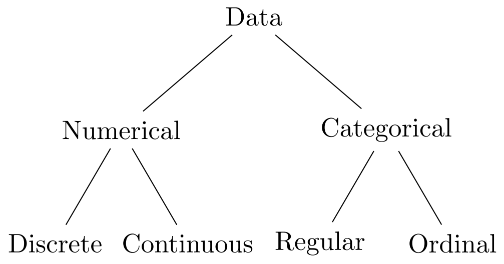
1 Descriptive Statistics



Observational data come from observing the world as it is.

Experimental data are generated by designing an experiment to test the effect of some explanatory variable, e.g. giving a treatment to the treatment group while not giving it to the control group (/only pretending to treat them).

A summary **statistic** is a number summarising the data, e.g. the mean, median (middle value), mode (most common value), variance.

Imagine we take a sample of n observations from a population and calculate a sample statistic. Now imagine we take another n observations and another n observations, etc., and each time we calculate the sample statistic. We can then plot the distribution of the sampling statistic - this is a **sampling distribution**. By the CLT, for a large number of successive random samples (big n), the distribution of sample means calculated for each sample will become approximately normally distributed.

If you take a lot of sample means from the same population, you may get a different result each time and perhaps none of the sample means would exactly equal the true population mean. Therefore, we need to specify a **margin of error** - a confidence interval. Point estimates vary from sample to sample, and we quantify this variability with what is called the standard error - the standard deviation of the sampling distribution:

$$SE = \sqrt{\mathrm{Var}(\bar{X})} = \sqrt{\frac{\sigma^2}{n}}$$

Confidence interval: point estimate $\pm z^* \times SE$, where $z^* \times SE$ is the margin of error.

1.1 Connection with Probability Theory

Definition

Consider a dataset consisting of n repeated measurements. Then the observations can be modelled by a **statistical model** as realisations of random variables $X_1, X_2, \dots, X_n$ such that they are **i.i.d.** (independent and identically distributed):

1. $X_1, X_2, \dots, X_n$ have the same probability distribution.
2. $X_1, X_2, \dots, X_n$ are independent.

Dataset with observations $x_1, \dots, x_n$	**Model with random variables** $X_1, \dots, X_n \sim f$
Sample mean $\bar{x}_n = \frac{1}{n}\sum_{i=1}^n x_i$	Expectation $E[X_i]$
Sample median $m = \text{median}(x_1, \dots, x_n)$	50-th percentile $q_{0.5} = F^{-1}(\frac{1}{2})$
Sample variance $s_n^2 = \frac{1}{n-1}\sum_{i=1}^n (x_i - \bar{x}_n)^2$	Variance $\mathrm{Var}(X_i)$
Sample standard deviation $s_n = \sqrt{s_n^2}$	Standard deviation $\sqrt{\mathrm{Var}(X_i)}$
Empirical quantile $q_n(p)$ s.t. $\frac{\# x_i \leq q_n(p)}{n} \leq p$	p-th quantile $q_p = F^{-1}(p)$
Sample correlation coefficient $r_{x,y}$	Correlation coefficient $\rho(X, Y)$

1.2 Univariate Descriptive Statistics

Definition

For a dataset $x_1, x_2, \dots, x_n$, the **sample variance** is defined as the unbiased estimator

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

The sample standard deviation s is the square root of the variance.

A boxplot and a histogram can be used to visualise a univariate dataset with its statistics and distribution.

A normalised **histogram** has area equal to one. The height of the bar of a given bin is equal to the proportion of datapoints divided by the size of the bin.

1.2 Bivariate Descriptive Statistics

Definition

For a bivariate dataset $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, the **sample correlation coefficient** is

$$r_{x,y} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}} = \frac{s_{xy}}{\sqrt{s_{xx} s_{yy}}}$$

Properties:

1. $-1 \leq r_{x,y} \leq 1$.
2. Thus, the sample correlation coefficient is independent of units of measurement.

A **scatterplot** can be used to investigate the relationship between two variables.

A **spurious correlation** is one where there is correlation without causation. A **latent variable** is an unobserved third variable causing a change in two strongly correlated variables.

```
data(mtcars)
# View(mtcars)
min(mtcars$wt)
max(mtcars$mpg)
mtcars[mtcars$X == "Duster 360",]
median(c(4, 18, 11, 9, 12, 4, 6, 7))
help(mtcars)
boxplot(mtcars$wt)
round(quantile(mtcars$wt), 3)
round(IQR(mtcars$wt), 3)

data(airquality)
hist(airquality$Temp, breaks=25)
qqnorm(airquality$Temp)
qqline(airquality$Temp, col='red')
hist(airquality$Ozone)
qqnorm(airquality$Ozone)
qqline(airquality$Ozone, col='red')
qqplot(qexp(ppoints(airquality$Ozone)), airquality$Ozone)
qqline(airquality$Ozone, distribution=qexp, col='blue') # not exponential either

set.seed(0)
x <- rnorm(5, mean=0, sd=1)
x
qqnorm(x)
qqline(x, col='red')
# The points are generated randomly from a normal distribution.
# So, it is extremely unlikely that they lie on a straight line.
# When there are more points, small individual deviations do not matter as much,
# and we will be able to draw an almost straight line through the points.

x <- c(3, 5, 7)
y <- c(8, 4, 6)
plot(x, y, xlim = c(0, 10), ylim = c(0, 10), pch = 16, col = "blue", xlab = "x", ylab = "y")
text(x, y, labels = paste("(", x, ",", y, ")", sep = ""), pos = 3)
correlation_coefficient <- cor(x, y)
correlation_coefficient # -0.5

# install.packages("ggplot2movies")
library(ggplot2movies)
data(movies)
plot(movies$year, movies$votes, xlab = "Year", ylab = "Votes")
round(cor(movies$year, movies$votes), 3)

set.seed(0)
x <- rexp(10, 3)
lambda_hat <- 1 / mean(x) # mean = 1 / lambda
round(lambda_hat, 2)
lambda_hat <- log(2) / median(x) # median = log(2) / lambda
round(lambda_hat, 2)
lambda_hat <- sqrt(1 / var(x)) # var = 1 / lambda^2
round(lambda_hat, 2)
set.seed(0)
x <- rexp(100, 3)
lambda_hat <- 1 / mean(x) # mean = 1 / lambda
round(lambda_hat, 2)
lambda_hat <- log(2) / median(x) # median = log(2) / lambda
round(lambda_hat, 2)
lambda_hat <- sqrt(1 / var(x)) # var = 1 / lambda^2
round(lambda_hat, 2)
# The estimates get better as the number of data points increases.
```

2 Estimator Theory

Often, an unknown quantity of interest is represented by some parameter of the model distribution, and one wants to estimate this parameter by means of the observations.

