dm25s1

Topic 07 : Regression1

Part 01 : Regression - Overview

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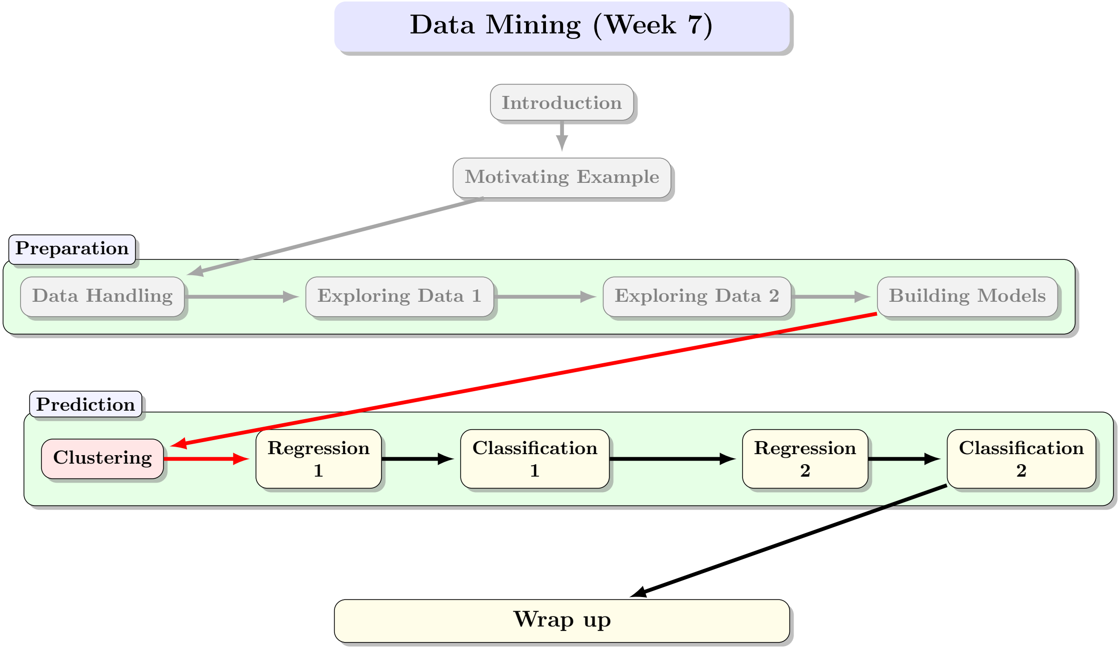
Outline

- 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
- Role of residuals


Data Mining (Week 7)
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

Regression - Overview — Summary

1. Introduction

2. Linear regression assumptions

3. Reviewing regression results

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    - Generated data (various)
    - 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?
- In terms of Week 3's ML models taxonomy: regression is geometric and parametric
- In terms of Week 3's Components of a Machine Learning Problem
  - Representation is based on (fitting) hyperplanes to point clouds
  - Evaluation usually based on MSE, with assumption checks to help identify the best model family
  - Optimization is one-step (no search needed) because we have a constraint on the errors we allow
- Hyperparameter tuning: polynomial degree, regularisation λ, weights, loss function, . . .

Review: Linear combinations and scalar products

Definition 1 (Scalar (dot) product of two vectors)

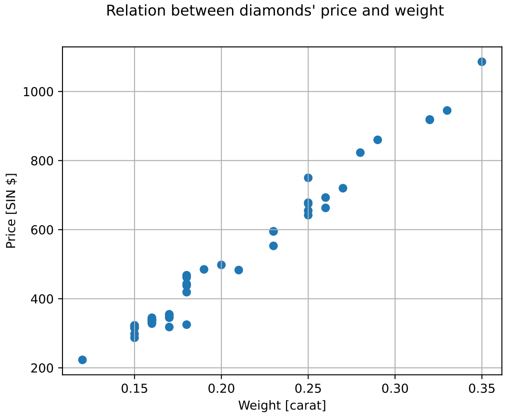
Given two vectors $\mathbf{a}$ and $\mathbf{b}$, each with n elements, the *scalar product* (c) of $\mathbf{a}$ and $\mathbf{b}$ is

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

Remarks

- The scalar product of 2 vectors is a scalar, which can be seen as "mixing" two vectors.
- Matrix-vector multiplication $X\mathbf{a}$ can be seen as the scalar product of each row in the matrix X, which is $X(i,:)$ for row i, with the column vector $\mathbf{a}$.
- Alternatively, matrix-vector multiplication can be seen as the *linear combination* of the matrix columns, such as $X(:,j)$, with the column multipliers being the elements of $\mathbf{a}$.
- For linear regression, the matrix columns are the feature vectors $X(j)$ and the column multipliers are the regression parameters $\mathbf{a}$.
- Two nonzero vectors $\mathbf{a}$ and $\mathbf{b}$ can have a scalar product that is zero if $\cos(\mathbf{a}, \mathbf{b}) = 0$, i.e., the $\mathbf{a}$ and $\mathbf{b}$ vectors are perpendicular to each other.

