Statistics

Collection of Formulas

Contents

1 Descriptive Statistics

1.1 Summary Statistics

1.1.1 Location

Mode Most frequent value of x_i. Two or more modes are possible (bimodal).

Median

$$\tilde{x}_{0.5} = \begin{cases} x_{((n+1)/2)} & \text{falls } n \text{ ungerade} \\ \frac{1}{2}(x_{(n/2)} + x_{(n/2+1)} & \text{falls } n \text{ gerade} \end{cases}$$

Quantile

$$\tilde{x}_\alpha = \begin{cases} x_{(k)} & \text{falls } n\alpha \notin \mathbb{N} \\ \frac{1}{2}(x_{(n\alpha)} + x_{(n\alpha+1)}) & \text{falls } n\alpha \text{ ganzzahlig} \end{cases}$$

with

$$k = \min x \in \mathbb{N}, \quad x > n\alpha$$

Minimum/Maximum

$$x_{\min} = \min_{i \in \{1,\dots,N\}}(x_i) \qquad x_{\max} = \max_{i \in \{1,\dots,N\}}(x_i)$$

Arithmetic Mean

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Estimates the expectation $\mu = E[X]$ (first moment).

Calculation Rules:

- ⋆ $E(a + b \cdot X) = a + b \cdot E(X)$
- ⋆ $E(X \pm Y) = E(X) \pm E(Y)$

Geometric Mean

$$\bar{x}_G = \sqrt[n]{\sum_{i=1}^{n} x_i}$$

For growth factors: $\bar{x}_G = \sqrt[n]{\frac{B_n}{B_0}}$

Harmonic Mean

$$\bar{x}_H = \frac{\sum_{i=1}^{n} w_i}{\sum_{i=1}^{n} \frac{w_i}{x_i}}$$

1.1.2 Dispersion

Range

$$R = x_{(n)} - x_{(1)}$$

Interquartile Range

$$d_Q = \tilde{x}_{0.75} - \tilde{x}_{0.25}$$

(Empirical) Variance

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

Estimates the second centralized moment.

Calculation Rules:

- ⋆ $Var(aX + b) = a^2 \cdot Var(X)$
- ⋆ $Var(X \pm Y) = Var(X) + Var(Y) + 2Cov(X, Y)$

(Empirical) Standard Deviation

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

Coefficient of Variation

$$\nu = \frac{s}{\bar{x}}$$

Average Absolute Deviation

$$e = \frac{1}{n}\sum_{i=1}^{n}|x_i - \bar{x}|$$

Estimates the first absolute centralized moment.

1.1.3 Concentration

Gini Coefficient

$$G = \frac{2\sum_{i=1}^{n} i x_{(i)} - (n+1)\sum_{i=1}^{n} x_{(i)}}{n\sum_{i=1}^{n} x_{(i)}} = 1 - \frac{1}{n}\sum_{i=1}^{n}(v_{i-1} + v_i)$$

with

$$u_i = \frac{i}{n}, \quad v_i = \frac{\sum_{j=1}^{i} x_{(j)}}{\sum_{j=1}^{i} x_{(j)}} \qquad (u_0 = 0, \quad v_0 = 0)$$

These are also the values for the Lorenz curve.

Range: $0 \le G \le \frac{n-1}{n}$

Lorenz-Münzner Coefficient (normed G)

$$G^+ = \frac{n}{n-1}G$$

Range: $0 \le G^+ \le 1$

1.1.4 Shape

(Empirical) Skewness

$$\nu = \frac{n}{(n-1)(n-2)} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s} \right)^3$$

Estimates the third centralized moment, scaled with $(\sigma^2)^{\frac{2}{3}}$

(Empirical) Kurtosis

$$k = \left[n(n+1) \cdot \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s} \right)^4 - 3(n-1) \right] \cdot \frac{n-1}{(n-2)(n-3)} + 3$$

Estimates the fourth centralized moment, scaled with $(\sigma^2)^2$

Excess

$$\gamma = k - 3$$

1.1.5 Dependence

for two nominal variables

χ^2-Statistic

$$\chi^2 = \sum_{i=1}^{k} \sum_{j=1}^{l} \frac{(n_{ij} - \frac{n_{i+}n_{+j}}{n})^2}{\frac{n_{i+}n_{+j}}{n}} = n \left(\sum_{i=1}^{k} \sum_{j=1}^{l} \frac{n_{ij}^2}{n_{i+}n_{+j}} - 1 \right)$$

Range: $0 \leq \chi^2 \leq n(\min(k,l) - 1)$

Phi-Coefficient

$$\Phi = \sqrt{\frac{\chi^2}{n}}$$

Range: $0 \leq \Phi \leq \sqrt{\min(k,l) - 1}$

Cramér's V

$$V = \sqrt{\frac{\chi^2}{\min(k,l) - 1}}$$

Range: $0 \leq V \leq 1$

Contingency Coefficient C

$$C = \sqrt{\frac{\chi^2}{\chi^2 + n}}$$

Range: $0 \leq C \leq \sqrt{\frac{\min(k,l)-1}{\min(k,l)}}$

Corrected Contingency Coefficient C_{corr}

$$C_{corr} = \sqrt{\frac{\min(k,l)}{\min(k,l) - 1}} \cdot \sqrt{\frac{\chi^2}{\chi^2 + n}}$$

Range $0 \leq C_{corr} \leq 1$

Odds-Ratio

$$OR = \frac{ad}{bc} = \frac{n_{ii}n_{jj}}{n_{ij}n_{ji}}$$

Range: $0 \leq OR < \infty$

for two ordinal variables

Gamma (Goodman and Kruskal)

$$\gamma = \frac{K - D}{K + D}$$

$K = \sum_{i<m} \sum_{j<n} n_{ij} n_{mn}$ Number of concordant pairs
$D = \sum_{i<m} \sum_{j>n} n_{ij} n_{mn}$ Number of reversed pairs

Range: $-1 \leq \gamma \leq 1$

Kendall's τ_b

$$\tau_b = \frac{K - D}{\sqrt{(K + D + T_X)(K + D + T_Y)}}$$

with
$T_X = \sum_{i=m} \sum_{j<n} n_{ij} n_{mn}$ Number of ties w.r.t. X
$T_Y = \sum_{i<m} \sum_{j=n} n_{ij} n_{mn}$ Number of ties w.r.t. Y

