which is termed the *error* ϵ.

Geometrical interpretation of regression: n rows, p features, $n > p$



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- Grey plane represents all the colours mixable from those colours.
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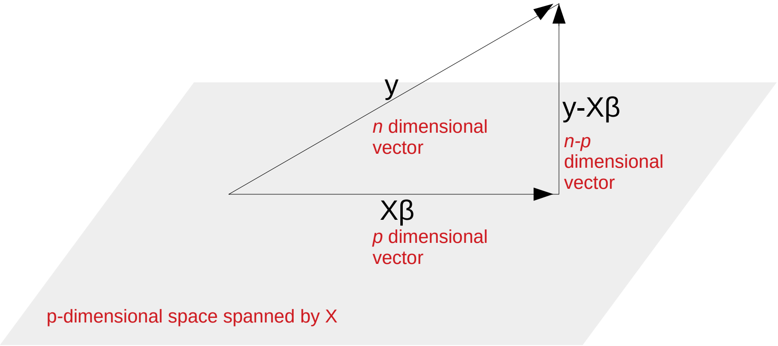

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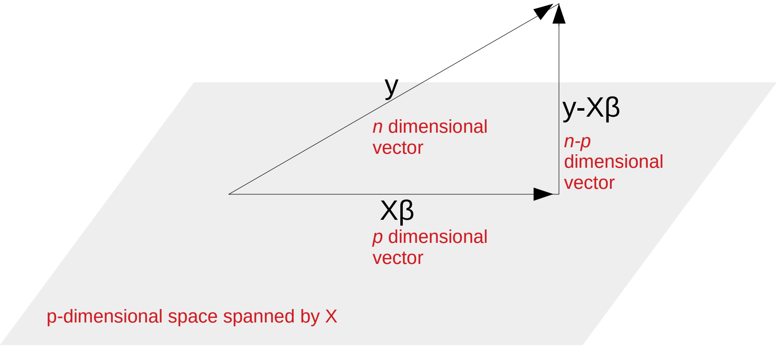

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This decomposition of n data dimensions (observations) into p model parameters and n residuals with rank $n - p$ is helpful when interpreting regression diagnostics.

OLS and Linear Regression

Definition 3 (BLUE)

According to the Gauss-Markov theorem, *Ordinary Least Squares* (OLS), which uses the Normal equations to minimise the sum of the squares of the errors ($\|\epsilon\|_2 \equiv \sqrt{e_1^2 + e_2^2 + e_3^2 + \ldots + e_n^2}$), is the *Best, Linear, Unbiased, Estimator* of that model that can be derived from the training data, provided some reasonably loose assumptions hold.

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In practice, the assumptions required for OLS to be appropriate can be stated in terms of properties of the residual vector ϵ.
In the rest of this lecture, we will generalise from Simple to Multiple Linear Regression, where $\beta = (\beta_0, \beta_1, \beta_2, \ldots, \beta_p)$ and $2 \leq p \leq n$, so instead of fitting lines, we fit (hyper)planes to data.

Assumptions required for the linear model to be meaningful

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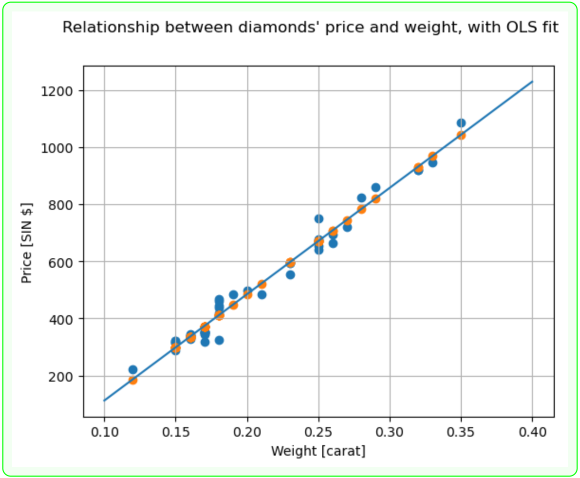
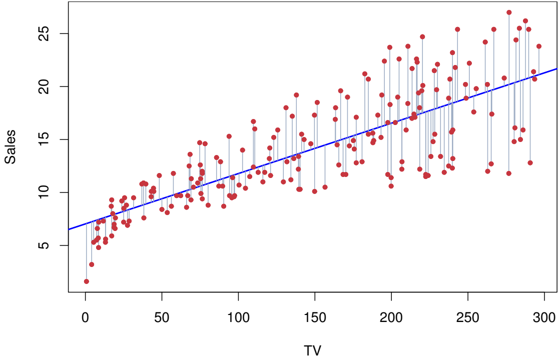
Because these assumptions depend both on the data and on the model fitted to that data, it is meaningless to say that “Data set A does not satisfy the linear regression assumptions”, because this observation might not apply to all formulations of all models applied to that data.
Consequently, these assumptions can be used constructively, when model building, or as checks, when validating models.

