Monte Carlo Simulation

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1 Introduction

Regression is a tool in statistics used to understand the relationship between one dependent variable and one or more independent variables. For regression to be both accurate and reliable, a set of assumptions needs to be met. These assumptions are independence of errors, linearity, homoscedasticity, normality of errors, multicollinearity, and correct model specifications. If these assumptions are not met, it can introduce bias and inaccuracies in the regression model.

1.1 Independence of Errors

This assumption states that the errors from the model are not correlated with each other but are independent. This means that one error cannot be used to predict the next one.

1.2 Linearity

This assumption states that the relationship between the independent variables and the parameters, also known as the coefficients, is linear. This does not mean that the regression model itself has to be linear. For example, in polynomial regression, the relationship between the independent variables and the coefficients is still linear, but the independent variables can be transformed using powers.

1.3 Homoscedasticity

This is the assumption of constant variance across errors for all levels of the independent variables.

1.4 Normality of Errors

This assumption states that the errors between the model and the observed values, also called residuals, are normally distributed. If this is not met, it may result in a biased model and a worse model fit.

1.5 Multicollinearity

This occurs when two or more independent variables in a regression model are highly correlated with each other. This means that changes in one independent variable are associated with changes in another, making it difficult to determine the individual effect of each independent variable on the dependent variable.

1.6 Correct Model Specifications

This assumes that the provided dependent variables for the models are the correct ones. If one is missing or the model is overfitting, this may result in incorrect coefficients and introduce errors into the model.

2 Statistical Theory

2.1 Probability space

The **sample space**, S, is the set of all possible outcomes.
If a sample space contains a finite number of possibilities or an unending sequence with as many elements as there are whole numbers, it is called a **discrete sample space**.
Example: When rolling a standard six-sided die form the discrete sample space, the possible outcomes are $S = 1, 2, 3, 4, 5, 6$

If a sample space contains an infinite number of possibilities equal to the number of points on a line segment, it is called a **continuous sample space**.
Example: Measuring the heights of people in a population. This is a continuous sample space, because height can take any real value within a given range.
An **event** is a subset, $A \subseteq S$, of the sample space. The event is the amount that contains all possible events. An example of a discrete event could be rolling a die and getting an uneven number, this would be the event $A = 1, 3, 5$.
For the continuous event, it could be that a person is between 160 cm and 170 cm tall.

The probability of an event A, $P(A)$, is the sum of the weights of all sample points in A. The probability of the whole sample space is 1, $P(S) = 1$ The probability of any event being between 0 and 1,$0 < P(A) < 1$ The probability of the empty set being 0, $P(\emptyset) = 0$

Probability of mutually exclusive events
If A and B are mutually exclusive, $A \cap B = \emptyset$, then
$P(A \cup B) = P(A) + P(B)$

Where A and B never occur at the same time, so their union is equal to the two events added together.
Probability of union
$P(A \cup B) = P(A) + P(B) - P(A \cap B)$
Here, the union of the two events is A added to B, but minus their common event, since it otherwise would be added twice.
Two events A and B are independent, if
$P(A|B) = P(A)$
The equivalent definition to this is:
Two events A and B are independent if and only if
$P(A \cap B) = P(A)P(B)$ This says that the probability of both event A and B happening, is equal to the product of the two events.

2.2 Random variables

test A random variable is defined as a function that associates a real number with each element in the sample space. We use capital letters to denote a random variabel, for example X, and then the corresponding small letter, in this case x, for one of its values. As an example we roll a dice 3 times, which gives us a sample space of the different combinations. Each point in the sample space gets a numerical value assigned between 0 and 3.These values are random quantities and are assumed by the random variabel X, which for example could assume the amount of 5's rolled. In that case $X(5,1,2) = 1$ and $X(3,6,1) = 0$.

A random variable X can be discrete, which means that its set of possible outcomes is countable. The dice example is a discrete random variable, because you can count how many times 5 is rolled. The outcomes of some statistical experiments may be neither finite nor countable. For example when something is measured such as temperature or speed where the set of possible values is an entire interval of numbers, it is not discrete. The random variable X then takes values on a continues scale, which therefore is called a continuous random variable.

2.2.1 Discrete random variable

A discrete random variable assumes each of its values with a certain probability. Frequently, it is convenient to represent all the probabilities of a random variable X by a formula. Let X be a discrete random variable which can take the values $x_1, x_2, ...$ Then the distribution of X is given by the probability function:

$$f(x_i) = P(X = x_i), \quad i = 1, 2, ...$$

For a discrete random variable this function is also called the probability mass function, where following holds for each possible outcome x:

- $P(X = x) = f(x)$.
- $f(x) \geq 0$,
- $\sum_x f(x) = 1$.

In addition to the probability mass function f, the discrete random variable X also has a distribution function $F(x)$ given by:

$$F(x) = P(X \leq x) = \sum_{x_i \leq x} f(x_i), \quad x \in \mathbf{R}.$$

This helps decide the probability that the random variable assumes a value equal to or smaller than x. Its sums up the probability mass functions's values.