Definition

Suppose we model a dataset $x_1, x_2, \ldots, x_n$ as the realisation of random variables $X_1, X_2, \ldots, X_n$.

Then the random variable $T = h(X_1, X_2, \ldots, X_n)$ is called an **estimator** and any $t = h(x_1, x_2, \ldots, x_n)$ for some function h is called an **estimate**. The distribution of T is called the **sampling distribution**.

Definition

Let $X_1, X_2, \ldots, X_n$ be random variables with a distribution that depends on some parameter θ. Let $T = h(X_1, X_2, \ldots, X_n)$ be an estimator for θ.

Then the **mean squared error (MSE)** for T with respect to θ is

$$\begin{aligned}\text{MSE}(T;\theta) &= E_\theta[(T-\theta)^2] \\ &= \text{Var}_\theta(T-\theta) + (E_\theta[T-\theta])^2 && \text{by definition} \\ &= \text{Var}_\theta(T) + (E_\theta[T]-\theta)^2 && \text{as } \text{Var}_\theta(\theta)=0, \\ & && E_\theta[\theta]=\theta\end{aligned}$$

That is, the MSE is composed of variance and bias:

- $\text{Var}_\theta(T)$ measures the variation of T around $E_\theta[T]$,
- $E_\theta[T] - \theta$ measures the average deviation of T from θ.

Definition

Let T be an estimator with a sampling distribution that depends on θ.

Then $E_\theta[T] - \theta$ is called the **bias** of T with respect to θ.

- When the bias is positive, the estimator T systematically produces values that are larger than θ.
- When the bias is negative, the estimator systematically produces values that are smaller than θ.
- Only when the bias is zero, the realisations of T are on average equal to θ.

Definition

Let T be an estimator with a sampling distribution that depends on θ.

When $E_\theta[T] = \theta$, T is an **unbiased** estimator for θ.

Example: The sample mean is an unbiased estimator for the mean:

$$E[\bar{X}_n] = E\Big[\frac{1}{n}\sum_{i=1}^{n} X_i\Big] = \frac{1}{n}\sum_{i=1}^{n} E[X_i] = \frac{1}{n} n\mu = \mu$$

Theorem

Suppose T is an unbiased estimator for a parameter θ. Suppose we want to estimate $g(\theta)$ for some function g.

Then $g(T)$ is not necessarily an unbiased estimator for $g(\theta)$.

Generally, expectation only carries over by linearity, but not necessarily for non-linear functions.

Example: If T is unbiased for θ, $E[T] = \theta$. Then $g(T) = 2 + 3T$ is unbiased for $g(\theta)$: $E[2 + 3T] = 2 + 3E[T] = 2 + 3\theta$.

Example: The sample variance is an unbiased estimator for the model variance, but the sample standard deviation is a biased estimator for the model standard deviation:

$$\begin{aligned}E[S_n^2] &= \frac{1}{n-1} E\Big[\sum_{i=1}^{n}(X_i - \bar{X}_n)^2\Big] \\ &= \frac{1}{n-1}(n-1)\sigma^2 \\ &= \sigma^2\end{aligned}$$

By Jensen's inequality, for the convex function $E[S_n^2]$:

$$\sigma^2 = E[S_n^2] > (E[S_n])^2 \Rightarrow E[S_n] < \sigma$$

Thus, S_n has negative bias with respect to σ.

A good estimator should ideally have both low variance and low bias.

Zero bias $E_\theta[T] = \theta$ is a desirable property but **overall the MSE, composed of variance and bias, determines the performance of an estimator T.**

For this reason, in some situations a biased estimator with small variance may be preferable over an unbiased estimator.

Different methods of estimation arise from different principles:

- Method of moments: based on the *moments* of the distribution.
- Maximum likelihood method: based on the *form* of the distribution.

However, although different distributions may have the same moments, the forms of their distributions may be different. For example, the two distinct distributions $X \sim \text{Exp}(1)$ and $Y \sim \mathcal{N}(1, 1)$ both have first and second-order moments $E[X] = 1 = E[Y]$, $E[X^2] = 2 = E[Y^2]$.

In such a case, an estimation method based on the form of the distribution (rather than its moments) provides more information; and likely a better estimator (with a lower MSE).

2.1 The Method of Moments

Definition

Given a random variable X, for $k = 1, 2, \ldots$, the expectation of X^k is called the k-th **moment**:

$$M^{(k)} = E[X^k]$$

Definition

Given a dataset $x_1, x_2, \ldots, x_n$, for $k = 1, 2, \ldots$, the mean of x_i^k is called the k-th **sample moment**:

$$M_n^{(k)} = \frac{1}{n}\sum_{i=1}^{n} x_i^k$$

Example: If $X \sim \mathcal{N}(\mu, \sigma^2)$, then

$$\begin{aligned}\sigma^2 = \mathrm{Var}(X) &= E[X^2] - (E[X])^2\\ &= \frac{1}{n}\sum_{i=1}^{n} x_i^2 - \left(\frac{1}{n}\sum_{i=1}^{n} x_i\right)^2\\ &= \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x}_n)^2\end{aligned}$$

(Note: The *sample* variance is commonly divided by $(n-1)$ so it will be an unbiased estimator.)

The Method of Moments

1. If the model distribution has more than one parameter, use more than one equation to solve for the parameters.
2. When multiple moments can be expressed in terms of the same parameters, then use the smallest value of k for which the k-th moment can be expressed in the parameters.