Range: $-1 \leq \tau_b \leq 1$

Kendall's/Stuart's τ_c

$$\tau_c = \frac{2\min(k,l)(K - D)}{n^2(\min(k,l) - 1)}$$

Range: $-1 \leq \tau_c \leq 1$

Spearman's Rank Correlation Coefficient

$$\rho = \frac{n(n^2-1) - \frac{1}{2}\sum\limits_{j=1}^{J} b_j(b_j^2 - 1) - \frac{1}{2}\sum\limits_{k=1}^{K} c_k(c_k^2 - 1) - 6\sum\limits_{i=1}^{n} d_i^2}{\sqrt{n(n^2-1) - \sum\limits_{j=1}^{J} b_j(b_j^2 - 1)}\sqrt{n(n^2-1) - \sum\limits_{k=1}^{K} c_k(c_k^2 - 1)}}$$

or

$$\rho = \frac{s_{rg_x rg_y}}{\sqrt{s_{rg_x rg_x} s_{rg_y rg_y}}}$$

Without ties:

$$\rho = 1 - \frac{6\sum\limits_{i=1}^{n} d_i^2}{n(n^2 - 1)}$$

with
$d_i = R(x_i) - R(y_i)$ rank difference

Range: $-1 \leq \rho \leq 1$

for two metric variables

Correlation Coefficient (Bravais-Pearson)

$$r = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}} = \frac{s_{xy}}{\sqrt{s_{xx}s_{yy}}}$$

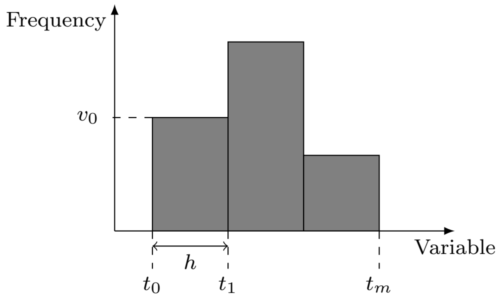
with
$S_{xy} = \sum\limits_{i=1}^{n}(x_i - \bar{x})^2(y_i - \bar{y})^2$ or $s_{xy} = \frac{S_{xy}}{n}$
$S_{xx} = \sum\limits_{i=1}^{n}(x_i - \bar{x})^2$ or $s_{xx} = \frac{S_{xx}}{n}$
$S_{yy} = \sum\limits_{i=1}^{n}(y_i - \bar{y})^2$ or $s_{yy} = \frac{S_{yy}}{n}$

Range: $-1 \leq r \leq 1$

1.2 Tables

1.3 Diagrams

1.3.1 Histogram



sample: $X = \{x_1, x_2, ...; x_n\}$
k-th bin: $B_k = [t_k, t_{k+1}), k = \{0, 1, ..., m-1\}$
Number of observations in the k-th bin: v_k
bin width: $h = t_{k+1} - t_k, \forall k$

Scott's Rule

$$h^* \approx 3.5\sigma n^{-\frac{1}{3}}$$

For approximately normal distributed data (min. MSE)

2 Probability

2.1 Combinatorics

		without replacement	with replacement
Permutations		$n!$	$\frac{n!}{n_1!\cdots n_s!}$
Combinations:	without order	$\binom{n}{m}$	$\binom{n+m-1}{m}$
	with order	$\binom{n}{m}m!$	n^m

with:
$n! = n \cdot (n-1) \cdot ... \cdot 1$
$\binom{n}{m} = \frac{n!}{m!(n-m)!}$

2.2 Probability Theory

Laplace

$$P(A) = \frac{|A|}{|\Omega|}$$

Kolmogorov Axioms mathematical definition of probability

(1) $0 \leq P(A) \leq 1 \qquad \forall A \in \mathcal{A}$
(2) $P(\Omega) = 1$
(3) $P(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$
$\forall A_i \in \mathcal{A}, i = 1, ..., \infty$ with $A_i \cap A_j = \emptyset$ for $i \neq j$

Implications:

- $P(\bar{A}) = 1 - P(A)$
- $P(\emptyset) = 0$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
- $A \subseteq B \Rightarrow P(A) \leq P(B)$
- $P(B) = \sum_{i=1}^{n} P(B \cap A_i)$, for $A_i, ..., A_n$ complete decomposition of Ω into pairwise disjoint events

Probability (Mises) frequentist definition of probability

$$P(A) = \lim_{n\to\infty} \frac{n_A(n))}{n}$$

with n repetitions of a random experiment and $n_A(n)$ events A

Conditional Probability

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \qquad \text{für } P(B) > 0$$

$$\Rightarrow P(A \cap B) = P(B|A)P(A) = P(A|B)P(B)$$

Law of Total Probability

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

Bayes' Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \qquad \text{for } P(A), P(B) > 0$$

Stochastic Independence

A, B independent $\Leftrightarrow P(A \cap B) = P(A) + P(B)$

X, Y independent $\Leftrightarrow f_{XY}(x,y) = f_X(x) \cdot f_Y(y) \qquad \forall x, y$

2.3 Random Variables/Vectors

Random Variables $\in \mathbb{R}$

Definition

$$Y : \Omega \to \mathbb{R}$$

The Subset of possible values for $\mathbb{R}$ is called support.
Notation: Realisations of Y are depicted with lower case letters.
$Y = y$ means, that y is the realisation of Y.

Discrete and Continuous Random Variables
If the support is uncountably infinite, the random variable is called *continuous*, otherwise it is called *discrete*.

- **Density $f(\cdot)$:**

  For continuous variables: $P(Y \in [a,b]) = \int_a^b f_Y(y)dy$

  For discrete variables the density (and other functions) can be depicted like the corresponding function for continuous variables, if the notation is extended as follows: $\int_{-\infty}^{y} f_Y(\tilde{y})d\tilde{y} := \sum_{k:k\leq y} P(Y = k)$. This notation is used.

- **Cumulative Distribution Function $F(\cdot)$:**
  $F_Y(y) = P(Y \leq y)$

Relationship:

$$F_Y(y) = \int_{-\infty}^{y} f_Y(\tilde{y})d\tilde{y}$$

Moments

- **Expectation (1. Moment)**: $\mu = E(Y) = \int y f_Y(y)dy$
- **Variance (2. centralized Moment)**:
  $\sigma^2 = Var(Y) = E(\{Y - E(Y)\}^2) = \int (y - E(Y))^2 f(y)dy$
  Note: $E(\{Y - \mu\}^2) = E(Y^2) - \mu^2$

  > Proof:
  > $E(\{Y-\mu\}^2) = E(Y^2 - 2Y\mu + \mu^2) = E(Y^2) - 2\mu^2 + \mu^2 = E(Y^2) - \mu^2$

- **kth Moment**: $E(Y^k) = \int y^k f_Y(y)dy$,
  k. centralized Moment: $E(\{Y - E(Y)\}^k)$

Moment Generating Function

$$M_Y(t) = \mathrm{E}(e^{tY})$$

with $\left.\frac{\partial^k M_Y(t)}{\partial t^k}\right|_{t=0} = \mathrm{E}(Y^k)$

Cumulant Generating Function $K_Y(t) = \log M_Y(t)$

A random variable is uniquely defined by its moment generating function and vice versa (as long as moments and cumulants are finite).