The mean of a discrete variabel X, with a distribution function $f(x_i)$ is given by:

$$\mu = E(X) = \sum_i x_i P(X = x_i) = \sum_i x_i f(x_i).$$

The mean is typically the expected value. It is a weighed average of the possible values of X. The values are weighed by its probability in the sample space.

In addition to the mean, we should also mention the variance. The variance is the mean squared distance between the values of the variable and the mean value. It is given by:

$$\sigma^2 = E\left[(X - \mu)^2\right] = \sum_i (x_i - \mu)^2 f(x_i).$$

The variance indicates whether the values of X are far from the mean values or close. A high variance means that the values of X have a high probability of being far from the mean values and vice versa. Along with the variance, the standard deviation is also often used. It is given by the square root of the variance:

$$\sigma = +\sqrt{\sigma^2}.$$

The advantage of the standard deviation over the variance is that it is measured in the same units as X.

2.2.2 Continuous random variable

Contrary to a discrete random variable, a continuous random variable can take values that are not countable. A continuous random variable can take infinetly many possible values within a certain range or interval. For a continuous random variable X the distribution is given by the probability density function f, which satisfies:

- $f(x)$ is defined for all x in $\mathbf{R}$,
- $f(x) \geq 0$ for all x in $\mathbf{R}$,
- $\int_{-\infty}^{\infty} f(x)\, dx = 1$.

Condition 3. ensures that $P(-\infty < X < \infty) = 1$, which means that the probability of the random variable X being between $-\infty$ and ∞ is 100%. Furthermore the probability of X assuming a specific value a is zero, in other words: $P(X = a) = 0$. That means that the values of the density function should not be interpreted as a probability of a given outcome. Instead the probability of X is found by integrating over the probability density function. So, the probability that a continuous random variable X lies between the values a and b is:

$$P(a < X < b) = \int_a^b f(x)\, dx.$$

A continuous random variable X also has a distribution function $F(x)$, that also predicts whether X assumes a value equal to or smaller than x. For a continuous random variable it is again given by integrating over the probability density function in the interval from $-\infty$ to x:

$$F(x) = P(X \leq x) = \int_{-\infty}^{x} f(y)\ dy$$

. That also means that $P(a < X < b)$ can be calculated by $F(b) - F(a)$.

For a continuous random variabel X the mean, variance and standard deviation the same interpretation applies. Just given by different formulars, which are:

$$\mu = E(X) = \int_{-\infty}^{\infty} x f(x)\, dx$$

and

$$\sigma^2 = E\left[(X-\mu)^2\right] = \int_{-\infty}^{\infty} (x-\mu)^2 f(x)\, dx,$$

(The standard deviation is still given by til square root of the variance).

2.3 Estimator and estimates

If we are interested in certain parameters of a population distribution, we can look at a sample. From this, we can make a **point estimate**.
Examples of this are,
$\bar{x}$ is a point estimate of μ
s is a point estimate of σ

This is often supplemented with a **confidence interval**
This is an interval around the point estimate, where we are confident that the population parameter is located.

For μ, we have different ways of estimating it. We can use the sample mean $\bar{X}$, or the average X_T of the sample upper and lower quartiles. But in this case, we have to look out for **bias**. If the distribution of a population is skewed, then X_T is biased. The result of this is, that in the long run, this estimator will systematically over or under estimate the value of μ. This is written as,
$E(X_T) \neq \mu$.
It is generally preferred that the estimator is **unbiased**. In this case, $\bar{X}$ is an unbiased estimate of the population mean μ.

The standard error of $\bar{X}$ is $\frac{\sigma}{\sqrt{n}}$. Here, the standard error decreases, when the sample size increases. If an estimator has this property, it is called **consistent**. If we compare, the estimator X_T is also consistent, but has a greater variance than $\bar{X}$.
It is generally preferred that the estimator has the smallest possible variance,

and in that case it is called efficient. So $\bar{X}$ is an efficient estimator.
When estimating a parameter, the symbol ˆ is used above it. For μ, $\hat{\mu} = \bar{X}$.
We can calculate $\bar{X}$ using the following formula,

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

For the variance σ, we can estimate it by using the formula for S^2,

$$S^2 = \frac{1}{n-1}\sum_{i=1}(X_i - \bar{X})$$

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2.4 Probability distribution

Data can come in various distributions depending on different parameters such as degrees of freedom. The distribution is the shape of the data and it will have an effect on statistical models. Therefore it is important to have an understanding of distributions.

2.4.1 Normal distribution

In the world of statistics, the most common distribution is the normal distribution. It is constructed as a bell shape. The normal distribution is a continuous distribution, with this density function:

$$n(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)}{2\sigma^2}}$$

The distribution is dependent on the mean(μ) and the standard deviation(σ), where changes to the mean will result in a change in the positioning of the normal distribution. Whereas a change in the standard deviation will change the spread of the curve. The normal distribution also always contains an area under the curve that is equal to one. This is to ensure that the normal distribution correctly models probability.