Motivating example: Diamond data



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 3 other factors that might affect the price?

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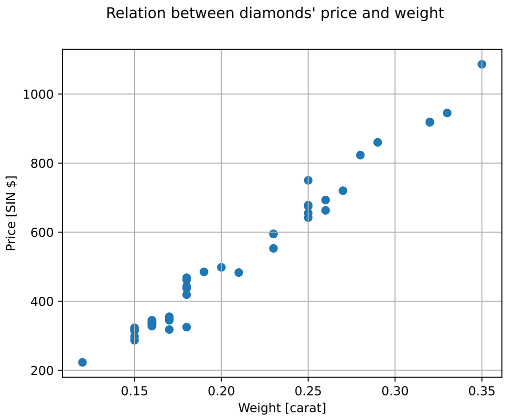

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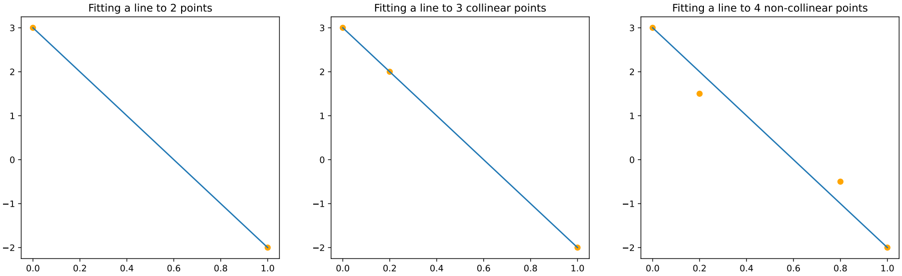
- Can you think of at least 3 other factors that might affect the price?
- Various(!) - some examples: clarity, cut, provenance, part of a set, . . .

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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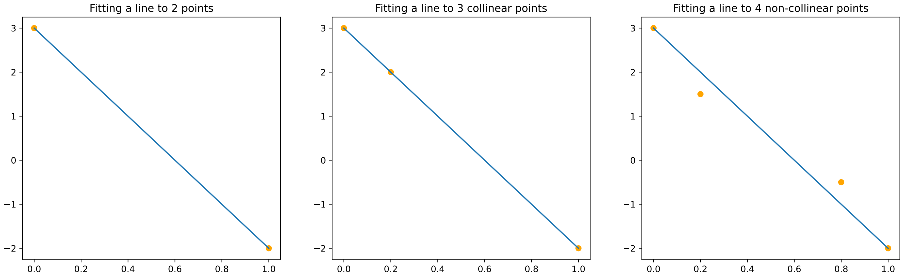

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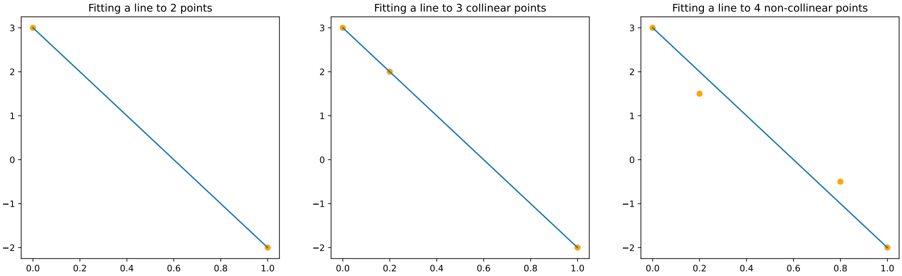

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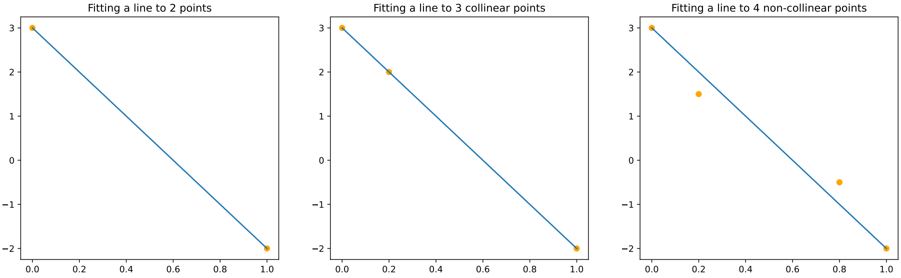