Example: $X_1, X_2, \ldots, X_n \sim \mathcal{N}(\mu, \sigma^2)$ has two parameters:

$$\frac{1}{n}\sum_{i=1}^{n} x_i = E[X_1] = \mu \quad \Rightarrow \quad \hat{\mu} = \bar{X}_n$$

$$\frac{1}{n}\sum_{i=1}^{n} x_i^2 = E[X_1^2] = \mathrm{Var}(X_1) + (E[X_1])^2 = \sigma^2 + \mu^2$$

$$\Rightarrow \quad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n} X_i^2 - \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i^2 - \bar{X}_n = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2$$

Example: $X_1, X_2, \ldots, X_n \sim \mathcal{N}(0, \sigma^2)$ has one parameter, but the first moment is zero: $E[X_1] = 0$.

$$E[X_1^2] = \mathrm{Var}(X_1) + (E[X_1])^2 = \sigma^2 + 0 \quad \Rightarrow \quad \hat{\sigma} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} X_i^2}$$

Definition

The **moment generating function** of a random variable X for $t \in \mathbb{R}$ is

$$M_X(t) = M(t) = E[e^{tX}] = \begin{cases}\sum_x e^{tx} p_X(x) & \text{if } X \text{ is discrete}\\ \int_{-\infty}^{\infty} e^{tx} f_X(x) & \text{if } X \text{ is continuous}\end{cases} \quad \text{s.t.} \quad M(0) = 1 = \begin{cases}\sum_x p_X(x) & \text{if } X \text{ is discrete}\\ \int_{-\infty}^{\infty} f_X(x) & \text{if } X \text{ is continuous}\end{cases}$$

Theorem

The derivatives of the moment generating function of a random variable generate its moments, evaluated at $t = 0$:

$$M^{(k)} = E[X^k] = \frac{d^k}{dt^k} M(t)\Big|_{t=0}, \quad k = 1, 2, 3, \ldots$$

Theorem

The moment generating function of the sum of X, Y independent random variables is the product of their generating functions:

$$M_{X+Y}(t) = M_X(t) M_Y(t)$$

Examples: $E[X] = M'(0)$, $\quad \mathrm{Var}(X) = M''(0) - M'(0)^2$

$\mathrm{Ber}(p) : M(t) = pe^t + 1 - p$, $\quad \mathrm{Bin}(n, p) : M(t) = (pe^t + 1 - p)^2$, $\quad \mathcal{N}(\mu, \sigma^2) : M(t) = e^{t\mu + t^2\sigma^2/2}$

2.2 The Maximum Likelihood Method

Definition

Consider a dataset $x_1, x_2, \ldots, x_n$ modelled as realisations of independent discrete random variables $X_1, X_2, \ldots, X_n$ whose distribution depends on a parameter θ. The **likelihood** is the product of marginal probabilities:

$$L(\theta) = P_\theta(X_1 = x_1) P_\theta(X_2 = x_2) \ldots P_\theta(X_n = x_n)$$

The **maximum likelihood estimate (MLE)** for θ is the value of θ that maximises $L(\theta)$ over all values of θ:

$$\hat{p} = \arg\max_\theta L(\theta) = \arg\max_\theta \log L(\theta)$$

(In practice, maximising $\log L(\theta)$ is often easier.)

Definition

Consider a dataset $x_1, x_2, \ldots, x_n$ modelled as realisations of independent continuous random variables $X_1, X_2, \ldots, X_n$ whose density f_θ depends on a parameter θ. The **likelihood** is the product of marginal densities:

$$L(\theta) = f_\theta(x_1) f_\theta(x_2) \ldots f_\theta(x_n)$$

The **maximum likelihood estimate (MLE)** for θ is the value of θ that maximises $L(\theta)$ over all values of θ:

$$\hat{p} = \arg\max_\theta L(\theta) = \arg\max_\theta \log L(\theta)$$

In general it is often true that the maximum likelihood estimator has the lowest MSE (for large n), of the asymptotically unbiased estimators.

```
set.seed(0)
n <- 10
n_exp <- 10000
# Estimator based on variance
K_hat_var <- 1:n_exp
for (i in 1:n_exp) {
  x <- sample(1:1000, n, replace=FALSE)
  K_hat_var[i] <- sqrt(12 * var(x) + 1)
}
mean(K_hat_var)
var(K_hat_var)
# Estimator based on median
K_hat_median <- 1:n_exp
for (i in 1:n_exp) {
  x <- sample(1:1000, n)
  K_hat_median[i] <- 2 * median(x) - 1
}
mean(K_hat_median)
var(K_hat_median)
# Estimator based on mean
K_hat_mean <- 1:n_exp
for (i in 1:n_exp) {
  x <- sample(1:1000, n)
  K_hat_mean[i] <- 2 * mean(x) - 1
}
mean(K_hat_mean)
var(K_hat_mean)
# Plot estimators
hist(K_hat_var, col=’green’, breaks=seq(0, 2000, 100), density=50)
hist(K_hat_median, col=’red’, breaks=seq(0, 2000, 100), density=50, add=TRUE)
hist(K_hat_mean, col=’blue’, breaks=seq(0, 2000, 100), density=50, add=TRUE)
# Why is the estimator based on the median different from the estimator based on the average, even though
# their theoretical values are the same?
# The estimators happen to have the same expectation, but they are different random variables.

m <- 500
n <- 100
p <- 0.5
N <- 1000
T1 <- 1:N
T2 <- 1:N
for (i in 1:N) {
  X <- rbinom(m, size=1, prob=p)
  Y <- rbinom(n, size=1, prob=p)

  T1[i] <- (mean(X) + mean(Y)) / 2
  T2[i] <- (sum(X) + sum(Y)) / (m + n)
}
mean(T1)
mean(T2)
MSE_T1 <- mean((p - T1)^2)
MSE_T2 <- mean((p - T2)^2)
MSE_T1
MSE_T2
# Smaller MSE gives a better estimator.
```

3 Hypothesis Testing

Definition

The **p-value** for a hypothesis test is the probability, under the assumption of H_0, that the test statistic has its observed value as an outcome, or a value that is even more extreme in the direction of H_1.

A small p-value implies that random variation because of the sampling process alone is not likely to account for the observed difference.

Therefore, with a small p-value, we reject H_0:

Definition

Statistical significance: If the p-value is less than some reference value, usually $\alpha = 0.05$, then data provide statistically significant evidence against the null hypothesis.

- Reject if $p \leq \alpha$.
- Fail to reject if $p > \alpha$.