There is a special case of the normal distribution, called the standard normal distribution, where the mean is zero and the standard deviation is one. All variations of a normal distribution can be standardized by a transformation of the distribution, using the Z-score formula.

$$Z = \frac{X - \mu}{\sigma}$$

Z in the Z-score represents the amount of standard deviations a given X value, deviates from the mean.

2.4.2 The central limit theorem

A very effective theorem in statistics is the central limit theorem. This theorem states that if a random sample $\overline{X}$, with the size n, is taken from a population with a mean and a finite variance, then as n goes towards infinity, the distribution will resemble a normal distribution. If used with the Z-score formula, the distribution will resemble a standard normal distribution. The formula for the Z-score, when in conjunction with the central limit theorem, looks like this:

$$Z = \frac{\overline{X} - \mu}{\sigma/\sqrt{n}}$$

Where $\overline{X}$ is a random sample of size n and μ is the mean of the true population. The standard error i represented by $\sigma/\sqrt{n}$, where σ is the standard deviation and n is the sample size. Usually the standard deviation is unknown, for these situations it's possible to use the estimator S^2. This estimates the variance of the population from the variance of the sample, by this formula:

$$s^2 = \sum_{i=1}^{n} \frac{(x_i - \overline{x})}{n-1}$$

The square root of the variance is the standard deviation, therefore the square root of the estimator S^2 would be the estimated standard deviation. The problem with using the estimator S^2, is that with small samples the variance is small and therefore it contains a lot of bias. In this situation the t-distribution would be used instead of the normal distribution, because the t-distribution takes the bias into account the bias of the standard deviation. It does this by having thicker tails, meaning that the probability of more extreme values are higher.

2.4.3 The t-distribution

The t-distribution is shaped as the standard normal distribution, in a bell shape and symmetrical around the mean of zero, the difference is that the t-distribution is more variable. This comes from the fact that the t-distribution is dependent on the degrees of freedom. When the degrees of freedom surpasses 30, the rule of thumb is that the distribution will resemble a normal distribution. So before 30 degrees of freedom, the distribution contains more variance. The t-distribution will come to resemble the standard normal distribution, when in surpasses 30 degrees of freedom, this makes sense, since the two distributions have the same formula:

$$T = \frac{\overline{X} - \mu}{S/\sqrt{n}}$$

The only difference is the estimated standard deviation S.

2.5 Statistical methods

2.5.1 Confidence intervals

The confidence interval is a good tool to use, when trying to estimate a parameter of a population. Its used to create an interval, where the parameter has a probability to lie inside of. This probability is called the confidence level and it's a chosen value, usually the chosen confidence level is either 95% or 99%. The confidence interval will become bigger with a larger confidence level. A good confidence interval is small with a large confidence level, this will usually occur when the sample size is large. The chosen confidence level relates to an α-value, where as an example the chosen confidence level is 95%, then the α-value would be 5% or normally written as 0.05. The α-value will sometimes be needed to find the critical value, that is used to calculate the margin of error, as an example it's used when trying to find the critical value of the confidence interval, when working with a t-distribution.
To set up a confidence interval, the margin of error needs to be computed and then that will be both added and subtracted from the point estimate. This will give the values of the outer bounds of the interval. The margin of error is calculated from this formula:

$$Margin\_of\_error = critical\_value \pm standard\_error$$

The standard error will change depending on which parameter that the confidence interval is estimating, but the general formula for the standard error is:

$$\frac{\sigma}{\sqrt{n}}$$

An example of computing a confidence interval of the mean while working with a standard normal distribution, then the formula for the confidence interval would be this:

$$P(-z_{\alpha/2} < Z < z_{\alpha/2}) = 1 - \alpha$$

Where $1 - \alpha$ is the confidence level. As it's the mean that is being estimated, then instead of Z-score, then μ must be isolated and that is done by multiplying $\frac{\sigma}{\sqrt{n}}$ and subtracting $\bar{X}$ on all sides, then multiplying all side by -1 to remove the minus sign. So the formula for a confidence interval of the mean will look like this:

$$P(\bar{X} - z_{\alpha/2}\frac{\sigma}{\sqrt{n}} < \mu < \bar{X} + z_{\alpha/2}\frac{\sigma}{\sqrt{n}}) = 1 - \alpha$$

This formula will give the upper and lower bounds of the confidence interval.