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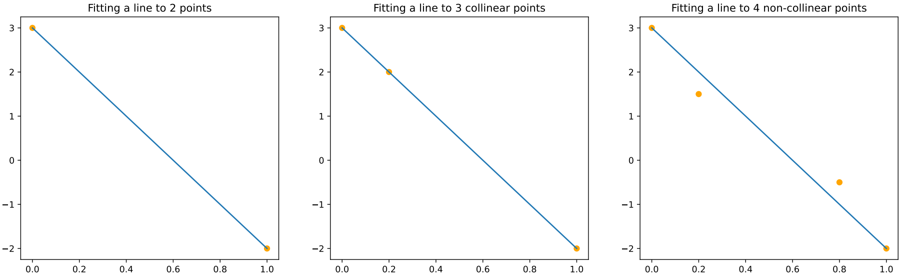
- For $n > 2$ collinear points, just pick any two points and solve as before.
- Otherwise the problem is overdetermined so need a more general formulation to solve for β_0, β_1.



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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- Matrix form is $\mathbf{y} = X\beta$. Remember matrix-vector multiplication: inner product of i^{th} row of X times the vector β = $1 \times \beta_0 + x_i \times \beta_1 = \hat{y}_i$.

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- So: our task is to solve the *overdetermined* (number of rows exceeds the number of columns) system of equations $\mathbf{y} = X\beta$ for β
- 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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\mathbf{y} &\approx X\beta \\
\mathbf{y} &= X\beta + \epsilon \\
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because $X^{\mathsf{T}}\epsilon \equiv 0$ implies the fitted line gives balanced errors and so is 'best". Swapping sides, we have

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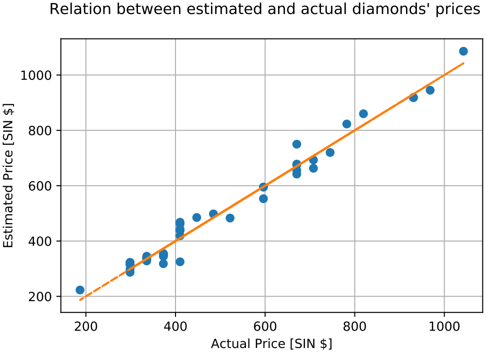
Note that everything on the right is a set of operations on the data.

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

Simple Linear Regression: Balanced Errors



What makes this look like a good fit?
The fitted line passes through the data centroid and errors pass are balanced *- cf. see-saw*

- More generally: a weighted sum of the errors should be 0.
- Weights should depend on the features.
- The $X^\top \epsilon = 0$ criterion works well, so we apply it.
- If you imagine the centroid as being the fulcrum of the line, viewed as a lever, we wish to “balance” the errors around that point

Simple Linear Regression: Implementation

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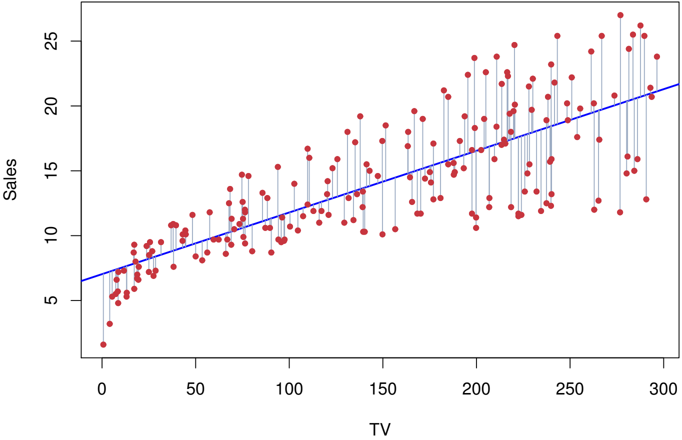
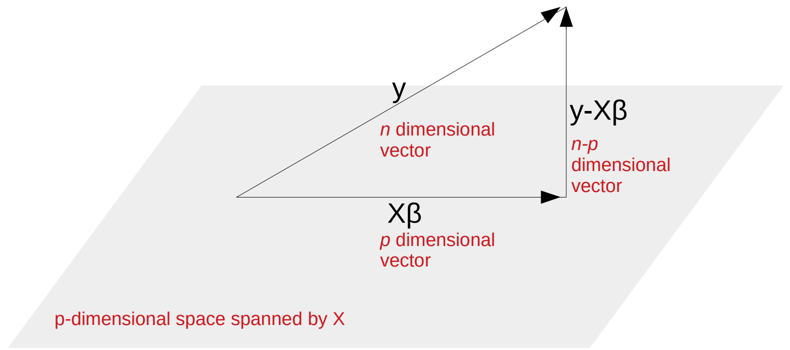
Remember: after *learning* the β parameters using the training data $\{\mathbf{x}_i, y_i\}$, with the model encoded in the feature matrix X, it is then possible to predict $\hat{y}_k$ for “new” (test) $\mathbf{x}_k$ values, using separate *prediction* function calls.