Definition

Errors:

- Type I Error (false positive): Rejecting the null hypothesis when it's actually true.
- Type II Error (false negative): Accepting the null hypothesis when it's actually false.

By reducing the rate of one type of error, you risk increasing the rate of the other type.

But with more and better data it is possible to reduce both error rates simultaneously.

Definition

Power: the probability of correctly rejecting the null hypothesis: (where β is the probability of a type I error)

$$1 - \beta = P(X \geq c)$$

Example: Suppose you are given a number v, which is a realisation of a random variable $V \sim \mathcal{N}(\mu, 1)$. Consider the following hypotheses: $H_0 : \mu = 0, H_1 : \mu \neq 0$. You decide to reject H_0 when $|v| \geq 2.5$.

The probability of committing a type I error is $P(|V| \geq 2.5) = P(V \leq -2.5) + P(V \geq 2.5) = 2 \cdot P(V \leq -2.5) = 2 \cdot P\big(\frac{V-\mu}{\sigma} \leq \frac{-2.5-\mu}{\sigma}\big) = 2 = P\big(Z \leq \frac{-2.5-0}{1}\big) = 2 \cdot P(Z \leq -2.5) = 2 \cdot 0.0062 = 0.0124$.

A z-score measures the number of standard deviations that a datapoint x is from the mean μ.

- When x is 1 standard deviation larger than the mean, then $z = 1$.
- When x is 2 standard deviations smaller than the mean, then $z = -2$.

3.1 The One-Sample t-Test

Let $H_0 : \mu = \mu_0, H_1 : \mu \neq \mu_0$ for some μ_0. Since $\bar{X}_n \approx \mu$ by the LLN, so $||\bar{X}_n - \mu_0|| \approx 0$ is in favour of the null hypothesis and $||\bar{X}_n - \mu_0|| \gg 0$ is in favour of the alternative hypothesis.

However, a difference is not a representative test statistic unless it is compared with something - the standard deviation:

$$\begin{aligned}\sqrt{\mathrm{Var}(\bar{X}_n - \mu_0)} = \sqrt{\mathrm{Var}(\bar{X}_n)} &= \sqrt{\mathrm{Var}\Big(\frac{1}{n}\sum_{i=1}^{n} X_i\Big)} \\ &= \sqrt{\frac{1}{n^2}\sum_{i=1}^{n} \mathrm{Var}(X_i)} \qquad \text{for independent } X_i \\ &= \sqrt{\frac{1}{n^2} n\sigma^2} \\ &= \frac{\sigma}{\sqrt{n}}\end{aligned}$$

Because the true value of σ is unknown, it is replaced by the sample standard deviation $\frac{S_n}{\sqrt{n}}$, where $S_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2$.

Definition

Let $H_0 : \mu = \mu_0, H_1 : \mu \neq \mu_0$ for some μ_0. The **test statistic** T for a hypothesis test is

$$T = \frac{\bar{X}_n - \mu_0}{S_n/\sqrt{n}}$$

$T \approx 0$ is in favour of the null hypothesis, while $|T| \gg 0$ is against the null hypothesis.

Since independent $X_1, X_2, \ldots, X_n \sim \mathcal{N}(\mu, \sigma^2)$, the sample mean $\bar{X}_n \sim \mathcal{N}\big(\mu, \frac{\sigma^2}{n}\big)$ and the hypothetical test statistic $\frac{\bar{X}_n - \mu_0}{\sigma\ \sqrt{n}} \sim \mathcal{N}(0, 1)$.

Theorem

Let $X_1, X_2, \ldots, X_n$ be independent normally distributed random variables. Then the random variable

$$T|H_0 = \frac{\bar{X}_n - \mu_0}{S_n/\sqrt{n}} \sim t(n-1)$$

that is, the test statistic follows a t-distribution with $n-1$ degrees of freedom.

Definition

A continuous random variable has a **t-distribution** with parameter m, if it has a probability density

$$f(x) = k_m\big(1+\frac{x^2}{m}\big)^{-\frac{m+1}{2}} \text{ for } -\infty < x < \infty$$

The distribution is denoted by $t(m)$. The parameter m is called the **degrees of freedom**.
k_m is a normalising constant such that $\int_{-\infty}^{\infty} f(x)\,dx = 1$.

- When $m = 1$, the distribution equals the Cauchy distribution:

$$f(x) = \frac{1}{\pi}(1+x^2)^{-1}$$

- As $m \to \infty$, the distribution approaches a Normal distribution:

$$f(x) \to \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$$

Therefore, a t-distribution is somewhere between these two extremes. The density is symmetric around zero and it is bell-shaped like the standard normal. The distinguishing feature is that densities of the t-distribution have heavier tails - the mean is smaller and the density goes to zero more slowly than the standard normal density as $s \to \pm\infty$.

Variation of the CLT

Let $X_1, X_2, \dots, X_n$ be independent random variables with a (non-normal) distribution with finite expectation μ and finite variance σ^2. Then (by the CLT),

$$\frac{\bar{X}_n - \mu_0}{S_n/\sqrt{n}} \xrightarrow{d} \mathcal{N}(0,1) \text{ as } n \to \infty$$

Consequently,

$$P\Big(a < \frac{\bar{X}_n - \mu_0}{S_n/\sqrt{n}} < b\Big) \to P(a < Z < b), \quad Z \sim \mathcal{N}(0,1)$$

3.2 Two-Sample Testing

One-sample t-test: $T = \frac{\bar{X}_n}{(S_n/\sqrt{n})} \sim t(n-1)$

Definition

A **paired two-sample t-test** compares the means of two groups of paired samples (i.e. *not independent*):

$$H_0 : \mu_1 = \mu_2 \iff \mu_D = 0, D_i = X_i - Y_i$$

$$H_1 : \mu_1 \neq \mu_2 \iff \mu_D \neq 0$$

$$T = \frac{\bar{D}_n}{(S_D)_n/\sqrt{n}} \sim t(n-1)$$

Examples:

- Blood pressure of patients before and after a treatment
- Market capitalisation of companies now and in two years
- Air resistance of an airplane wing before and after a coating is applied
- Lung closing capacity for smokers and non-smokers

Definition

The **pooled variance** of two groups of observations $x_1, \dots, x_{n_x}$ and $y_1, \dots, y_{n_y}$ is given by

$$s_p^2 = \frac{(n_x-1)s_X^2 + (n_y-1)s_Y^2}{n_x+n_y-2}$$

The **pooled standard deviation** is

$$s_p = \sqrt{s_p^2}$$

Theorem

The pooled variance is an unbiased estimator for the common variance σ^2, i.e. $E[S_p^2] = \sigma^2$.