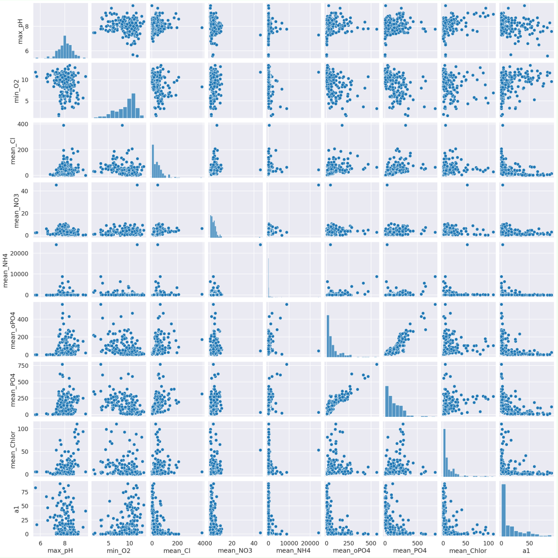
Linear relationship





- In both cases, the relationship between predictor (feature) and target is approximately linear.
- Given a feature value, we can predict the target value using a simple linear formula.
- The predicted parameters are the *intercept* β_0 and *slope* β_1 of the line.
- Usually the vertical distance between a data point x_i and its predicted value $\hat{y}_i$ is $\epsilon_i \neq 0$.

Collinearity (high pairwise correlation) among the algae bloom predictors



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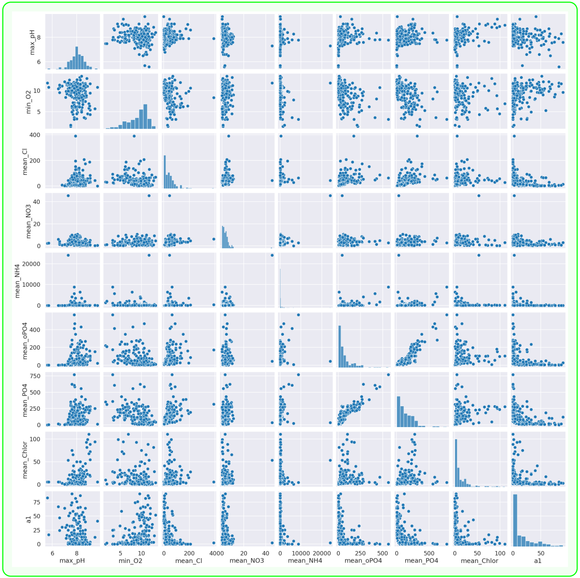

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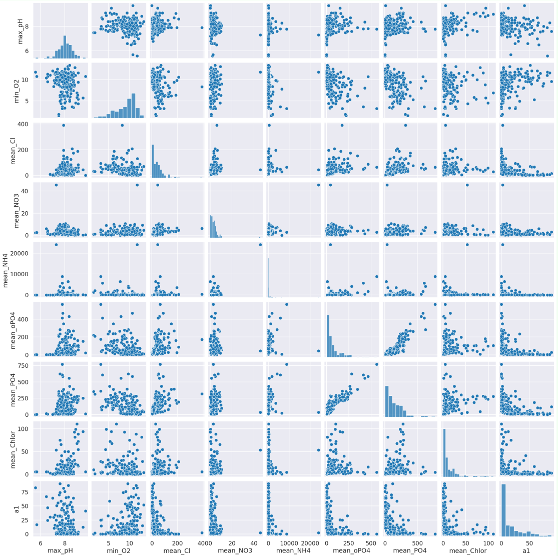