Random Vectors $\in \mathbb{R}^q$

Density and Cumulative Distribution Function

$$F(y_1,...,y_q) = P(Y_1 \leq y_1,...,Y_q \leq y_q)$$

$$P(a_1 \leq Y_1 \leq b_1,...,a_q \leq Y_q \leq b_q)$$
$$= \int_{a_1}^{b_1} ... \int_{a_q}^{b_q} f(y_1,..,y_q) dy_1...dy_q$$

Marginal Density

$$f_{Y_1}(y_1) = \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} f(y_1,...,y_k) dy_2...dy_k$$

Conditional Density

$$f_{Y_1|Y_2}(y_1|y_2) = \frac{f(y_1,...,y_2)}{f(y_2)} \text{ for } f(y_2) > 0$$

Iterated Expectation

$$\mathrm{E}(Y) = \mathrm{E}_X(\mathrm{E}(Y|X))$$

Proof:

$$\mathrm{E}(Y) = \int y f(y) dy = \int\int y f(y|x) dy f_X(x) dx = \mathrm{E}_X(\mathrm{E}(Y|X))$$

$$\mathrm{Var}(Y) = \mathrm{E}_X(\mathrm{Var}(Y|X)) + \mathrm{Var}_X(\mathrm{E}(Y|X))$$

Proof:

$$\begin{aligned}
\mathrm{Var}(Y) &= \int (y-\mu_Y)^2 f(y) dy \\
&= \int (y-\mu_Y)^2 f(y|x) f(x) dy dx \\
&= \int (y-\mu_{Y|x} + \mu_{Y|x} - \mu_Y)^2 f(y|x) f(x) dy dx \\
&= \int (y-\mu_{Y|x})^2 f(y|x) f(x) dy dx + \\
&\quad \int (\mu_{Y|x} - \mu_Y)^2 f(y|x) f(x) dy dx + \\
&\quad 2\int (y-\mu_{Y|x})(\mu_{Y|x} - \mu_Y) f(y|x) f(x) dy dx \\
&= \int \mathrm{Var}(Y|x) f(x) dx + \int (\mu_{Y|x} - \mu_Y)^2 f(x) dx \\
&= \mathrm{E}_X(\mathrm{Var}(Y|X)) + \mathrm{Var}_X(\mathrm{E}(Y|X))
\end{aligned}$$

2.4 Probability Distributions

2.4.1 Discrete Distributions

Discrete Uniform

$$Y \sim \mathrm{U}(\{y_1,...,y_k\}),\ y \in \{y_1,...,y_k\}$$
$$P(Y = y_i) = \frac{1}{k},\ i = 1,...,k$$
$$\mathrm{E}(Y) = \frac{k+1}{2},\ \mathrm{Var}(Y) = \frac{k^2-1}{12}$$

Binomial Successes in independent trials

$$Y \sim \mathrm{Bin}(n,\pi) \text{ with } n \in \mathbb{N}, \pi \in [0,1],\ y \in \{0,...,n\}$$
$$P(Y = y|\lambda) = \binom{n}{y} \pi^k (1-\pi)^{n-y}$$
$$\mathrm{E}(Y|\pi,n) = n\pi,\ \mathrm{Var}(Y|\pi,n) = n\pi(1-\pi)$$

Poisson Counting model for rare events
only one event at a time, no autocorrelation, mean number of events over time is constant and proportional to length of the considered time interval

$$Y \sim \mathrm{Po}(\lambda) \text{ with } \lambda \in [0,+\infty],\ y \in \mathbb{N}_0$$

$$P(Y = y|\lambda) = \frac{\lambda^y exp^{-\lambda}}{y!}$$
$$\mathrm{E}(Y|p) = \lambda,\ \mathrm{Var}(Y|p) = \lambda$$

The model tends to overestimate the variance (Overdispersion).
Approximation of the Binomial for small p

Geometric

$$Y \sim \mathrm{Geom}(\pi) \text{ with } \pi \in [0,1],\ y \in \mathbb{N}_0$$
$$P(Y = y|\pi) = \pi(1-\pi)^{y-1}$$
$$\mathrm{E}(Y|\pi) = \frac{1}{\pi},\ \mathrm{Var}(Y|\pi) = \frac{1-\pi}{\pi^2}$$

Negative Binomial

$$Y \sim \mathrm{NegBin}(\alpha,\beta) \text{ with } \alpha,\beta \geq 0,\ y \in \mathbb{N}_0$$
$$P(Y = y|\alpha,\beta) = \binom{\alpha+y-1}{\alpha-1} \left(\frac{\beta}{\beta-1}\right)^\alpha \left(\frac{1}{\beta+1}\right)^y$$
$$\mathrm{E}(Y|\alpha,\beta) = \frac{\alpha}{\beta},\ \mathrm{Var}(Y|\alpha,\beta) = \frac{\alpha}{\beta^2}(\beta+1)$$

2.4.2 Continuous Distributions

Continuous Uniform

$$Y \sim \mathrm{U}(a,b) \text{ with } \alpha,\beta \in \mathbb{R}, a \leq b,\ y \in [a,b]$$
$$p(y|a,b) = \frac{1}{b-a}$$
$$\mathrm{E}(Y|a,b) = \frac{a+b}{2},\ \mathrm{Var}(Y|a,b) = \frac{(b-a)^2}{12}$$

Univariate Normal symmetric with μ and σ^2

$$Y \sim \mathrm{N}(\mu,\sigma^2) \text{ with } \mu \in \mathbb{R}, \sigma^2 > 0,\ y \in \mathbb{R}$$
$$p(y|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$
$$\mathrm{E}(Y|\mu,\sigma^2) = \mu,\ \mathrm{Var}(Y|\mu,\sigma^2) = \sigma^2$$

Multivariate Normal symmetric with μ_i and Σ

$$Y \sim \mathrm{N}(\mu,\Sigma) \text{ with } \mu \in \mathbb{R}^d, \Sigma \in \mathbb{R}^{d\times d} s.p.d.,\ y \in \mathbb{R}^d$$
$$p(y|\mu,\Sigma) = (2\pi)^{-\frac{d}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(y-\mu)^T\Sigma^{-1}(y-\mu)\right)$$
$$\mathrm{E}(Y|\mu,\Sigma) = \mu,\ \mathrm{Var}(Y|\mu,\Sigma) = \Sigma$$