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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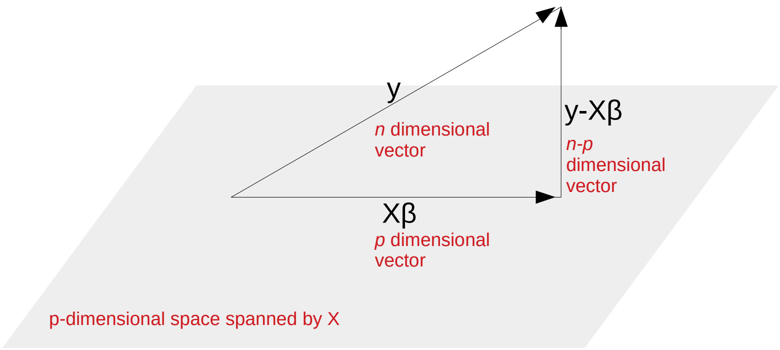

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- But $\mathbf{y}$ has $n > p$ dimensions and so is represented by a point that lies outside the grey plane.
- When $\mathbf{y}$ is projected onto the nearest point in the X space,
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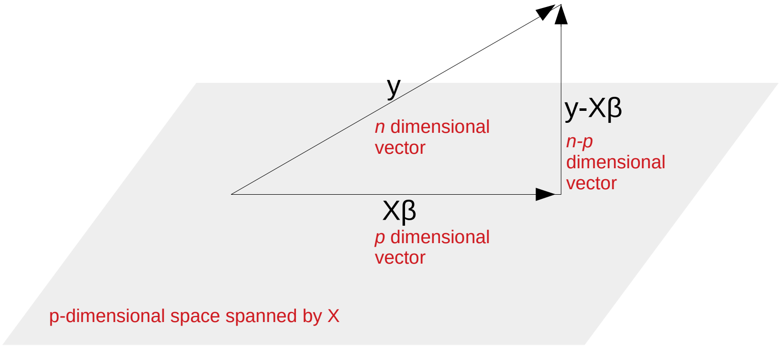

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This decomposition of n data dimensions (observations) into p model parameters and n residuals with rank $n - p$ is helpful when interpreting regression diagnostics.

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.

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4. There is no auto-correlation in $\mathbf{y}$: each observation is independent of its "neighbours".

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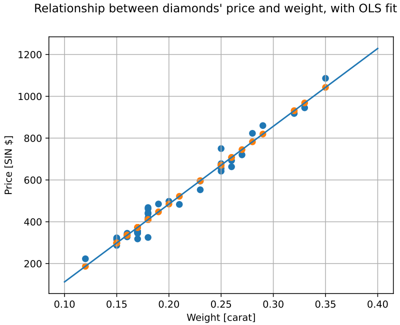
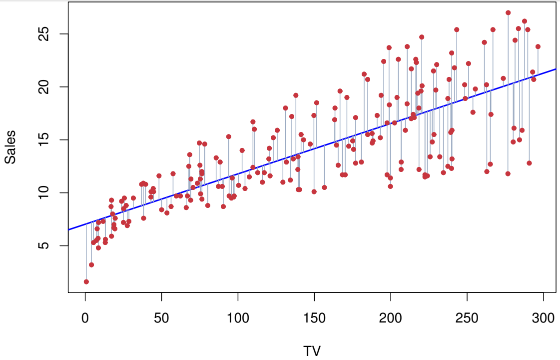
Consequently, these assumptions can be used constructively, when model building, or as checks, when validating models.

Linear relationship





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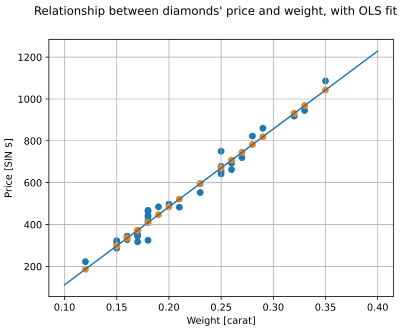

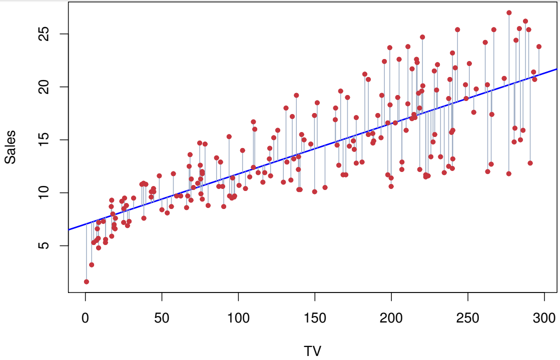

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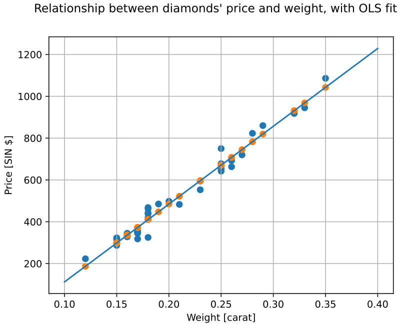