The interpretation of a confidence interval
To interpret a confidence interval, it would be incorrect to interpret the confidence level of some value x, as the probability of the true parameter being inside of the interval. The reason behind this is that the computed interval is static, so either the value x is inside the interval or it's not. So the correct way of interpreting the confidence interval is by taking multiple samples and computing the confidence interval for all samples, then the value x would reside inside 95% of the confidence intervals. **Kilde for fortolkningen af kofidense intervaller:**
$http://www.drhuang.com/science/mathematics/book/probability_and_statistics_for_engineering_and_the_scienc$

2.5.2 Hypothesis testing

A hypothesis test is used to test an assumption about a population. This is done from a sample of the population, as the information about the population is usually hard to come by. A hypothesis test is set up, by having a null hypothesis and an alternate hypothesis.

$$H_0 = Null\ hypothesis$$

$$H_a = Alternate\ hypothesis$$

When working with hypothesis testing, the hypothesis H_0 is usually represented as the status quo, where as the hypothesis H_a is represented as the opposition. It is also important to note that there is only two outcomes of a hypothesis test, either H_0 is rejected in favor of H_a or H_0 is failed to be rejected. Therefore in no situation can H_0 be stated to be an absolute truth, as there might be other samples where H_0 will be rejected. Therefore in a hypothesis test H_0 needs to be the thing that can be rejected and if H_0 gets rejected, then H_a will become the new status quo until proven otherwise.
In a hypothesis test H_0 will be the assumption that a parameter for two populations is the same, where as H_a can be either one of three assumptions, depending on the intention of the hypothesis test.

$$H_0 : \theta = \theta_0$$

1. $H_a : \theta \neq \theta_0$
2. $H_a : \theta < \theta_0$
3. $H_a : \theta > \theta_0$

When the direction of the rejection is not important and also is unknown, then (1) will be the case. This scenario sets up a two-tailed-test, where the hypothesis test is used to reject H_0 if H_a is either significantly larger or smaller than H_0, this means that the critical area is on both sides of the difference of θ and θ_0. Either (2) or (3) will set up a one-tailed-test, where depending on what is important, either the hypothesis test is used to determine if H_a is significantly bigger or smaller than H_0. This means that the critical area only spans one side

of the difference between θ and θ_0.

Error in hypothesis testing
When making a hypothesis test there is four different possible outcomes. The results are separated by correct decisions and errors. There exist two types of hypothesis errors, called type 1 error and type 2 error. The type 1 error occurs when H_0 is mistakenly rejected and H_0 is true. Type 2 error is the opposite, where H_a is rejected and H_a is true. The types of outcomes occurring from a hypothesis test can be seen in Table 1

	H_0 is true	H_0 is false
Does not reject H_0	Correct decision	Type 2 error
Reject H_0	Type 1 error	Correct decision

Table 1: Outcomes of a hypothesis test

It is possible to compute the probability of a type 1 error occurring, this value is the same as the significance level α. To calculate the probability of a type 2 error occurring, the H_a needs to be defined, more specifically the mean of the sample is needed. Depending on the which parameter is known, different formulas are taking into use. As an example where the standard deviation is known, its a normal distribution and its a one tailed test, then the formula for the Z-score is used, but $\overline{X}$ is changed with $\overline{x}_{crit}$ and μ is changed with μ_1:

$$Z = \frac{\overline{x}_{crit} - \mu_1}{\sigma/\sqrt{n}}$$

The value of $\overline{x}_{crit}$ is the value that separates whether H_0 is rejected or not and μ_1 is the value of the alternative hypothesis. The value of the calculated Z-score is used in a table of areas under the normal curve. This value will be used as the probability of a type 2 error occurring.

3 Polynomial Regression

Polynomial Regression

Linear regression is a model that estimates the relationship between a dependent variable, y, and one or more independent variables, x.

A reasonable relationship between the two in simple regression is the linear relationship:

$$Y = \beta_0 + \beta_1 x$$

Where β_0 is the intercept, and β_1 is the slope.

In a lot of cases, there will be more independent variables, so the relationship for multiple regression will look like this:

$$Y = \beta_0 + \beta_1 x_1 + ... + \beta_n x_n$$

Where n is the number of independent variables, and

$$\beta_2$$

and further shape the curvature and complexity of the curve. Linear models use the method of least squares of the residuals to estimate parameters, in order to find the best fitting line for the data.

In simple linear regression, the random error ϵ is included:

$$Y = \beta_0 + \beta_1 x + \epsilon$$

It is assumed that ϵ is distributed with $\epsilon = 0$ and $\epsilon) = \sigma^2$, and it has consistent variance, which is usually called the *homogeneous variance assumption*. The random error ϵ adds randomness to account for the natural variability in real data, making the model more realistic.

Polynomial regression is a form of linear regression, but the relationship between x and y is an nth-degree polynomial. It fits a nonlinear relationship between the value of x and the corresponding conditional mean of y, meaning the model predicts the expected value of y given x.

That is why it is used when the relationship between the independent variable and the dependent variable is better represented by a curve rather than a straight line, since it can show the nonlinear patterns in the data. In polynomial regression, as mentioned before, there are six assumptions, that always need to be met.

3.1 The method of least squares

To find connections in data, it is necessary to estimate coefficients, β_0 and β_1, in linear models. A widely used method to estimate the coefficients, is the least squares method that was previously mentioned.