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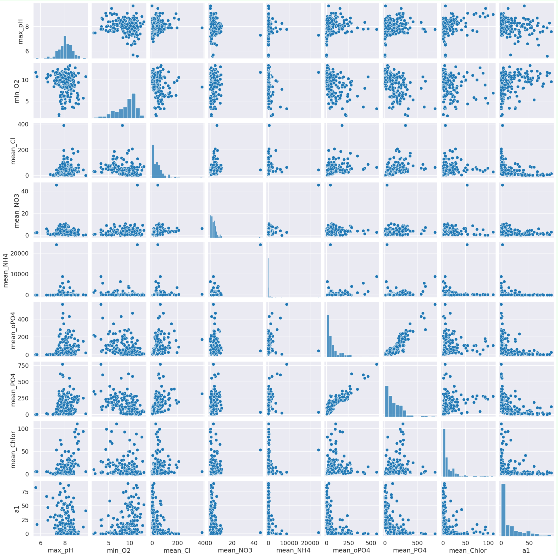

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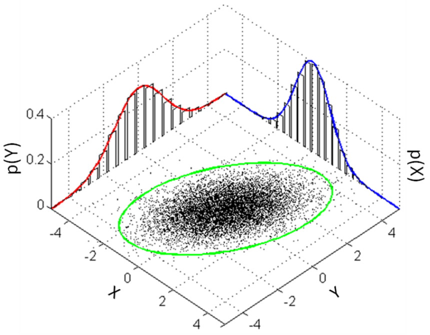
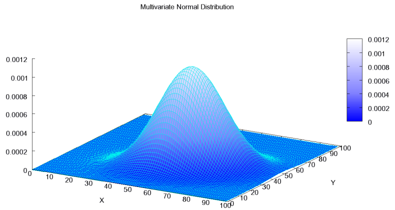
- Also, the individual predictors do not have a strong linear relationship with `a1` (look at the scatterplots in the last row and column) so, on their own, they are not likely to predict `a1` well with a linear model.
- However, it is still possible that a combination of predictors might predict a1 well.

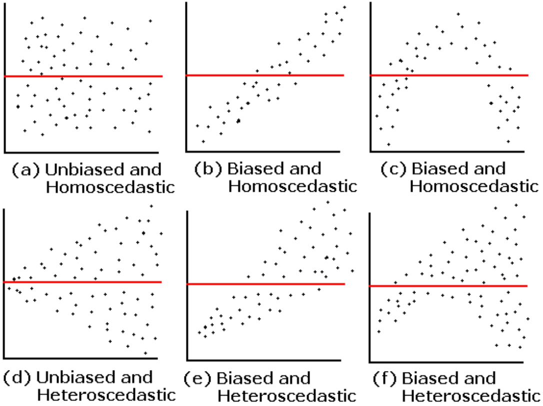
Errors are normally distributed

- Centred on zero so small errors are more common
- Symmetric so positive and negative balance out
- Normal distribution is a also called the Gaussian distribution and is “bell-shaped”.





Bias and variance in regression

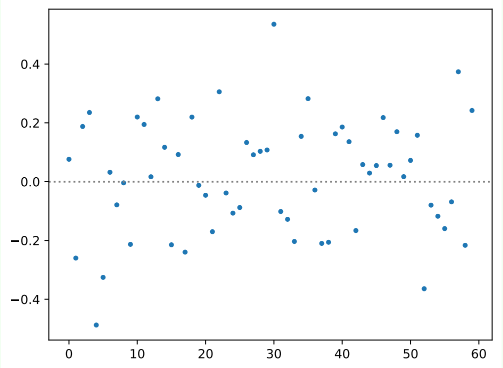


Source: `https://bit.ly/3vC9zK7`

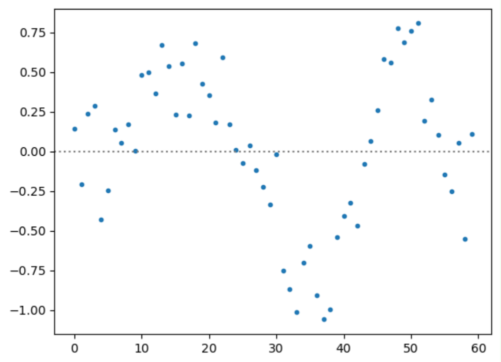
- Bias is caused by underfitting.
- Fix bias by adding suitable predictors.
- Overfitting causes large variance.
- If variance changes over the range, some errors get undue attention.
- Fix this by weighting the errors so they are balanced.