Theorem

If $X_i \sim \mathcal{N}(\mu, \sigma^2)$ for $1 \leq i \leq n_x$ and $Y_i \sim \mathcal{N}(\mu, \sigma^2)$ for $1 \leq i \leq n_y$ are *independent*, then

$$T = \frac{\bar{X_{n_x}} - \bar{Y_{n_y}}}{S_p\sqrt{\frac{1}{n_x} + \frac{1}{n_y}}} \sim t(n_x + n_y - 2)$$

Definition

An **unpaired two-sample t-test** compares the means of two groups of unpaired samples:

$$H_0 : \mu_1 = \mu_2 \iff \mu_D = 0, D_i = X_i - Y_i$$

$$H_1 : \mu_1 \neq \mu_2 \iff \mu_D \neq 0$$

$$T = \frac{\bar{D}_n}{(S_D)_n/\sqrt{n}} \sim t(n-1)$$

If the two samples have different variances, **Welch's test** can be applied.

```
set.seed(42)

# Suppose you toss a fair coin 10 times. To compute the probability of a certain
# number of heads, you can use the command dbinom. It returns the value of the
# probability mass function at that number.
dbinom(5, size=10, prob=0.5)

# To compute the probability of computing at most a certain number of heads, you
# can use the command pbinom. It returns the value of the cumulative density
# function at that number. What is the probability of at most 6 and at least 3?
pbinom(6, size=10, prob=0.5) - pbinom(2, size=10, prob=0.5)

dbinom(500, size=1000, prob=0.5)
range <- 425:575
plot(range, dbinom(range, size=1000, prob=0.5))
plot(range, pbinom(range, size=1000, prob=0.5))
# To compute the number of heads, such that the probability of flipping that many
# heads has a certain value, you can use the command qbinom. It returns the value
# of the inverse cumulative density function or quantile function at that probability.
# The first quartile (Q1) is the point where you expect the cumulative density function to be 0.25.
qbinom(0.25, size=1000, prob=0.5)

# To draw random samples of the binomial distribution, you can use the command rbinom.
# Flip 1000 coins 10 times. What is the mean?
rsample <- rbinom(10, size=1000, prob=0.5)
mean(rsample)

# What’s the probability of 133 successes in 175 trials?
dbinom(133, size=175, prob=0.68)
range <- 85:150
plot(range, dbinom(range, size=175, prob=0.68))
# What’s the probability of at least 133 successes?
1 - pbinom(132, size=175, prob=0.68)
# This is the p-value for hypotheses H_0: mu=0.68, H_1: mu > 0.68
binom.test(133, n=175, p=0.68, alternative = "greater", conf.level = 0.95)

data("iris")
head(iris)
only_versicolor <- iris[iris$Species == "versicolor",]
sep_len <- only_versicolor$Sepal.Length
hist(sep_len)
qqnorm(sep_len)
t.test(sep_len, mu=5.731)

data("chickwts")
sunfl <- subset(chickwts, feed == "sunflower")[,1]
soyb <- subset(chickwts, feed == "soybean")[,1]
var.test(sunfl, soyb)
# The high p-value tells you not to reject the equality of variances.
# This means we now know which t-test to apply: the two-sample unpaired t-test, equal variances.
t.test(sunfl, soyb, alternative = "greater", paired = FALSE, var.equal = TRUE)
```

4 Confidence Intervals

Definition

A **pivotal quantity** or **pivot** T is a function of observations and unknown parameters such that the distribution of T does not depend on any unknown parameters.

Example: The test statistic $T = \frac{\bar{X}_n - \mu}{S_n \ \sqrt{n}} \sim t(n-1)$ depends both on observations and unknown parameters, while its distribution does not. T is a pivot.

Definition

Assuming normality:
Given i.i.d. $X_i \sim \mathcal{N}(\mu, \sigma^2)$, $T = \frac{\bar{X}_n - \mu}{S_n \ \sqrt{n}} \sim t(n-1)$. Hence

$$P\big(\bar{X}_n - t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}} \le \mu \le \bar{X}_n + t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}}\big) = 1 - \alpha = \gamma$$

Thus there is a $\gamma\%$ probability that μ lies in the **confidence interval**

$$\Big[\bar{X}_n - t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}}, \bar{X}_n + t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}}\Big]$$

NB: The statement "μ has $\gamma\%$ probability of lying in this interval" is not correct!

Definition

Normal approximation given a large sample size:
Without normality, for large n, it follows from the CLT that $T = \frac{\bar{X}_n - \mu}{S_n \ \sqrt{n}} \overset{d}{\approx} \mathcal{N}(0,1)$. Hence

$$P\big(\bar{X}_n - z_{\alpha/2}\frac{S_n}{\sqrt{n}} \le \mu \le \bar{X}_n + z_{\alpha/2}\frac{S_n}{\sqrt{n}}\big) = 1 - \alpha = \gamma$$

The $(1-\alpha)$ confidence interval for μ in this case then is

$$\Big[\bar{X}_n - z_{\alpha/2}\frac{S_n}{\sqrt{n}}, \bar{X}_n + z_{\alpha/2}\frac{S_n}{\sqrt{n}}\Big]$$

Disadvantages of the CLT approximation:

1. The CLT only gives an approximate interval.
2. The approximation may not be very good for small n.
3. It is more accurate to use the *actual distribution*.

Definition

$\gamma (= 1 - \alpha)$ is the **confidence level**. Common choices are 90%, 95%, 99.9%.

Theorem

Connection to hypothesis testing: The two following statements are equivalent:

1. $H_0 : \mu = \mu_0$ is rejected at significance level α in a two-sided test.
2. The $1 - \alpha$ confidence interval does not contain the value μ_0.

That is, the confidence interval is the set of all μ_0 for which $H_0 : \mu = \mu_0$ would not be rejected in a two-sided hypothesis test (with the same α).