Least squares considers the deviation of Y_i for its expected value, where the observations are (X_i, Y_i). This method also requires, that we consider the sum of the n squared deviations. This is denoted by the following function,

$$Q = \sum_{i=1}^{n} (Y_1 - \beta_0 - \beta_1 X_i)^2$$

According to the method of least squares, the estimations of β_0 and β_1 that minimize Q for the given sample observations $(X_1, Y_1), (X_2, Y_2), ..., (X_n, Y_n)$, are called b_0 and b_1.

If an analytical approach is used, the values b_0 and b_1 that minimize Q for any particular set of sample data are given by these simultaneous equations:

$$\sum Y_i = nb_0 + b_1 \sum X_i$$

$$\sum X_i Y_i = b_0 \sum X_i + b_1 \sum X_1^2$$

These equations are called $normalequations$, where b_0 and b_1 are the $pointestimators$ of β_0 and β_1. It is possible to calculate these normal equations simultaneously for b_0 and b_1 through these expressions,

$$b_1 = \frac{\sum (X_1 - \bar{X})(Y_i - \bar{Y})}{\sum (X_i - \bar{X})^2}$$

$$b_0 = \frac{1}{n}(\sum Y_i - b_1 \sum X_i) = \bar{Y} - b_1 \bar{X}$$

Here, $\bar{X}$ and $\bar{Y}$ are the means of X_i and Y_i.

The normal equations can also be derived by differentiating with respect to β_0 and β_1:

$$\frac{\partial Q}{\partial \beta_0} = -2 \sum (Y_i - \beta_0 - \beta_1 X_i)$$

$$\frac{\partial Q}{\partial \beta_1} = -2 \sum X_i (Y_i - \beta_0 - \beta_1 X_i)$$

Then b_0 and b_1 can be set to equal zero,

$$-2 \sum (Y_i - b_0 - b_1 X_1) = 0$$

$$-2 \sum X_i (Y_i - b_0 - b_1 X_1) = 0$$

This can be simplified,

$$\sum_{i=1}^{n} (Y_i - b_0 - b_1 Xi) = 0$$

$$\sum_{i=1}^{n} X_1 (Y_i - b_0 - b_1 Xi) = 0$$

And it can be expanded, so the normal equations are obtained,

$$\sum Y_1 - nb_0 - b_1 \sum X_1 = 0$$

$$\sum X_1 Y_1 - b_0 \sum X_1 - b_1 \sum X_i^2 = 0$$

Solving this will lead to values of b_0 and b_1, that minimize Q, and these are the estimates for β_0 and β_1.

The estimates b_0 and b_1 obtain the minimum when checking the second partial derivatives.

Linear models:

Equations for linear models can be written in matrix terms, where the normal error regression model for simple linear regression is.

$$Y_i = \beta_0 + \beta_1 X_i 0 \epsilon_i$$

Which implies that,

$$Y_1 = \beta_0 + \beta_1 X_1 + \epsilon_1$$
$$Y_2 = \beta_0 + \beta_2 X_2 + \epsilon_2$$
$$\vdots$$
$$Y_n = \beta_0 + \beta_n X_n + \epsilon_n$$

The observations vector Y is,

$$Y_{n\times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}$$

The X matrix is,

$$X_{n\times 2} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$$

The β vector is,

$$\beta_{2\times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

And the ϵ vector is,

$$\epsilon_{n\times 1} = \begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

This can be written in matrix terms as,

$$Y_{n\times 1} = X_{n\times 2} \cdot \beta_{2\times 1} + \epsilon_{n\times 1}$$

Where,
Y is a vector of response
β is a vector of parameters
X is a matrix of constants, called det design matrix
ϵ is a vector of independent normal random variables with expectation

This can be shown in columns,

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

If the dependent variable Y has more than one independent variable in a linear model, the equation looks like this,

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + ... + \beta_p - 1X_{i,p-1} + \epsilon_i$$

In matrix terms it is,

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & ... & X_{1,p-1} \\ 1 & X_{21} & ... & X_{2,p-1} \\ \vdots & \vdots & & \vdots \\ 1 & X_{n1} & ... & X_{n,p-1} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p - 1 \end{bmatrix} + \begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

The Y and ϵ vectors are the same as in the simple linear regression matrix. The β vector has additional parameters, and the X matrix now has a column of n observations for each $p - 1X$ variables.