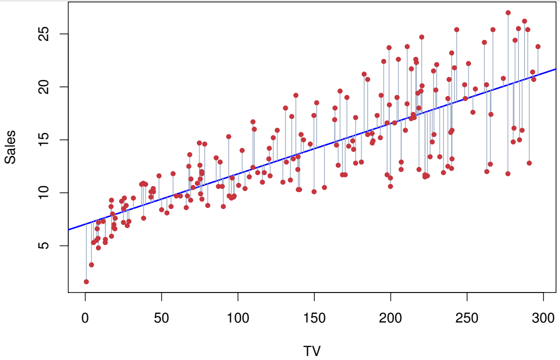

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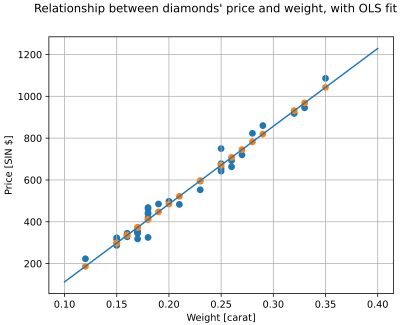

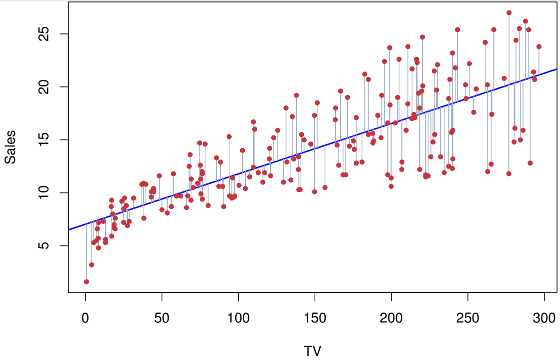

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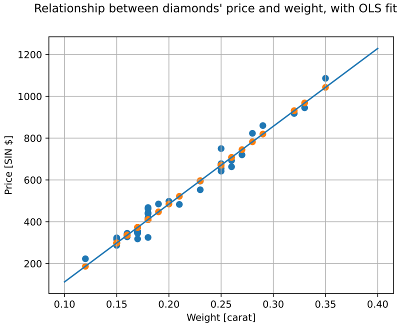

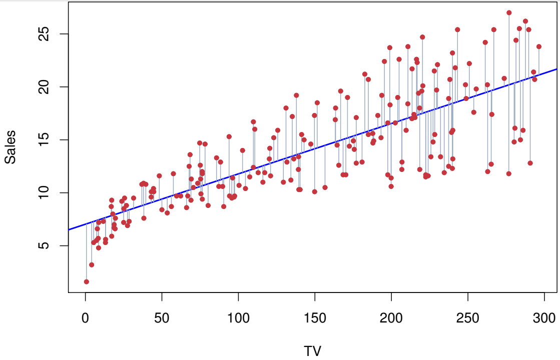

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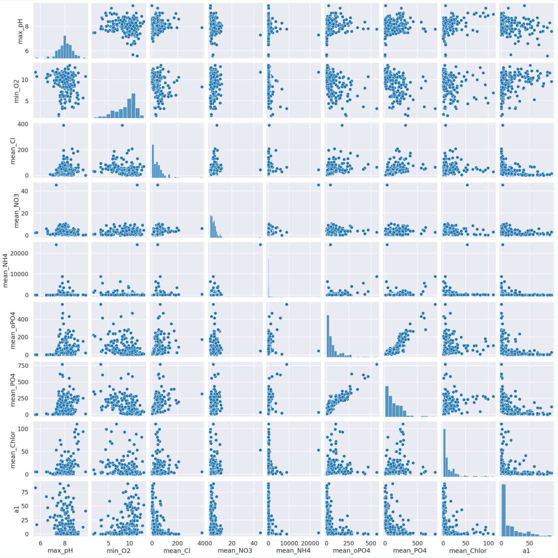
- Usually the vertical distance between a data point x_i and its predicted value $\hat{y}_i$ is $\epsilon_i \neq 0$.
- ϵ_i is the *residual error*. It quantifies data behaviour not included in our model.