Theorem

The sum of n independent $\text{Exp}(\lambda)$ random variables follows a $\Gamma(n, 1/\lambda)$ distribution.

Definition

A continuous random variable follows a **Gamma distribution** with parameters $n \in \mathbb{Z}$ and $1/\lambda > 0$ if it has a probability density

$$f(x) = \frac{\lambda^n}{(n-1)!}x^{n-1}e^{-\lambda x} \text{ for } x \ge 0$$

Problem: The Gamma distribution depends on an **unknown parameter** $1/\lambda$. Therefore, a random variable $S \sim \Gamma(n, 1/\lambda)$ is not a pivot.

Theorem

Scaling property of the Gamma distribution: If $X \sim \Gamma(n, 1/\lambda)$ then $aX \sim \Gamma(n, a/\lambda)$

(The Gamma scaling property follows from a similar scaling property of the Exponential distribution.)

Solution: $\lambda S \sim \Gamma(n, 1)$ is a pivot. Thus you can avoid the CLT approximation and instead use the known distribution.

Definition

The $(1-\alpha)$ confidence interval for λ based on n observations is given by

$$\left[\frac{q_{n,\alpha/2}}{\sum_{i=1}^n X_i}, \frac{q_{n,1-\alpha/2}}{\sum_{i=1}^n X_i}\right]$$

where $q_{n,\rho}$ is the ρ-quantile of the $\Gamma(n, 1)$ distribution.

Example: Given a random variable $X \sim \text{Bin}(n, p)$, its test statistic is not a pivot because its distribution depends on an unknown parameter, p. By the CLT,

$$\frac{X - np}{\sqrt{np(1-p)}} \xrightarrow{d} \text{ as } n \to \infty \Rightarrow \frac{X - np}{\sqrt{np(1-p)}} \overset{d}{\approx} \mathcal{N}(0,1)$$

Approximating p by its sample estimate $\hat{p} = \frac{X}{n}$,

$$\frac{X - np}{\sqrt{n\hat{p}(1-\hat{p})}} \xrightarrow{d} \text{ as } n \to \infty \Rightarrow \frac{X - np}{\sqrt{n\hat{p}(1-\hat{p})}} \overset{d}{\approx} \mathcal{N}(0,1)$$

This leads to the approximate confidence interval $\approx 1 - \alpha$, with $\hat{p} = X/n$, for p:

$$\left[\hat{p} - z_{\alpha/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}, \hat{p} + z_{\alpha/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}\right] = \hat{p} \pm z_{\alpha/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}$$

Definition

A random variable which is not a pivot but can be approximated by a standard normal distribution, by the CLT, is called a **near-pivot**.

The critical value for a t-based confidence interval is always larger than the equivalent z-based critical value, because not only are we uncertain about the population mean, we are also uncertain about the population standard deviation. As sample size increases, t converges to z.

```
# Suppose you are given a dataset that is sampled from a normally distributed population.
# The size of your dataset is 26, the sample mean is 23, and the sample standard deviation is 10.
# Compute the lower limit of the 80% confidence interval for mu.
sample_mean <- 23
sample_sd <- 10
sample_size <- 26
confidence_level <- 0.8
alpha <- 1 - confidence_level
critical_value <- qt(1 - alpha/2, df = sample_size - 1)
margin_of_error <- critical_value * (sample_sd / sqrt(sample_size))
lower_limit <- sample_mean - margin_of_error
print(lower_limit)

# Use R to generate a random sample of size 100 from a normal distribution with parameters mu=25, sigma=3.
# Compute the sample mean and standard deviation.
# Set the parameters
x <- rnorm(100, mean = 25, sd = 3)
sd(x)
mean(x)
t.test(x, mu = 25)
# If 1000 of your fellow MOOC students correctly solve this exercise, how many do you expect will answer "yes"
# 950. There is a 95% probability of obtaining a random sample that gives rise to a confidence interval (compu

set.seed(10)

# Run a simulation making one million 95% confidence intervals for the parameter lambda,
# based on samples of size 15 from an exponential distribution with parameter 0.923.
count1 <- 0
count2 <- 0
for (i in 1:1000000) {
  decays <- rexp(15, 0.923)
  CI_lower <- qgamma(0.025, 15, 1) / sum(decays)
  CI_upper <- qgamma(0.975, 15, 1) / sum(decays)
  if (CI_lower > 0.923) {
    count1 <- count1 + 1
  }
  if (CI_upper < 0.923) {
    count2 <- count2 + 1
  }
}
# What is the value of count1, the number of confidence intervals for which the
# lower bound is higher than the real value of the parameter?
count1
# How many intervals do contain the exact value of lambda?
count2
# Notice this means that ~95% of the confidence intervals contained the true parameter as expected.
```

5 Analysis of Variance (ANOVA)

With ANOVA and the associated F test, one can examine the equality of multiple means using a single test:

$$H_0 : \mu_1 = \mu_2 = \mu_3 = \ldots, \quad H_A : \text{ At least one mean is different.}$$

Three conditions:

- **Independence** of observations within and between groups.
- **Normality**, which can be investigated by checking if the group sizes are sufficiently large.
- **Constant variance** σ^2 in all groups (σ^2 may be known or unknown).

By default, we reject a null hypothesis when we get a p-value less than $\alpha = 0.05$.

The F statistic compares the between group variability (MSG) with the within group variability (MSE):

$$F = \frac{\text{MSG}}{\text{MSE}}$$

- The MSG is the variance of k means, so it has $k-1$ degrees of freedom.
- The MSE is an average of k individual group variances. It has $(n_1 - 1) + (n_2 - 1) + \cdots = N - k$ degrees of freedom.

All else equal, the larger is F, the more inclined you should be to reject the null hypothesis.

If the null hypothesis is true, F should be close to 1 because the variability between groups with match the overall variability in the data.

If the null hypothesis is rejected (i.e. the F test indicates that at least one mean is different), one can proceed with multiple pairwise comparisons.

$$t = \frac{\bar{x}_1 - \bar{x}_2}{s\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

- It is good practice to use more stringent significance levels in pairwise comparisons to avoid making a Type I error.
- In addition, a pooled standard deviation should be used.
- **Bonferroni correction**: For a desired overall Type I error rate of α, the Bonferroni correction suggests that a significance level α/K should be used for pairwise comparisons where K is the number of pairwise comparisons.