Errors should not be serially correlated

No serial correlation



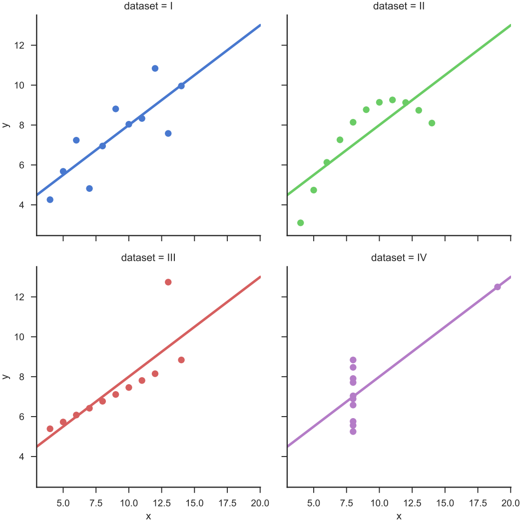
Positive serial correlation



Apparent seasonal effects - can they be removed?

1. Add feature to the model
2. Include autoregressive terms (but then it is no longer Ordinary Least Squares (OLS)!)

Anscombe's quartet (1973)



Francis Anscombe devised 4 data sets to show different forms of misalignment between data and models. Sets I,II,III share the same x values. All 4 sets share approximately the same descriptive statistics (mean and variance), but little else is common to all 4!

Only I appears suited as it stands. The other data sets require some work, particularly IV.

What do you think needs to be done for each data set?

Common Cost Functions in Regression Models

Remember: we are trying to minimise a loss function based on the error, which we approximate with the residuals of the training set.

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Measure	Definition	Purpose
Mean square error (MSE)	$\frac{(p_1-a_1)^2+\cdots+(p_m-a_m)^2}{m}$	Mathematically tractable but places greater emphasise on observations with large error
Root mean square error (RMSE)	$\sqrt{\frac{(p_1-a_1)^2+\cdots+(p_m-a_m)^2}{m}}$	Has same units as data
Mean absolute error (RMAE)	$\frac{\lvert p_1-a_1\rvert+\cdots+\lvert p_m-a_m\rvert}{m}$	Does not overemphasise observations with large error (like MSE does)
Relative square error (RSE)	$\frac{(p_1-a_1)^2+\cdots+(p_m-a_m)^2}{(p_1-\bar{a})^2+\cdots+(p_m-\bar{a})^2}$	Relative metric compares the error in the predictions with errors in the simplest model possible (a model just always predicting the average value of y)
Root Relative square error (RRSE)	$\sqrt{\frac{(p_1-a_1)^2+\cdots+(p_m-a_m)^2}{(p_1-\bar{a})^2+\cdots+(p_m-\bar{a})^2}}$	
Relative absolute error (RAE)	$\frac{\lvert p_1-a_1\rvert+\cdots+\lvert p_m-a_m\rvert}{\lvert p_1-\bar{a}\rvert+\cdots+\lvert p_m-\bar{a}\rvert}$	

where a_j is the actual value, p_j is the predicted value, m is the number of observations, and $\bar{a}$ represents the mean of the a_j.

Choices of Vector norms

Definition 5 (Manhattan norm)

$\ell_1(\dots) = \|\dots\|_1$ is the *Manhattan* norm (length) of a vector. Let $\mathbf{x} = (x_1, x_2, \dots, x_m)$. Then $\ell_1(\dots) = \|\dots\|_1 = |x_1| + |x_2| + \dots + |x_m|$ is the *Manhattan* distance of $\mathbf{x}$ from the origin. Think of having to *walk* from one junction in Manhattan to another, the distance is the difference in the Street numbers plus the difference in the Avenue numbers.

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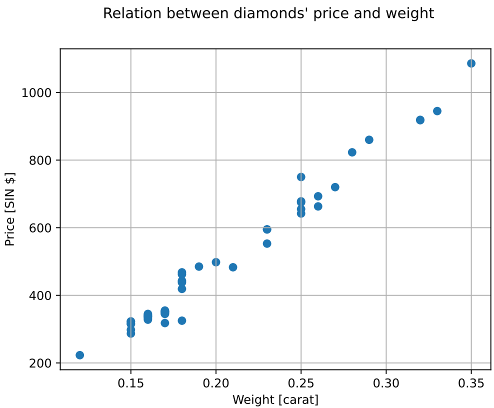
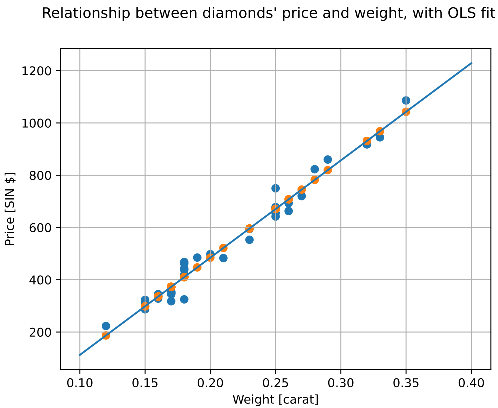
The Euclidean norm is very common, but the Manhattan norm is gaining popularity, because it is robust to outliers and computers are becoming powerful enough. However we generally use Euclidean norm in this module.