Collinearity (high pairwise correlation) among the algae bloom predictors



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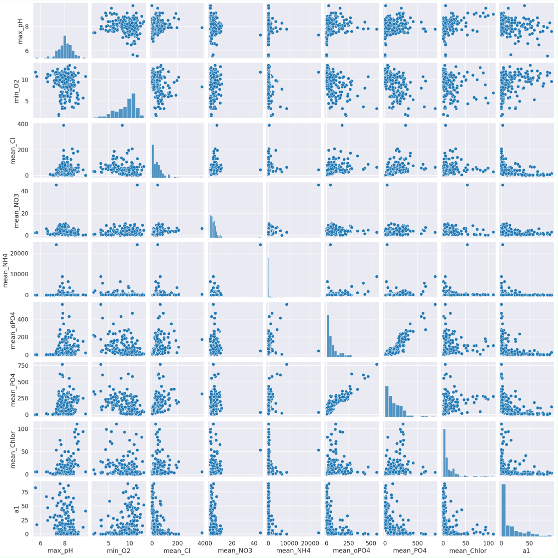

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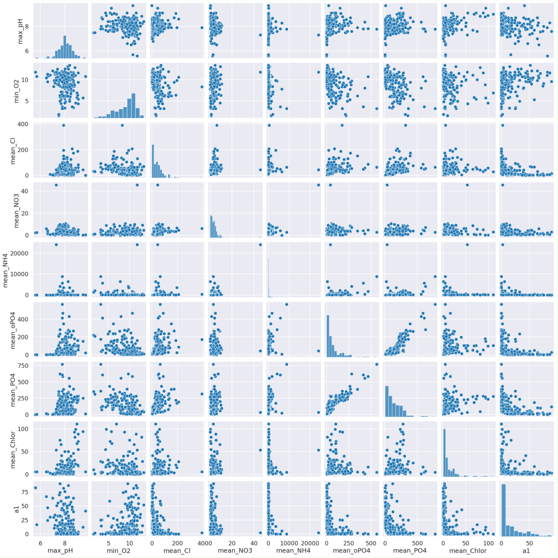

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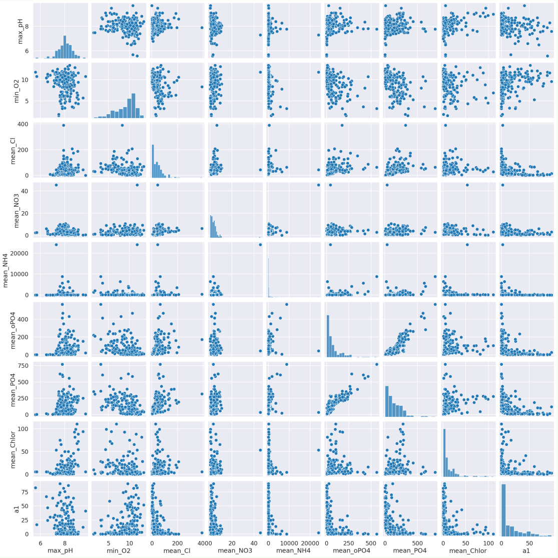

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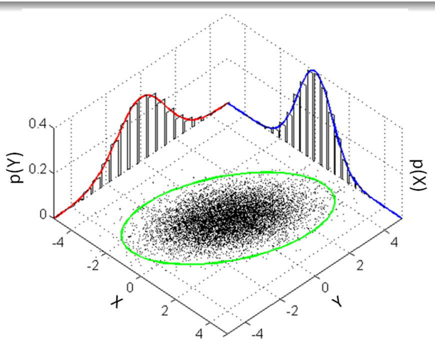
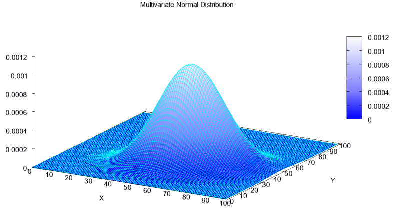
- Also, the individual predictors do not have a strong linear relationship with `a1` (look at the scatterplots in the last row and column) so, on their own, they are not likely to predict `a1` well with a linear model.
- However, it is still possible that a combination of predictors might predict a1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

Errors are normally distributed

- Centred on zero so small errors are more common





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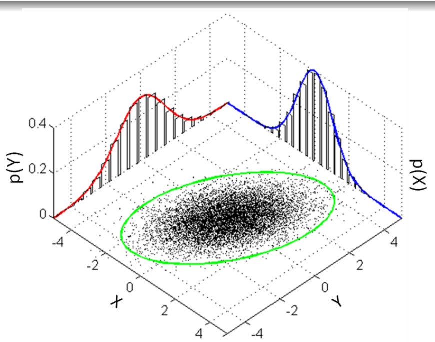