For multiple linear regression, the coefficients can still be found through the method of least squares,

$$Q = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i 1 - ... - \beta_{p-1} X_{i,p-1})^2$$

3.2 Assumptions

3.2.1 Homoscedasticity

One of the assumptions of a polynomial regression is that homoscedasticity is fulfilled. Homoscedasticity is the assumption of constant error variance, where observations in a dataset would exhibit errors that have roughly the same spread across all levels of the independent variable.
If this assumption is not upheld, then this will cause the standard error to be

biased and therefore not trustworthy. This problem causes further testing involving this standard error to become wrong, an example is the hypothesis test. The reason for the assumption needs to be upheld, comes from how the regression is created. The regression is created via the ordinary least square method, that requires the assumption of homoscedasticity to be upheld.
A way to display homoscedasticity is through the variance-covariance matrix. The matrix shows whether the data contains homoscedasticity or heteroscedasticity through the diagonal values. If the matrix contains all the same values through the diagonal, then the assumption of homoscedasticity is upheld, else the data contains heteroscedasticity. This is a showcase of the variance-covariance matrix with homoscedasticity:

Every position in the matrix is calculated, then the diagonal will tell if the data contains homoscedasticity or heteroscedasticity. The positions that are not on the diagonal should be zero else the data contains another problem, that is autocorrelation, meaning that the observations in the data set are correlated.

Source: https://openpublishing.library.umass.edu/pare/article/id/1590/

3.2.2 No multicollinearity

Perfect multicollinearity is a term used for describing a perfect linear relationship between two or more independent variables. This relationship occurs when an independent variable can be perfectly predicted from other independent variables. In mathematical terms, this could be written as a linear regression:

$$X_1 = c + \beta_1 \cdot X_2 + ... + \beta_n \cdot X_n$$

Where $X_1...X_n$ is all the independent variables that have a perfect linear relationship. The coefficients are represented by $\beta_1...\beta_n$ and they are the amount that X_1 changes when their relative independent variable changes. Lastly c is the intercept and represents the value of X_1, when all other independent variables are zero.
The regression model can feel the effects of multicollinearity even without there being perfect multicollinearity. A strong linear relationship is enough to have an effect on the model. The problem caused by multicollinearity, is that as it increases the variance of the value that the coefficients can receive also increases. Where as perfect multicollinearity will make the model unable to estimate a value of one coefficient, due to the perfect linearity between the independent variables.
Source: https://ekja.org/upload/pdf/kja-19087.pdf

Detecting multicollinearity

To check for multicollinearity in a dataset, a good approach is pearson´s correlation coefficient. This will make a table of all pairwise correlation, this means that all combinations of independent variables are checked for multicollinearity. This can be seen in **table...**. The correlation coefficient is calculated through this formula:

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

Where n is the number of observations, with x and y representing the two variables tested for correlation and the pairwise correlation coefficient is denoted as r. When computing the value of r, the value will be in a range: $-1 \leq r \leq 1$. If the value of r is -1 or 1, that indicates a perfect either negative or positive correlation and if the value is 0, then there is no correlation between the variables.

4 Pseudo Random Number Generator

To generate the dataset, we use a Pseudo-Random Number Generator (PRNG). PRNGs are algorithms that produce sequences of numbers that appear random but are actually deterministically generated from an initial seed value. While these numbers are not truly random, they are sufficiently unpredictable for many practical applications. Random numbers are widely used in fields such as statistics, game theory, cryp- tography, and simulations. These applications require numbers that behave as if they were random, yet can be reproduced when needed. This is where PRNGs come in—they allow for repeatable randomness, making them ideal for controlled experiments, testing, and security. This chapter will explore the key concepts behind PRNGs. Before going into the mechanics of these generators, it is important to first understand what 'random' means and the characteristics that define truly random numbers.

4.1 Properties of PRNGs

The quality of a PRNG is determined by several key factors that influence its use for different applications. Some of the properties of a good PRNG is properties: Independency, a large period and reproducibility The numbers produced by the PRNG should be statistically independent, en- suring that each generated value exhibits no correlation with previous numbers or other sequences. This implies that knowledge of previously generated num- bers or sequences provides no advantage in predicting the next output. A PRNG operates within a specific interval before its sequence begins to repeat. A high-quality PRNG has a long interval, delaying repetition and enhancing its unpredictability. Conversely, a PRNG with a shorter period becomes more pre- dictable and less suitable for practical use. A key feature of a PRNG is its ability to reproduce the same sequence of num- bers when given a specific seed. This property is particularly useful in testing and simulation scenarios, where it is essential to generate identical sequences multiple times for consistency and reproducibility In addition, a PRNG must be fast and efficient to prevent it from introducing performance bottlenecks within an application. The speed of number generation directly impacts computational efficiency, especially in applications requiring a large volume of random numbers. An inefficient PRNG can significantly slow down processes, undermining the overall performance of the system. Therefore, balancing randomness and efficiency is essential for practical applications

4.2 Linear Congruential Generator

Linear Congruential Sequence (LCS) is a commonly used approach to generate pseudo-random numbers. LCS generates a sequence of numbers using a linear recurrence relation LCS is expressed as:

$$X_{n+1} = (aX_n + c) \bmod m.$$

where X_0 is the seed, a is the multiplier, c is the increment, and m is the modulus.