Case Study 2: Diamonds - Check relationship





Clearly there is a linear relationship between a diamond's weight (in carats) and its price (in Singapore dollars, as here). So that is one assumption satisfied!

Sometimes the dependent variable has a linear dependence on a function of an attribute. Example functions include log, exp, sqrt, polynomial, etc. Even if the function is nonlinear in the attribute, that does not matter, as long as the model is linear in the regression parameters β.

Case Study 2: Diamonds - Check residual distribution

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resFig = "res/residHist.pdf"
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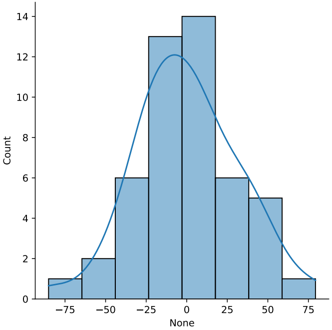

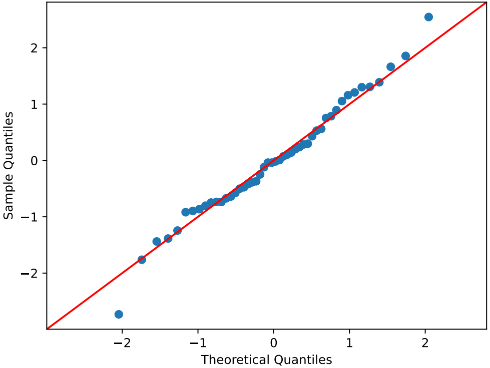

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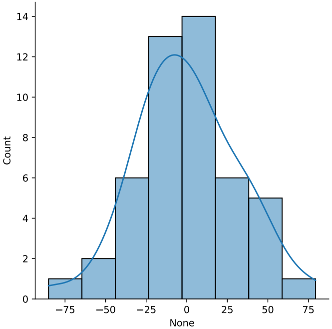

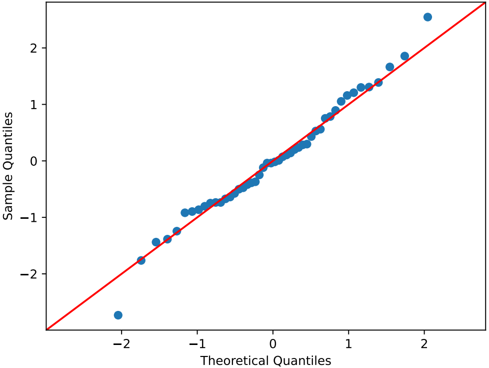

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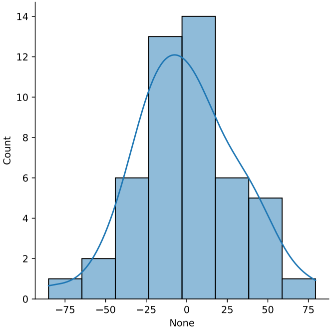

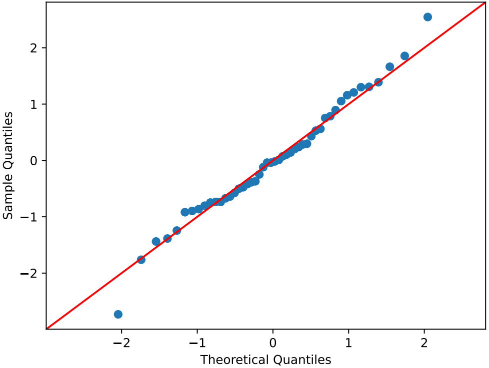

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OLS Regression Results

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Model:	OLS	**Adj. R-squared:**	0.978
Method:	Least Squares	**F-statistic:**	2070.
Date:	Fri, 25 Oct 2024	**Prob (F-statistic):**	6.75e-40
Time:	10:54:56	**Log-Likelihood:**	-233.20
No. Observations:	48	**AIC:**	470.4
Df Residuals:	46	**BIC:**	474.1
Df Model:	1		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
const	-259.6259	17.319	-14.991	0.000	-294.487	-224.765
carats	3721.0249	81.786	45.497	0.000	3556.398	3885.651