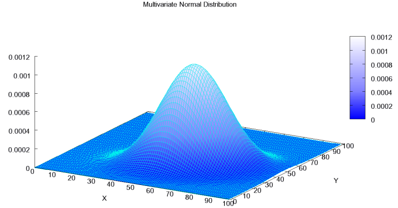

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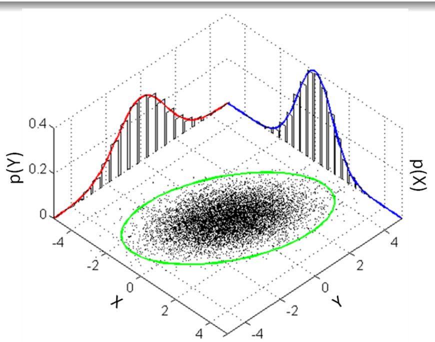
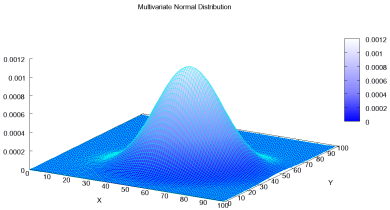
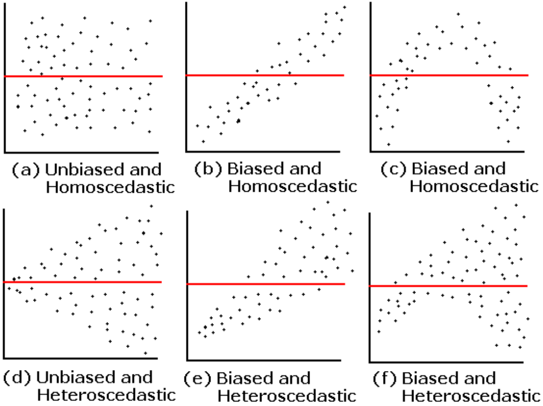
- Normal distribution is a also called the Gaussian distribution and is “bell-shaped”.





Bias and variance in regression



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

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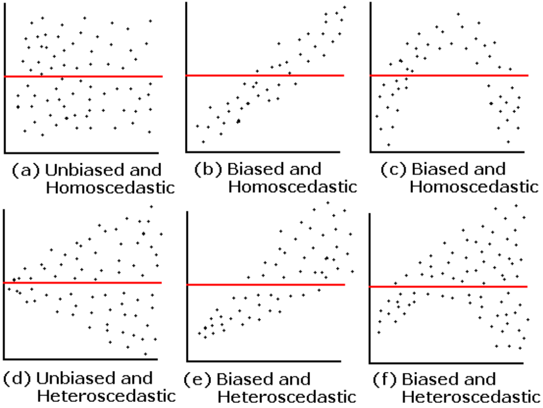

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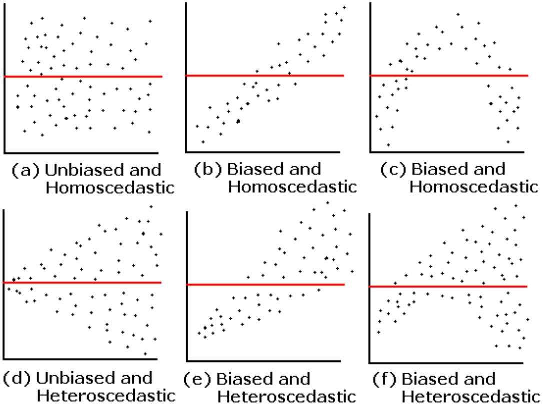

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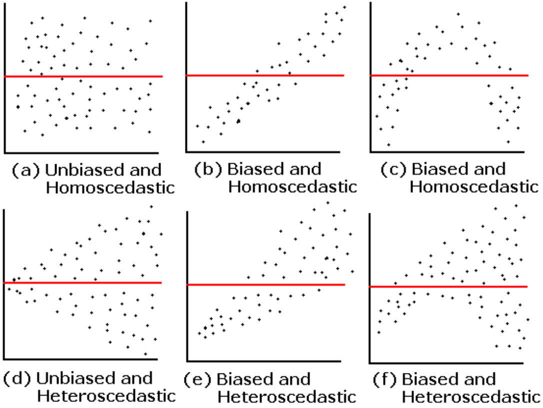

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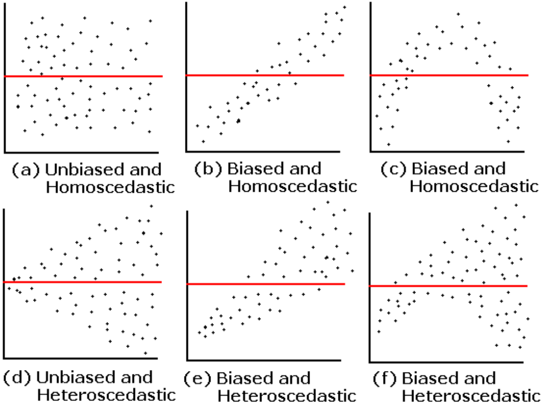