Log-Normal

$$Y \sim \mathrm{LogN}(\mu,\sigma^2) \text{ eith } \mu \in \mathbb{R}, \sigma^2 > 0,\ y > 0$$
$$p(y|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2 y}} \exp\left(-\frac{(\log y-\mu)^2}{2\sigma^2}\right)$$
$$\mathrm{E}(Y|\mu,\sigma^2) = \exp(\mu + \frac{\sigma^2}{2}),$$
$$\mathrm{Var}(Y|\mu,\sigma^2) = \exp(2\mu+\sigma^2)(\exp(\sigma^2)-1)$$

Relationship: $\log(Y) \sim \mathrm{N}(\mu,\sigma^2) \Rightarrow Y \sim \mathrm{LogN}(\mu,\sigma^2)$

non-standardized Student's t statistical Tests for μ with unknown (estimated) variance and ν degrees of freedom

$$Y \sim \mathrm{t}_\nu(\mu,\sigma^2) \text{ with } \mu \in \mathbb{R}, \sigma^2, \nu > 0,\ y \in \mathbb{R}$$
$$p(y|\mu,\sigma^2,\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma(\frac{\nu}{2})\Gamma(\sqrt{\nu\pi}\sigma)} \left(1 + \frac{(y-\mu)^2}{\nu\sigma^2}\right)^{-\frac{\nu+1}{2}}$$
$$\mathrm{E}(Y|\mu,\sigma^2,\nu) = \mu \text{ for } \nu > 1,$$
$$\mathrm{Var}(Y|\mu,\sigma^2,\nu) = \sigma^2\frac{\nu}{\nu-2} \text{ for } \nu > 2$$

Relationship: $Y|\theta \sim \mathrm{N}(\mu, \frac{\sigma^2}{\theta}),\ \theta \sim \mathrm{Ga}(\frac{\nu}{2},\frac{\nu}{2}) \Rightarrow Y \sim \mathrm{t}_\nu(\mu,\sigma)$
$t_\nu(\mu,\sigma^2)$ has heavier tails then the normal distribution.
$t_\infty(\mu,\sigma^2)$ approaches $\mathrm{N}(\mu,\sigma^2)$.

Beta

$$Y \sim \mathrm{Be}(a,b) \text{ with } a,b > 0,\ y \in [0,1]$$
$$p(y|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} y^{a-1}(1-y)^{b-1}$$
$$\mathrm{E}(Y|a,b) = \frac{a}{a+b},$$
$$\mathrm{Var}(Y|a,b) = \frac{ab}{(a+b)^2(a+b+1)},$$
$$\mathrm{mod}(Y|a,b) = \frac{a-1}{a+b-2} \text{ for } a,b > 1$$

Gamma

$$Y \sim \mathrm{Ga}(a,b) \text{ with } a,b > 0,\ y > 0$$
$$p(y|a,b) = \frac{b^a}{\Gamma(a)} y^{a-1}\exp(-by)$$
$$\mathrm{E}(Y|a,b) = \frac{a}{b},$$
$$\mathrm{Var}(Y|a,b) = \frac{a}{b^a},$$
$$\mathrm{mod}(Y|a,b) = \frac{a-1}{b} \text{ for } a \geq 1$$

Inverse-Gamma

$$Y \sim \mathrm{IG}(a,b) \text{ with } a,b > 0,\ y > 0$$
$$p(y|a,b) = \frac{b^a}{\Gamma(a)} y^{-a-1}\exp(-\frac{b}{y})$$
$$\mathrm{E}(Y|a,b) = \frac{b}{a-1} \text{ for } a > 1,$$
$$\mathrm{Var}(Y|a,b) = \frac{b^2}{(a-1)^2(a-2)} \text{ for } a \geq 2,$$
$$\mathrm{mod}(Y|a,b) = \frac{b}{a+1}$$

Relationship: $Y^{-1} \sim \mathrm{Ga}(a,b) \Leftrightarrow Y \sim \mathrm{IG}(a,b)$

Exponential Time between Poisson events

$$Y \sim \mathrm{Exp}(\lambda) \text{ with } \lambda > 0,\ y \geq 0$$
$$p(y|\lambda) = \lambda\exp(-\lambda y)$$
$$\mathrm{E}(Y|\lambda) = \frac{1}{\lambda},\ \mathrm{Var}(Y|\lambda) = \frac{1}{\lambda^2}$$

Chi-Squared squared standard normal random variables with ν degrees of freedom

$$Y \sim \chi^2(\nu) \text{ with } \nu > 0, ,\ y \in \mathbb{R}$$
$$p(y|\nu) = \frac{y^{\frac{\nu}{2}-1}e^{-\frac{y}{2}}}{2^{\frac{\nu}{2}}\Gamma\left(\frac{\nu}{2}\right)}$$
$$\mathrm{E}(Y|\nu) = \nu,\ \mathrm{Var}(Y|\nu) = 2\nu$$

2.4.3 Exponential Family

Definition
The exponential family comprises all distributions, whose density can be written as follows:

$$f_Y(y,\theta) = \exp^{t^T(y)\theta-\kappa(\theta)} h(y)$$

with $h(y) \geq 0$, $t(y)$ vector of the canonical statistic, θ as parameter and $\kappa(\theta)$ the normalising constant.

Normalising Constant

$$1 = \int \exp^{t^T(y)\theta} h(y)dy \exp^{-\kappa(\theta)}$$

$$\Leftrightarrow \kappa(\theta) = \log \int \exp^{t^T(y)\theta} h(y) dy$$

$\kappa(\theta)$ is the cumulant generating function, therefore $\frac{\partial \kappa(\theta)}{\partial \theta} = \mathrm{E}(t(Y))$ and $\frac{\partial^2 \kappa(\theta)}{\partial \theta^2} = \mathrm{Var}(t(Y))$

Members

- **Poisson**
- **Geometric**
- **Exponential**
- **Normal** $t(y) = \left(-\frac{y^2}{2}, y\right)^T$, $\theta = \left(\frac{1}{\sigma^2}, \frac{\mu}{\sigma^2}\right)^T$, $h(y) = \frac{1}{\sqrt{2\pi}}$, $\kappa(\theta) = \frac{1}{2}\left(-\log\frac{1}{\sigma^2} + \frac{\mu^2}{\sigma^2}\right)$
- **Gamma**
- **Chi-Squared**
- **Beta**

2.5 Limit Theorems

Law of Large Numbers

Central Limit Theorem

$$Z_n \xrightarrow{d} \mathrm{N}(0, \sigma^2)$$

with $Z_n = \sum_{i=1}^n \frac{Y_i}{\sqrt{n}}$ and Y_i i.i.d. with expectation 0 and variance σ^2