Omnibus:	0.739	**Durbin-Watson:**	1.994
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- **What score(s) indicate that the residuals are not serially correlated?**

Case Study 2: Diamonds - model summary

OLS Regression Results

Dep. Variable:	price	**R-squared:**	0.978
Model:	OLS	**Adj. R-squared:**	0.978
Method:	Least Squares	**F-statistic:**	2070.
Date:	Fri, 25 Oct 2024	**Prob (F-statistic):**	6.75e-40
Time:	10:54:56	**Log-Likelihood:**	-233.20
No. Observations:	48	**AIC:**	470.4
Df Residuals:	46	**BIC:**	474.1
Df Model:	1		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
const	-259.6259	17.319	-14.991	0.000	-294.487	-224.765
carats	3721.0249	81.786	45.497	0.000	3556.398	3885.651

Omnibus:	0.739	**Durbin-Watson:**	1.994
Prob(Omnibus):	0.691	**Jarque-Bera (JB):**	0.181
Skew:	0.056	**Prob(JB):**	0.913
Kurtosis:	3.280	**Cond. No.**	18.5

Notes:
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```
simpleModel.summary()
```

The output from Python's statsmodels.summary() call has lots of information!

- **How much of the variability of the data is explained by the model?**
- **What is the probability that such data arose if price does not increase with weight?**
- **What score(s) indicate that the residuals are not serially correlated?**
- **What scores indicate that the distribution of the residuals is Normal?**

Model summary interpretation - 1

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Definition 7 (Dep. variable)

This is synonymous with the *target*, which is `price` (in this dataset).

Definition 8 (Model)

statsmodels uses it here in the sense of *problem formulation*. We wish to solve an Ordinary Least Squares problem (assumes all the regression assumptions are met, so no special treatment was applied).

Definition 9 (No. Observations)

This is the number of rows (also known as instances or cases) in the training set.

Model summary interpretation - 2

Definition 10 (Df Model)

The model has one named feature (carats (weight of the diamond)) and one unnamed feature (constant, independent of carats). df, the number of degrees of freedom counts the named features.

Definition 11 (Df Residuals)

The number of degrees of freedom in the residuals is the number of residuals minus the number of features. A higher value tends to go with smaller model variance.

Definition 12 (Covariance Type)

If residuals have the same variance (homoscedastic), nonrobust covariance (the default) can be used.

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Definition 13 (R-squared)

This is the ratio of the data variance explained by the model, to the variance of the data. It ranges from zero (model explains none of the data variance) to one (model explains all the data variance). A higher value is better, but be careful of overfitting the training set!

Definition 14 (Adj. R-squared)

Similar to R-squared, but it takes account of the number of features. Adding a feature generally increases R-squared, but if the feature did not help as much as its peers, adjusted R-squared shows a smaller increase than “normal” R-squared.

Model summary interpretation - 4

Definition 15 (F-statistic)

Ratio of the variance of a model with just the constant (intercept) feature to the variance of this model. Generally, large values of F are preferred.

Definition 16 (Prob (F statistic))

The value is assumed to follow the F distribution for given *dof*, so can lookup its probability. Small probability indicates that it is highly *unlikely* that the model is doing well purely by chance.

Definition 17 (log likelihood)

OLS is a special case of *maximum likelihood estimation*. Larger likelihood model fits the training data better.

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Definition 18 (AIC and BIC)

Akaike and Bayesian Information Criterion. These are calculated from the residuals and are derived from *information theory*. They allow for the number of features. Lower values are better.

Definition 19 (Features table: const,carats in this example)

coef is the parameter value for that feature, e.g., const=-259.6 here. $P > |t| = 0$ so it is highly unlikely the coef is zero, given the training data. We also have the 2.5% and 97.5% quantiles, giving the expected range of coef.

Model summary interpretation - 6

Definition 20 (Skew, Kurtosis)

Measures of asymmetry and of peak shape of the residual distribution. Ideal values are 0 (skew) and 3 (kurtosis).

Definition 21 (Durbin-Watson)

Measures the serial correlation of the residuals. Ideal value is 2 (no serial correlation).

Definition 22 (Cond. no)

OLS implementation solves a linear system of equations. Condition number measures column (hence feature independence). Large values mean the features are not independent (they are correlated), making the system more difficult to solve.

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  1. If a model does not do well, they can help to diagnose the problem(s).
  2. They can also be used constructively, to help identify promising candidate models.

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- Next time - we return to classification…