Example: Given $a = 5$, $c = 1$, $m = 16$, and $X_0 = 7$:

$$X_1 = (5 \cdot 7 + 1) \bmod 16 = 4$$

$$X_2 = (5 \cdot 4 + 1) \bmod 16 = 5$$

$$X_3 = (5 \cdot 5 + 1) \bmod 16 = 10$$

$$X_4 = (5 \cdot 10 + 1) \bmod 16 = 3$$

This sequence has a period of 16. In an LCG, the period can be as large as m, but choosing parameters carefully is crucial to achieving long periods. Therefore

5 Monte Carlo Bootstrap

5.1 Assumptions

6 Metrics

To evaluate the quality of a regression model, i. e. how well the model is performing. All the metrics provide some kind of score that reflects the reliability of the model's predictions..

Metrics in are measures used to evaluate how well a model performs. Metrics assess the accuracy of the model's predictions compared to actual values. Common metrics like R^2 and MBE help determine how closely predictions match real outcomes, while others like bias and variance reveal systematic errors and model stability. Metrics help model selection improvement by providing objective feedback on performance. They're essential for comparing models, detecting underfitting or overfitting, and ensuring predictions are reliable for real-world use.

6.1 R-Squared

The R^2 measures how much better the model is at guessing than guessing the mean of the variable. It is calculated using the Total Sum of Squares (TSS) and the Sum of Squared Errors (SSE) with this formula:

$$R^2 = \frac{TSS - SSE}{TSS}.$$

TSS explains how much the values of a dataset vary from the mean and is calculated by:

$$\sum_{i=1}^{n}(y_i - \overline{y})^2,$$

where y_1 is the actual value and $\overline{y}$ is the mean of all actual values.

The SSE is how far the predictions from the model are from the actual values and is calculated by:

$$\sum_{i=1}^{n}(y_i - \hat{y_i})^2,$$

where $\hat{y_i}$ is the predicted value from the model. The errors are squared to make all values positive, highlight larger mistakes more strongly, and stay consistent with how variance is calculated in statistics.

R^2 explains much of the variance explained by the model. The value of R^2 will therefore normally be $0 \leq R^2 \geq 1$, where 0 means that the model explains none of the variance, a value of 1 would mean that the model explains all the variance, while 0.5 means that the model explains 50% of the variance. If the R^2-value is negative, it means that the model is performing so bad, that it would be better so simply predict the mean for all observations.

Although widely used, the R^2-score should not be relied upon as the only metric of model performance due to several shortcomings. Primarily, it evaluates the proportion of variance in the dependent variable explained by the model, but does not reflect the accuracy of individual values. As a result, a model can achieve a high R^2 despite making major errors on specific data points. In addition, R^2 is vulnerable to overfitting, especially when the model becomes overly complex and starts fitting the noise in the data instead of underlying trends. Another critical issue is that R^2 does not adjust for the number of predictors in the model. It will never decrease when more features are added, even if those features are irrelevant. For a more reliable assessment, alternative metrics should be used alongside R^2 to evaluate a regression model.

6.2 Mean Bias Error

Mean Bias Error (MBE) is a metric that measures the average difference between the actual values and the model's predictions. Unlike other metrics, MBE does not emphasize the magnitude of the error but instead indicates whether the model systematically overestimates or underestimates, revealing potential bias in the predictions.

The formula for MBE is:

$$MBE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)$$

Here $\hat{y}_i$ is the predicted value, y_i is the actual value, and n is the number of observations.

When interpreting MBE there are three different cases. If the $\mathbf{MBE} \geq 0$, the model tends to over-predict the values compared to the actual values. If the $\mathbf{MBE} \leq 0$, the opposite is the case, and the model tends to under-predict the values. If the $\mathbf{MBE} \approx 0$ there is no consistent bias in either direction.

As mentioned, the MBE measures the bias of the model, if it generally predicts values too high or too low compared to the actual values. This means that we cannot use MBE to estimate the size of the error or the overall quality of the model. If two actual values are 100 and the model predicts 120 and 80 the error calculated with $\hat{y} - y$ is respectively $+20$ and -20. Because the absolute or squared values are not used, these errors will cancel each other out. Therefore, the size of the error is not computed. Instead, to understand the size of the errors, Root Mean Square Error can be used, which penalizes large deviations more heavily.

6.3 Root Mean Square Error

https://www.sciencedirect.com/topics/earth-and-planetary-sciences/root-mean-square-error
Root Mean Square Error (RMSE) is a metric used to evaluate regression models. It measures the average size of prediction errors. Since it squares the errors, it punishes larger mistakes harder than smaller ones, which is useful if the objective is to emphasize the impact of larger deviations of the actual values.
The formula used to calculate RMSE:

$$\textbf{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y_i} - y_1)^2}$$

As before $\hat{y_i}$ is the predicted value, y_i is the actual value, and n is the number of observations.
The idea is to find the error by subtracting the actual value from its prediction, square the error so negatives and positives do not cancel out (like in MBE) and large errors will stand out. Then the average of all squared errors is found, and the square root is taken to bring the result back to the original scale.