Proof:
For normal random variables $Z \sim \mathrm{N}(\mu, \sigma^2)$: $K_Z(t) = \mu t + \frac{1}{2}\sigma^2 t^2$. The first two derivatives $\left.\frac{\partial^k K_Z(t)}{\partial t^k}\right|_{t=0}$ are μ and σ. All other moments are zero.
For $Z_n = (Y_1 + Y_2 + ... + Y_n)/\sqrt{n}$:

$$\begin{aligned} M_{Z_n}(t) &= \mathrm{E}\left(e^{t(Y_1+Y_2+...+Y_n)/\sqrt{n}}\right) \\ &= \mathrm{E}\left(e^{tY_1/\sqrt{n}} \cdot e^{tY_2/\sqrt{n}} \cdot ... \cdot e^{tY_n/\sqrt{n}}\right) \\ &= \mathrm{E}\left(e^{tY_1/\sqrt{n}}\right) \mathrm{E}\left(e^{tY_2/\sqrt{n}}\right) ... \mathrm{E}\left(e^{tY_n/\sqrt{n}}\right) \\ &= M_Y^n(t/\sqrt{n}) \end{aligned}$$

Analoguously: $K_{Z_n}(t) = nK_Y(t/\sqrt{n})$.

$$\left.\frac{\partial K_{Z_n}(t)}{\partial t}\right|_{t=0} = \frac{n}{\sqrt{n}} \left.\frac{\partial K_Y(t)}{\partial t}\right|_{t=0} = \sqrt{n}\mu$$

$$\left.\frac{\partial^2 K_{Z_n}(t)}{\partial t^2}\right|_{t=0} = \frac{n}{n} \left.\frac{\partial^2 K_Y(t)}{\partial t^2}\right|_{t=0} = \sigma^2$$

Using the Taylor Expansion, we can write$K_{Z_n}(t) = 0 + \sqrt{n}\mu t + \frac{1}{2}\sigma^2 t^2 + ...$, where the terms in ... are tending towards 0 as $n \to \infty$.
Therefore: $K_{Z_n}(t) \overset{n\to\infty}{\longrightarrow} K_Z(t)$ with $Z \sim \mathrm{N}(\sqrt{n}\mu, \sigma^2)$.

3 Inference

3.1 Method of Moments

The theoretical moments are estimated by their empirical counterparts:

$$\mathrm{E}_{\hat{\theta}_{MM}}(Y^k) = m_k(y_1, ..., y_n)$$

For the exponential family: $\hat{\theta}_{MM} = \hat{\theta}_{ML}$

3.2 Loss Functions

Loss

$$\mathcal{L} : \mathcal{T} \times \Theta \to \mathbb{R}^+$$

with parameter space $\Theta \subset \mathbb{R}$, $t \in \mathcal{T}$ with $t : \mathbb{R}^n \to \mathbb{R}$ a statistic, that estimates the parameter θ, $\mathcal{L}(\theta, \theta) = 0$ holds

- **absolute loss (L1)**: $\mathcal{L}(t, \theta) = |t - \theta|$
- **quadratic loss (L2)**: $\mathcal{L}(t, \theta) = (t - \theta)^2$

As θ is unknown, the loss is a theoretical measure. Additionally, it is the realisation of a random variable as it is dependent on a concrete sample.

Risiko

$$\begin{aligned} R(t(.), \theta) &= \mathrm{E}_\theta \left(\mathcal{L}(t(Y_1, ..., Y_n), \theta)\right) \\ &= \int_{-\infty}^{\infty} \mathcal{L}(t(Y_1, ..., Y_n), \theta) \prod_{i=1}^n f(y_i; \theta) dy_i \end{aligned}$$

Minimax Approach
The risk still depends ton the true parameter θ. Tentative estimation: Choose θ, so that the risk is maximal and then $t(.)$, so that the risk is minimized (minimizing the worst case):

$$\hat{\theta}_{minimax} = \arg\min_{t(.)} \left(\max_{\theta \in \Theta} R(t(.); \theta) \right)$$

Mean Squared Error (MSE)

$$\begin{aligned} MSE(t(.), \theta) &= \mathrm{E}_\theta \left(\{t(Y) - \theta\}^2 \right) \\ &= \mathrm{Var}_\theta \left(t(Y_1, ..., Y_n)\right) + Bias^2((t(.); \theta) \end{aligned}$$

with $Bias(t(.); \theta) = \mathrm{E}_\theta \left(t(Y_1, ..., Y_n)\right) - \theta$

Proof:
Let $\mathcal{L}(t, \theta) = (t - \theta)^2$

$$\begin{aligned} R(t(.), \theta) &= \mathrm{E}_\theta(\{t(Y) - \theta\}^2) \\ &= \mathrm{E}_\theta(\{t(Y) - \mathrm{E}_\theta(t(Y)) + \mathrm{E}_\theta(t(Y)) - \theta\}^2) \\ &= \mathrm{E}_\theta(\{t(Y) - \mathrm{E}_\theta(t(Y))\}^2) + \mathrm{E}_\theta(\{\mathrm{E}_\theta(t(Y)) - \theta\}^2) \\ &\quad + 2\mathrm{E}_\theta(\{t(Y) - \mathrm{E}_\theta\,(t(Y))\}\{\mathrm{E}_\theta(t(Y)) - \theta\}) \\ &= \mathrm{Var}_\theta(t(Y_1, ..., Y_n)) + Bias^2((t(.); \theta) + 0 \end{aligned}$$

Cramér-Rao Inequality

$$MSE(\hat{\theta}, \theta) \geq Bias^2(\hat{\theta}, \theta) + \frac{\left(1 + \frac{\partial Bias(\hat{\theta}, \theta)}{\partial \theta}\right)^2}{I(\theta)}$$

Proof:
For unbiased estimates: $\theta = \mathrm{E}_\theta(\hat{\theta}) = \int t(y) f(y; \theta) dy$

$$\begin{aligned} 1 &= \int t(y) \frac{\partial f(y; \theta)}{\partial \theta} dy \\ &= \int t(y) \frac{\partial \log f(y; \theta)}{\partial \theta} f(y; \theta) dy \\ &= \int t(y) s(y; \theta) f(y; \theta) dy \\ &= \int \left(t(y) - \theta\right) \left(s(\theta; y) - 0\right) f(y; \theta) dy && \text{1. Bartlett equation } \mathrm{E}_\theta\left(s(\theta; y)\right) = 0 \\ &= \mathrm{Cov}_\theta\left(t(Y); s(\theta; Y)\right) \\ &\geq \sqrt{\mathrm{Var}_\theta(t(Y))}\sqrt{\mathrm{Var}_\theta(s(\theta; Y))} && \text{Cauchy-Schwarz} \\ &= \sqrt{MSE(t(Y); \theta)}\sqrt{I(\theta)} \end{aligned}$$

Kullback-Leibler Divergence Comparing distributions

$$KL(t, \theta) = \int_{-\infty}^{\infty} \log \frac{f(\tilde{y}; \theta)}{f(\tilde{y}; t)} f(\tilde{y}; \theta) d\tilde{y}$$

The KL divergence is not a distance as it is not symmetric. It is 0 for $t = \theta$ and ≥ 0 otherwise.