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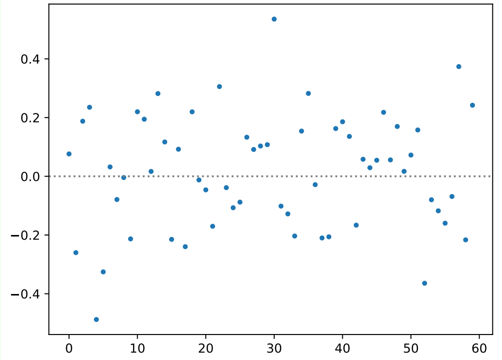
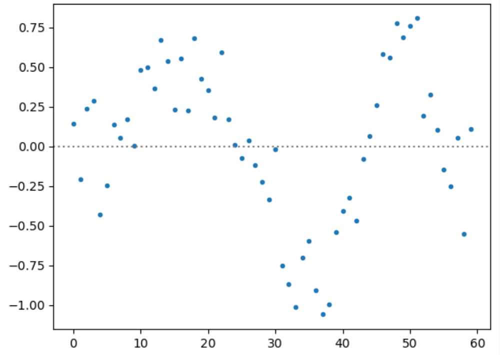
- Fix this by weighting the errors so they are balanced.

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

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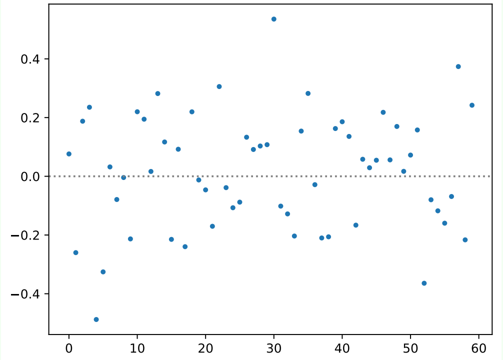

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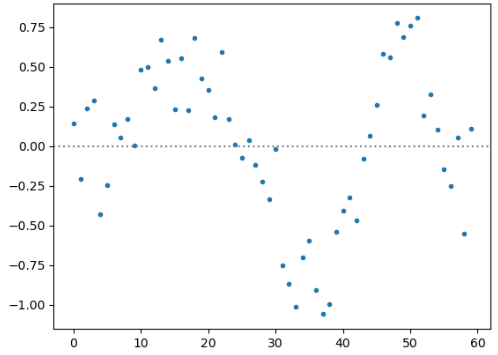
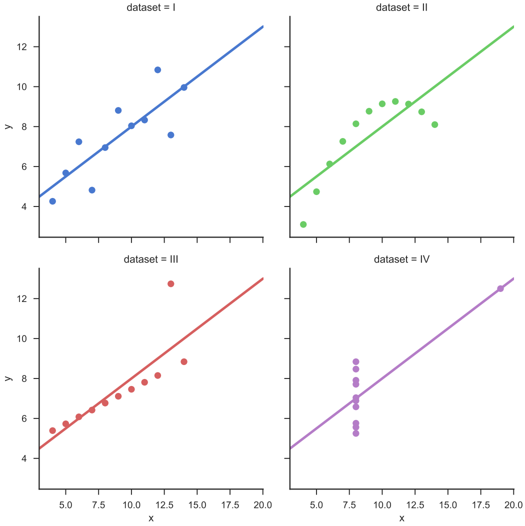


Apparent seasonal effects - can they be removed?

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)

$\ell_1(\ldots) = \|\ldots\|_1$ is the *Manhattan* norm (length) of a vector. Let $\mathbf{x} = (x_1, x_2, \ldots, x_m)$. Then $\ell_1(\ldots) = \|\ldots\|_1 = |x_1| + |x_2| + \ldots + |x_m|$ 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.

Sidebar: Distance Measures for numeric data

Definition 7 (Minkowski $p-$norm)

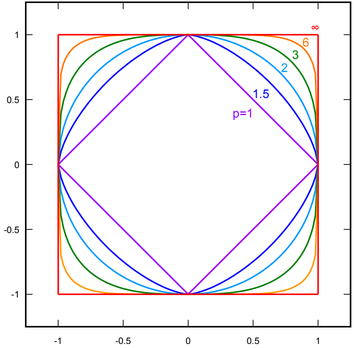
For a real number $1 \leq p < \infty$, the p-norm of $\mathbf{x}$ is defined by

$$\|\mathbf{x}\|_p \equiv \left(|x_1|^p + |x_2|^p + \ldots + |x_n|^p\right)^{\frac{1}{p}}.$$

The limiting case of $p = \infty$ is defined as

$$\|\mathbf{x}\|_\infty \equiv \max\{|x_1|, |x_2|, \ldots, |x_n|\}.$$

See the visualisation of the "unit balls" alongside, for $p = 1, 1.5, 2, 3, 6, \infty$.



Source: wikipedia

The most common norms are when $p = 1, 2, \text{or}, \infty$. Choice of p depends on the application scenario. Can you think of when you would use each?

Huber loss