Definition — Theorem

Description: Text

$$\mathbf{v} \cdot \mathbf{w} = 0 \iff \alpha = \frac{\pi}{2} \iff \mathbf{v} \perp \mathbf{w}$$

6 Analysis of Categorical Data

Definition

The **variance** of a categorical variable (0 or 1) is

$$\sigma^2 = p(1-p)$$

Proof: Recall the variance is defined as the average squared deviation from the mean. For 1, the squared deviation from the mean is $(1-p)^2$; for 0, it is p^2.

Definition

The **standard error** for a categorical variable is

$$\text{SE}_{\hat{p}} = \sqrt{\frac{p(1-p)}{n}}$$

Theorem

The sample size needed for a given confidence interval is

$$n = \frac{p(1-p)}{\text{SE}^2}$$

Theorem

Variance is maximised when $p = \frac{1}{2}$.

Definition

The standard error of a difference in proportions is

$$\text{SE}(p_1 - p_2) = \sqrt{\frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}}$$

Definition

The z-statistic of the difference is calculated as

$$z = \frac{\text{observed} - \text{expected}}{\text{SE}} = \frac{(p_1 - p_2) - 0}{\text{SE}}$$

Definition

The **Chi-Squared distribution** is such that, taking repeated samples from random variable(s) $z_i \sim \mathcal{N}(0,1), i = 1, 2, \ldots,$ and squaring them,

$$\chi^2(1) = z_1^2, \quad \chi^2(2) = z_1^2 + z_2^2, \quad \ldots$$

The **degrees of freedom** uniquely define each χ^2 distribution.

Definition

The χ^2 goodness-of-fit test: When the observed frequency is far from the expected frequency, the corresponding term in the sum is large (and vice versa).

$$\chi^2 = \sum \frac{(\text{observed frequency} - \text{expected frequency})^2}{\text{expected frequency}}$$

- When the null model is "good", the sum will be small.
- When the null model is "bad", the sum will be large.

Reject the null hypothesis when the result is large enough.

Example:

$$\begin{aligned}\chi^2 &= \frac{(4-10)^2}{10} + \frac{(6-10)^2}{10} + \frac{(17-10)^2}{10} \\ &= \frac{6^2}{10} + \frac{4^2}{10} + \frac{7^2}{10} \\ &= 10.1\end{aligned}$$

Reject the null hypothesis when the result of the χ^2 test is large enough - compare with the appropriate χ^2 distribution with $k-1$ degrees of freedom.

7 Linear Regression

Definition

In a **linear regression model** for $(x_1, y_1), \dots, (x_n, y_n)$ we assume that $x_1, \dots, x_n$ are non-random and $y_1, \dots, y_n$ are realisations of random variables $Y_1, \dots, Y_n$ s.t.

$$Y_i = \alpha + \beta x_i + U_i, \text{ for } i = 1, \dots, n$$

where measurement errors $U_1, \dots, U_n$ are independent (i.e. do not influence each other) Normal random variables with $E[U_i] = 0$ (i.e. no systematic deviation from zero in the error term) and $\mathrm{Var}(U_i) = \sigma^2$.

Theorem

If $U_1, \dots, U_n \sim \mathcal{N}(0, \sigma^2)$, the least squares estimators $\hat{\alpha}, \hat{\beta}$ obtained with the method of moments are the same as the maximum likelihood estimators $\hat{\alpha}_{ML}, \hat{\beta}_{ML}$.

In the case of multiple linear regression, the line becomes a hyperplane.

A regression coefficient β_j estimates the expected change in Y per unit change in X_j, with all other predictors held fixed.

Theorem

The least squares estimators $\hat{\alpha}, \hat{\beta}$ that minimise the sum of squared distances

$$\sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

over all $\alpha, \beta \in \mathbb{R}$ are given by

$$\hat{\alpha} = \bar{Y}_n - \hat{\beta}\bar{x}_n$$

$$\hat{\beta} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2} = \frac{s_Y}{s_X} r_{x,Y}$$

which are both unbiased; that is, $E[\hat{\alpha}] = \alpha, E[\hat{\beta}] = \beta$. Since, according to the model, $U_i = Y_i - \alpha - \beta x_i \approx Y_i - \hat{\alpha} - \hat{\beta} x_i$, the least squares estimator for σ^2 is given by

$$\hat{\sigma^2} = \frac{1}{n-2} \sum_{i=1}^{n} (Y_i - \hat{\alpha} - \hat{\beta} x_i)^2$$

where dividing by $n-2$ gives an unbiased estimator, given the expression contains two estimated parameters $\hat{\alpha}, \hat{\beta}$.

7.1 Model Assessment

Definition

Let $\hat{\alpha}, \hat{\beta}$ be the least-squares estimators. Then for each observation, the i-**residual** is the observed minus predicted:

$$R_i = Y_i - \hat{\alpha} - \hat{\beta} x_i, \; i = 1, 2, \dots, n$$

Since $\hat{\alpha}, \hat{\beta}$ are unbiased estimators, i.e. $E[\hat{\alpha}] = \alpha, E[\hat{\beta}] = \beta$, the residuals $R_i = Y_i - \hat{\alpha} - \hat{\beta} x_i$ mimic the unobservable measurement errors $U_i = Y_i - \alpha - \beta x_i$:

$$R_i \approx U_i$$

A *residual plot* can be used to check the model **assumptions**:

- Linearity: Is there a linear relationship?
- Is $E[U_i] = 0$?
- **Homoskedasticity**: Is $\mathrm{Var}(U_i) = \sigma^2$? That is, is the variation of the residuals constant along the line?
- Nearly-normal residuals: Is $U_i \sim \mathcal{N}(0, \sigma^2)$? (straight line in QQ-Plot)

Definition

The variation in Y is defined as the **total sum of squares**

$$\mathrm{TSS} = \sum_{i=1}^{n} (y_i - \bar{y}_n)^2$$

The variation in Y due to measurement error is quantified by the **residual sum of squares** (which the Least Squares approach minimises):

$$\mathrm{RSS} = \sum_{i=1}^{n} R_i^2 = \sum_{i=1}^{n} (Y_i - \hat{\alpha} - \hat{\beta} x_i)^2$$

The remaining variation in Y is due to the linear relationship with x, and the higher its share of the total variation the better the fit of the model:

Definition

Let TSS, RSS be the total sum of squares and the residual sum of squares. Then the **proportion of explained variance** is the **coefficient of determination**

$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}} \quad (= r_{x,Y}^2)$$

where r is the correlation coefficient between x and Y: $r_{x,Y} = \frac{\sum_{i=1}^{n}(x_i - \hat{x}_n)(y_i - \hat{y}_n)}{\sqrt{\sum_{i=1}^{n}(x_i - \hat{x}_n)^2}\sqrt{\sum_{i=1}^{n}(y_i - \hat{y}_n)^2}}$

The least squares estimate $\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^{n} R_i^2$, by definition.