Proof:
Follows from $\log(x) \leq x - 1 \forall x \geq 0$, with equality for $x = 1$.

$R_{KL}(t(.), \theta)$ is approximated by the MSE.

Proof:

$$\begin{aligned} & R_{KL}(t(.), \theta) = \\ &= \int_{-\infty}^{\infty} \mathcal{L}_{KL}(t(Y_1, ..., Y_n), \theta) \prod_{i=1}^n f(y_i; \theta) dy_i \\ &= \int \int \log \frac{f(\tilde{y}; \theta)}{f(\tilde{y}; t)} f(\tilde{y}; \theta) d\tilde{y} \prod_{i=1}^n f(y_i; \theta) dy_i \\ &= \int \int \left(\log f(\tilde{y}; \theta) - \log f(\tilde{y}; t)\right) f(\tilde{y}; \theta) d\tilde{y} - \prod_{i=1}^n f(y_i; \theta) dy_i \\ &\approx - \int \underbrace{\left(\int \frac{\partial \log f(\tilde{y}; \theta)}{\partial \theta} f(\tilde{y}; \theta) d\tilde{y} \right)}_{0} (t - \theta) \prod_{i=1}^n f(y_i; \theta) dy_i \\ &+ \frac{1}{2} \int \underbrace{\left(- \int \frac{\partial^2 \log f(\tilde{y}; \theta)}{\partial \theta^2} f(\tilde{y}; \theta) d\tilde{y} \right)}_{I(\theta)} (t - \theta)^2 \prod_{i=1}^n f(y_i; \theta) dy_i \end{aligned}$$

The last step is approximated by the Taylor Expansion: $\log f(\tilde{y}, t) \approx \log f(\tilde{y}, \theta) + \frac{\partial \log f(\tilde{y}, \theta)}{\partial \theta}(t - \theta) + \frac{1}{2} \frac{\partial^2 \log f(\tilde{y}, \theta)}{\partial \theta^2}(t - \theta)^2$

3.3 Maximum Likelihood (ML)

Prerequisites

- $Y_i \sim f(y;\theta)$ *i.i.d.*
- $\theta \in \mathbb{R}^p$
- $f(.;\theta)$ Fisher-regular:
  - $\{y : f(y;\theta > 0)\}$ independent of θ
  - Parameter space Θ is open
  - $f(y;\theta)$ twice differentiable
  - $\int \frac{\partial}{\partial\theta} f(y;\theta)dy = \frac{\partial}{\partial\theta}\int f(y;\theta)dy$

Central Functions

- **Likelihood** $L(\theta; y_1, ..., y_n)$: $\prod_{i=1}^n f(y_i;\theta)$
- **log-Likelihood** $l(\theta; y_1, ..y_n)$:
  $\log L(\theta; y_1, ..., y_n) = \sum_{i=1}^n \log f(y_i;\theta)$
- **Score** $s(\theta; y_1, ..., y_n)$: $\frac{\partial l(\theta;y_1,..y_n)}{\partial\theta}$
- **Fisher-Information** $I(\theta)$: $-\mathrm{E}_\theta\left(\frac{\partial s(\theta;Y)}{\partial\theta}\right)$
- **observed Fisher-Information** $I_{obs}(\theta)$: $-\mathrm{E}_\theta\left(\frac{\partial s(\theta;y)}{\partial\theta}\right)$

Attributes of the Score-Function

first Bartlett-Equation:

$$\mathrm{E}\left(s(\theta;Y)\right) = 0$$

Proof:

$$\begin{aligned} 1 &= \int f(y;\theta)dy \\ 0 = \frac{\partial 1}{\partial\theta} &= \int \frac{\partial f(y;\theta)}{\partial\theta}dy = \int \frac{\partial f(y;\theta)/\partial\theta}{f(y;\theta)} f(y;\theta)dy \\ &= \int \frac{\partial}{\partial\theta}\log f(y;\theta) f(y;\theta)dy = \int s(\theta;y)f(y;\theta)dy \end{aligned}$$

second Bartlett-Equation:

$$\mathrm{Var}_\theta\left(s(Y;\theta)\right) = \mathrm{E}_\theta\left(-\frac{\partial^2 log f(Y;\theta)}{\partial\theta^2}\right) = I(\theta)$$

Proof:

$$\begin{aligned} 0 = \frac{\partial 0}{\partial\theta} &= \frac{\partial}{\partial\theta}\int \frac{\partial}{\partial\theta}\log f(y;\theta)f(y;\theta)dy \qquad \text{see above} \\ &= \int\left(\frac{\partial^2}{\partial\theta^2}\log f(y;\theta)\right)f(y;\theta)dy \\ &\quad + \int \frac{\partial \log f(y;\theta)}{\partial\theta}\frac{\partial f(y;\theta)}{\partial\theta}dy \\ &= \mathrm{E}_\theta\left(\frac{\partial^2}{\partial\theta^2}\log f(Y;\theta)\right) \\ &\quad + \int \frac{\partial \log f(y;\theta)}{\partial\theta}\frac{\partial \log f(y;\theta)}{\partial\theta}f(y;\theta)dy \end{aligned}$$

$$\Leftrightarrow \mathrm{E}_\theta\left(s(\theta;Y)s(\theta;Y)\right) = \mathrm{E}_\theta\left(-\frac{\partial^2}{\partial\theta^2}\log f(Y;\theta)\right)$$

Bartlett's second equation holdds then as $\mathrm{E}\left(s(\theta;Y)\right) = 0$

ML-Estimate

$$\hat\theta_{ML} = \arg\max\ l(\theta; y_1, ...y_n)$$

for Fisher-regular distributions: $\hat\theta_{ML}$ has aysmptotically the smallest variance, given by the Cramér-Rao inequality,
$s\left(\hat\theta_{ML}; y_1, ..., y_n\right) = 0$
$\hat\theta \overset{a}{\sim} \mathrm{N}\left(\theta, I^{-1}(\theta)\right)$
The ML-estimate is invariant: $\hat\gamma = g(\hat\theta)$ if $\gamma = g(\theta)$.