The value of the result of RMSE will always be a non-negative number and the closer RMSE is to 0, the better the model is performing. The scale and unit of RMSE is the same as the target variable. So, if the data is about 'Miles Per Gallon', a RMSE of 2 means that the predictions of the model are 2 miles off, on average. Therefore, RMSE is most useful when the objective is comparing different models on the same dataset, or at least on datasets that are on the same scale, and in the same units. This also means an RMSE of 5 can be great if the values of the target variable ranges from 1-1000, but awful if the range is 1-10. As the other metrics, RMSE should be used alongside other metrics like better picture of the models performance. RMSE does not explain why a model performs well or bad. To investigate that, bias-variance decomposition can be used to split error into systematic bias and model instability.

6.4 Bias-Variance

To understand the sources of error in a model's predictions, the bias-variance decomposition framework can be used. Bias and variance describe two different ways a model can make mistakes. Bias measures how far, on average, the model's predictions are from the true values. Variance describes how sensitive the model is to changes in the training data; it measures how much the model's predictions vary when trained on different datasets.

The ideal case is when both bias and variance are low, meaning the model is both accurate and stable. This framework is especially useful for diagnosing underfitting, which is caused by high bias, and overfitting, which is caused by high variance. By examining both bias and variance, the decomposition helps in understanding the trade-off between model complexity and generalization.

6.4.1 Variance

The variance of a model, for a single input, can be calculated using this formula:

$$\mathbf{Var}[\hat{f}(x)] = \frac{1}{M}\sum_{j=1}^{M}(\hat{f}_j(x) - \overline{\hat{f}}(x))^2$$

Where:

- M is the number of models or simulations,
- $\hat{f}_j(x)$ is the prediction by model j at input x,
- $\overline{\hat{f}}(x)$ is the mean prediction across all M models at input x.

This formula measures how much predictions vary at a specific input x across multiple model runs. To calculate the overall variance across the input space, the average of the variances at all test inputs is taken:

$$\textbf{Overall Model Variance} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{Var}[\hat{f}(x_i)]$$

This overall measure is beneficial because it captures how the model's prediction variability behaves across the entire dataset, rather than at just one point. A model with high variance is likely too complex and sensitive to the noise in the data.

6.4.2 Bias

Bias measures how far the model's average prediction is from the true value. Since bias can be positive or negative, it is typically squared to focus on its magnitude. The squared bias for a specific input x is calculated as:

$$\mathbf{Bias}^2(x) = (\overline{\hat{f}}(x) - f(x))^2$$

The overall squared bias across all inputs is calculated by averaging over the test set:

$$\textbf{Bias}^2 = \frac{1}{n}\sum_{i=1}^{n}(\overline{\hat{f}}(x_i) - f(x_i))^2$$

High bias typically indicates that the model is too simple to capture the underlying structure of the data, resulting in systematic under- or over-prediction.

6.5 Confidence-intervals

7 Problem Statement

8 Classical Regression

9 Comparison between Regressions

Bootstrap	Lower	Upper
X.Intercept.	22.679714	24.215509
poly.acceleration..2.1	-7.872243	13.971982
poly.acceleration..2.2	0.829106	20.456479
poly.cylinders..2.1	-94.973539	-70.848648
poly.cylinders..2.2	-4.912405	13.539521
poly.model.year..2.1	47.874788	65.900777
poly.model.year..2.2	10.966639	26.904885
poly.origin..2.1	18.520674	39.663935
poly.origin..2.2	-12.998969	6.919619

klassisk model	Lower	Upper
(Intercept)	23.067281	23.824556
poly(acceleration, 2)1	-6.406934	12.842683
poly(acceleration, 2)2	2.348050	19.352905
poly(cylinders, 2)1	-94.611185	-71.254636
poly(cylinders, 2)2	-4.040154	12.576736
poly(model.year, 2)1	48.963118	65.465928
poly(model.year, 2)2	11.269143	26.988917
poly(origin, 2)1	19.473871	38.413961
poly(origin, 2)2	-11.324497	4.955582

	Bootstrap SE
X.Intercept.	0.39179151
poly.acceleration..2.1	5.57260870
poly.acceleration..2.2	5.00707501
poly.cylinders..2.1	6.15442196
poly.cylinders..2.2	4.70721037
poly.model.year..2.1	4.59855108
poly.model.year..2.2	4.06595361
poly.origin..2.1	5.39378812
poly.origin..2.2	5.08136578

	klassisk model SE
(Intercept)	0.193186
poly(acceleration, 2)1	4.910707
poly(acceleration, 2)2	4.338053
poly(cylinders, 2)1	5.958413
poly(cylinders, 2)2	4.239080
poly(model.year, 2)1	4.209978
poly(model.year, 2)2	4.010220
poly(origin, 2)1	4.831744
poly(origin, 2)2	4.153158

10 Discussion

11 Conclusion

12 Litteratur

13 latextables