Definition

The **residual standard error** is defined as

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} R_i^2} = \sqrt{\frac{1}{n-2} \mathrm{RSS}}$$

Definition

The **standard error** of an estimator reflects how it varies under repeated sampling.

$$\mathrm{SE}(\hat{\alpha})^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}$$

$$\mathrm{SE}(\hat{\beta})^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2} \right]$$

The standard errors of the estimators can be used to compute confidence intervals for the estimators.

7.2 Tests and Confidence Intervals

Theorem

Consider the simple linear regression model $Y_i = \alpha + \beta x_i + U_i, i = 1, 2, \dots, n$ with i.i.d. $U_i, U_2, \dots, U_n \sim \mathcal{N}(0, \sigma^2)$. Let $\hat{\alpha}, \hat{\beta}$ be the least squares estimators. Then

$$\frac{\hat{\alpha} - \alpha}{\text{se}(\hat{\alpha})}, \frac{\hat{\beta} - \beta}{\text{se}(\hat{\beta})} \sim t(n-2)$$

follow a t-distribution with $m = n - 2$ degrees of freedom.

Thus, **confidence intervals** can be constructed for the least squares estimators:

$$P\left(-t_{n-1,\alpha/2} \leq \frac{\hat{\beta} - \beta}{\text{SE}(\hat{\beta})} \leq t_{n-2,\alpha/2} \right) = 1 - \alpha$$

$$P\left(\hat{\beta} - t_{n-1,\alpha/2}\text{se}(\hat{\beta}) \leq \beta \leq \hat{\beta} + t_{n-1,\alpha/2}\text{SE}(\hat{\beta}) \right) = 1 - \alpha$$

Furthermore, standard errors can also be used to perform **hypothesis tests** on the coefficients. **Example**:

H_0: There is no relationship between X and Y: $\beta = 0$. (If $\beta =$, the model reduces to $Y = \alpha + U$ and X is not associated to Y.)

H_A: There is some relationship between X and Y: $\beta \neq 0$.

The t-statistic for the test is $t = \frac{\hat{\beta} - 0}{\text{SE}(\hat{\beta})}$ which follows a t-distribution with $n - 2$ degrees of freedom.

Note: There is in fact a one-to-one correspondence between confidence intervals and hypothesis tests; that is, if the null hypothesis of the test is rejected and $\beta \neq 0$, the corresponding confidence interval (i.e. with the corresponding level of confidence) for the parameter will not contain 0.

7.3 Model Selection

Potential fixes if model assumptions are not satisfied:

- A quadratic term is a potential fix for a parabola in the residual plot (and should result in a straight line).
- Log-scaling the independent variable is a potential fix for heteroskedasticity (and should result in constant variance in the residual plot, i.e. homoskedasticity).

Products of variables are called **interaction terms**.

Definition

The **Akaike Information Criterion (AIC)** is a measure of the suitability of the dependent variables in a model:

$$AIC = 2k - 2\log(L)$$

where k is the number of dependent variables, and L is the likelihood. Both terms increase with the number dependent variables.

Therefore, you want the AIC to be as low as possible.

8 Generalised Linear Models (GLMs)

Generalisations of the linear model include:

- Classification problems: logistic regression, support vector machines
- Non-linearity: kernel smoothing, splines and generalised additive models, nearest neighbour methods
- Interactions: tree-based methods, bagging, random forests and boosting
- Regularised fitting: Ridge and Lasso

Definition

A n^{th}-order spline with knots at $\xi_k, k = 1, \ldots, K$ is a piecewise n^{th}-order polynomial with continuous derivatives up to order $n-1$ at each knot.

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+n} b_{K+n}(x_i) + \epsilon_i$$

$$b_1(x_i) = x_i, \quad b_2(x_i) = x_i^2, \quad \ldots, \quad b_{k+n}(x_i) = (x_i - \xi_k)_+^n, \quad k = 1, \ldots, K$$

$$(x_i - \xi_k)_+^n = \begin{cases} (x_i - \xi_k)^3 & \text{if } x_i > \xi_k \\ 0 & \text{otherwise} \end{cases}$$

A cubic spline with K knots has $K+4$ parameters, or degrees of freedom. A **natural spline** with K knots has K degrees of freedom.

A natural cubic spline extrapolates linearly beyond the boundary knots. This adds $4 = 2 \times 2$ extra constraints, and allows us to put more internal knots for the same degrees of freedom as a regular cubic spline.

Smoothing splines avoid the knot-selection issue, leaving a single λ to be chosen. Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\min_{g \in S} \sum_{i=1}^{n} (y_i - g(x_i))^2 + \lambda \int g''(t)^2 \, dt$$

- The first term is the RSS, and tries to make $g(x)$ match the data at each x_i.
- The second term is a rougness penalty, and controls how wiggly $g(x)$ is. It is modulated by the tuning parameter $\lambda \geq 0$.
  - The smaller λ, the more wiggly the function, eventually interpolating y_i when $\lambda = 0$.
  - As $\lambda \to \infty$, the function $g(x)$ becomes linear.

The solution is a natural cubic spline with a knot at every unique value of x_i. The roughness penalty still controls the roughness via λ.

Definition — Theorem

Description: Text

$$\mathbf{v} \cdot \mathbf{w} = 0 \iff \alpha = \frac{\pi}{2} \iff \mathbf{v} \perp \mathbf{w}$$

References

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