Proof:
$\gamma = g(\theta) \Leftrightarrow \theta = g^{-1}(\gamma)$
For the log-likelihood of γ at the location $\hat\theta$ holds:

$$\frac{\partial l(g^{-1}(\hat\gamma))}{\partial\gamma} = \frac{\partial g^{-1}(\gamma)}{\partial\gamma}\underbrace{\frac{\partial l(\hat\theta)}{\partial\theta}}_{=0} = 0$$

Die Fisher-Information ist dann $\frac{\partial\theta}{\partial\gamma}I(\theta)\frac{\partial\theta}{\partial\gamma}$

Proof:

$$\begin{aligned} I_\gamma(\gamma) &= -\mathrm{E}\left(\frac{\partial^2 l(g^{-1}(\hat\gamma))}{\partial\gamma^2}\right) = -\mathrm{E}\left(\frac{\partial}{\partial\gamma}\left(\frac{\partial g^{-1}(\gamma)}{\partial\gamma}\frac{\partial l(\theta)}{\partial\theta}\right)\right) \\ &= -\mathrm{E}\left(\underbrace{\frac{\partial^2 g^{-1}(\gamma)}{\partial\gamma}\frac{\partial l(\theta)}{\partial\theta}}_{\text{Erwartungswert } 0} + \frac{\partial g^{-1}(\gamma)}{\partial\gamma}\frac{\partial^2 l(\theta)}{\partial\theta^2}\frac{\partial g^{-1}(\gamma)}{\partial\gamma}\right) \\ &= \frac{\partial g^{-1}(\gamma)}{\partial\gamma}I(\theta)\frac{\partial g^{-1}(\gamma)}{\partial\gamma} = \frac{\partial\theta}{\partial\gamma}I(\theta)\frac{\partial\theta}{\partial\gamma} \end{aligned}$$

Delta-Regel: $\gamma \overset{a}{\sim} \mathrm{N}(\hat\gamma, \frac{\partial\theta}{\partial\gamma}I^{-1}(\theta)\frac{\partial\theta}{\partial\gamma}$

Numerical computation of the ML estimate Fisher-Scoring as statistical version of the Newton-Raphson procedure

1. Initialize $\theta_{(0)}$
2. Repeat: $\theta_{(t+1)} := \theta_{(t)} + I^{-1}(\theta_{(t)})s(\theta_{(t)}; y)$
3. Stop if $\|\theta_{(t+1)} - \theta_{(t)}\| < \tau$; return $\hat\theta_{ML} = \theta_{(t+1)}$

Proof:

$$0 = s(\hat\theta_{ML}; y) \overset{Taylor}{\underset{Series}{\approx}} s(\theta; y) + \frac{\partial s(\theta;y)}{\partial\theta}(\hat\theta_{ML} - \theta) \Leftrightarrow$$

$$\hat\theta_{ML} \approx \theta - \left(\frac{\partial s(\theta;y)}{\partial\theta}\right)^{-1}s(\theta;y) \approx \theta - I^{-1}(\theta)s(\theta;y)$$

As $\frac{\partial s(\theta;y)}{\partial\theta}$ is often complicated, its expectation $I(\theta)$ is used.

The second part in 2 can be weighted with a step size δ or $\delta(t)$ $\in (0,1)$, e. g. to ensure convergence.
If $I(\theta)$ can't be analytically derived, simulation from $f(y;\theta_{(t)})$ can be used. For the exponential family, step 2 then changes to $\theta_{(t+1)} := \theta_{(t)} + \hat{\mathrm{Var}}_{\theta_{(t)}}(t(Y))^{-1}\mathrm{E}_{\theta_{(t)}}(t(Y))$ as the ML estimate is the expectation.

Log Likelihood Ratio

$$lr(\theta,\hat\theta) := l(\hat\theta) - l(\theta) = \log\frac{L(\hat\theta)}{L(\theta)}$$

with $2 \cdot lr(\theta,\hat\theta) \overset{a}{\sim} \chi^2_1$

Proof:

$$l(\theta) \overset{Taylor}{\underset{Series}{\approx}} l(\hat\theta) + \underbrace{\frac{\partial l(\hat\theta)}{\partial\theta}}_{=0}(\theta-\hat\theta) + \frac{1}{2}\underbrace{\frac{\partial^2 l(\hat\theta)}{\partial\theta^2}}_{\approx I^{-1}(\theta)s(\theta;Y)}(\underbrace{\theta-\hat\theta}_{\approx -I(\theta)})^2$$

$$\approx l(\hat\theta) - \frac{1}{2}\frac{s^2(\theta,Y)}{I(\theta)}$$

$s(\theta,Y)$ is asymptotically normal.

If $\theta \in \mathbb{R}^p$ the corresponding distribution is χ_p^2.

3.4 Sufficiency und Consistency

Statistic

$$t : \mathbb{R}^n \to \mathbb{R}$$

$t(Y_1, ..., Y_n)$ depends on sample size n and is a random variable

Suffizienz

A statistic $t(y_1, ..., y_n)$ is sufficient for θ, if the conditional distribution $f(y_1, ..., y_n|t_0 = t(y_1, ..., y_n); \theta)$ is independent of θ.

Neyman criterion:

$$t(Y_1, ..., Y_n) \text{ suffizient } \Leftrightarrow f(y;\theta) = h(y)g\left(t(y);\theta\right)$$

Proof:

"$\Rightarrow$":

$$f(y;\theta) = \underbrace{f(y|t=t(y);\theta)}_{h(y)}\underbrace{f_t(t|y;\theta)}_{g(t(y);\theta)}$$

"$\Leftarrow$":

$$f_t(t;\theta) = \int_{t=t(y)} f(y;\theta)dy = \int_{t=t(y)} h(y)g(t;\theta)dy$$

Therefore:

$$f\left(y|t=t(y);\theta\right) = \frac{f(y,t=t(y);\theta)}{f_t(t,\theta)} = \begin{cases} \frac{h(y)g(t;\theta)}{g(t;\theta)} & t = t(y) \\ 0 & \text{otherwise} \end{cases}$$

Minimal Sufficiency:

$t(.)$ is sufficient and $\forall\, \tilde t(.)\, \exists\, h(.)$ s.t. $t(y) = h(\tilde t(y))$

(Weak) Consistency

$$MSE(\hat\theta,\theta) \overset{n\to\infty}{\longrightarrow} 0 \Rightarrow \hat\theta \text{ consistent}$$

Proof:

$P(|\hat\theta - \mathrm{E}_{\hat\theta}| \geq \delta) \leq \frac{Var_\theta(\hat\theta)}{\delta^2}$ using the inequality of Chebyshev and $MSE(t(.),\theta) = \mathrm{Var}_\theta\left(t(Y_1, ..., Y_n)\right) + Bias^2((t(.);\theta)$

4 Statistical Hypothesis Testing

4.1 Significance and Confidence Intervals

Significance Test
Assuming two states H_0 and H_1 and two corresponding decisions "H_0" and "H_1", a decision rule (a threshold $c \in \mathbb{R}$ for the test statistic $T(X)$) is constructed s. t.:

$$P(\text{“}H_1\text{”}|H_0) \leq \alpha$$

	"H_0"	"H_1"
H_0	$1-\alpha$ (correct)	α (type I error)
H_1	β (type II error)	$1-\beta$ (correct)

Power concerns the type II error

$$power = P(\text{“}H_1\text{”}|H_1) = 1-\beta$$

p-Value measures the amount of evidence against H_0

$$p - value \leq \alpha \Leftrightarrow \text{“}H_0\text{”}$$

Confidence Interval

$$[t_l(Y), t_r(Y)] \text{ Confidence Interval}$$
$$\Leftrightarrow$$
$$P_\theta\left((t_l(Y) \leq \theta \leq t_r(Y)\right) \geq 1-\alpha$$

with $1-\alpha$ confidence level und α significance level

Corresponding Test

$$\theta \notin [t_l(y), t_r(y)] \Leftrightarrow \text{“}H_1\text{”}$$

Specificity or True Negative Rate (1−empirical type I error)

$$TNR = \frac{\#TN}{\#N} = \frac{\#TN}{\#TN + \#FP}$$

Sensitivity or True Positive Rate, Recall (empirical power)

$$TPR = \frac{\#TP}{\#P} = \frac{\#TP}{\#TP + \#FN}$$

4.2 Tests for One Sample

Normal Distribution $X_i \overset{iid}{\sim} N(\mu, \sigma^2)$

Test for μ, known σ^2 (Simple Gauss-Test)
$H_0\colon\ \mu = \mu_0 \quad vs. \quad H_1\colon\ \mu \neq \mu_0$

$$T(X) = \frac{\bar{X} - \mu_0}{\sigma} \overset{H_0}{\sim} \mathrm{N}(0,1)$$

Test for μ, unknown σ^2 (Simple t-Test)
$H_0\colon\ \mu = \mu_0 \quad vs. \quad H_1\colon\ \mu \neq \mu_0$

$$T(X) = \frac{\bar{X} - \mu_0}{\hat{\sigma}/\sqrt{n}} \overset{H_0}{\sim} t_{n-1}$$

with $\hat{\sigma} = \sqrt{\frac{1}{n-1}\sum_{i=1}^n (Y_i - \bar{Y})^2}$

ML Estimate $\hat{\theta} \overset{a}{\sim} \mathrm{N}(\theta, I^{-1}(\theta))$

Wald Test
$H_0\colon\ \theta = \theta_0 \quad vs. \quad H_1\colon\ \theta \neq \theta_0$

$$T(X) = |\hat{\theta} - \theta_0| \overset{H_0}{\sim} \mathrm{N}(0, I^{-1}(\theta_0))$$

As $\hat{\theta}$ converges to θ_0 under H_0, it can also be used to calculate the variance: $I^{-1}(\hat{\theta}$.

Score Test
$H_0\colon\ \theta = \theta_0 \quad vs. \quad H_1\colon\ \theta \neq \theta_0$

$$T(X) = |s(\theta_0; y)| \overset{H_0}{\sim} \mathrm{N}(0, I(\theta_0))$$

Advantage compared to the Wald Test: $\hat{\theta}$ does not have to be calculated.

Likelihood Ratio Test
$H_0\colon\ \theta = \theta_0 \quad vs. \quad H_1\colon\ \theta \neq \theta_0$

$$T(X) = 2(l(\hat{\theta}) - l(\theta)) \overset{H_0}{\sim} \chi_1^2$$

Neyman-Pearson Test
$H_0\colon\ \theta = \theta_0 \quad vs. \quad H_1\colon\ \theta = \theta_1$

$$T(X) = l(\theta_0) - l(\theta_1)$$

For a given significance level α, the Neyman Pearson Test is the most powerful test for comparing two estimates for θ.

Proof:

Decision rule of the NP-Test: $\varphi^* = \begin{cases} 1 & if\, \frac{f(y;\theta_0)}{f(y;\theta_1)} \leq \mathrm{e}^c \\ 0 & \text{otherwise} \end{cases}$

Need to show: $P(\varphi(Y){=}1|\theta_1) \leq P(\varphi^*(Y){=}1|\theta_1)\ \forall\varphi$

$$\begin{aligned}
&P(\varphi^*{=}1|\theta_1) - P(\varphi{=}1|\theta_1) = \\
&= \int \{\varphi^*(y) - \varphi(y)\} f(y;\theta_1) dy \\
&\geq \frac{1}{\mathrm{e}^c} \int_{\varphi^*=1} \{\varphi^*(y) - \varphi(y)\} f(y;\theta_0) dy \qquad f(y;\theta_1) \geq \frac{f(y;\theta_0)}{\mathrm{e}^c} \\
&+ \frac{1}{\mathrm{e}^c} \int_{\varphi^*=0} \{\varphi^*(y) - \varphi(y)\} f(y;\theta_0) dy \qquad f(y;\theta_1) \leq \frac{f(y;\theta_0)}{\mathrm{e}^c} \\
&= \frac{1}{\mathrm{e}^c} \int \{\varphi^*(y) - \varphi(y)\} f(y;\theta_0) dy = 0
\end{aligned}$$

As $\alpha = \int \varphi^*(y) f(y;\theta_0) dy = \int \varphi(y) f(y;\theta_0) dy$

4.3 Tests for Goodness of Fit

Discrete (Chi-Squared)
$H_0\colon\ X_i \sim F_0 \quad vs. \quad H_1\colon\ X_i \sim F \neq F_0$

$$T(X) = \sum_{k=1}^{K} \frac{(n_k - l_k)^2}{l_k} \overset{H_0}{\sim} \chi^2_{K-1-p}$$

with the following contingency table:

	1	2		K
observed	n_1	n_2	...	n_K
expected under H_0	l_1	l_2	...	l_K

$l_k > 5$ and $l_k > n-5$ for the χ^2_{K-1-p}-distribution to hold, F_0 needs to be known, but its p parameters can be estimated. The test can be applied to discretized continuous variables.

Continuous (Kolmogorov-Smirnov Test)
$H_0\colon\ X_i \sim F_0 \quad vs. \quad H_1\colon\ X_i \sim F \neq F_0$

$$T(X) = \sup_x |F_n(x) - F(x;\theta)| \overset{H_0}{\sim} KS$$

with the distribution function $F(x;\theta)$ and the empirical counterpart $F_n(x) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{X_i \leq x\}}$

Proof:

$$P(\sup_x |F_n(x) - F(x;\theta)| \leq t) =$$
$$= P(\sup_y |F^{-1}(y;\theta) - x| \leq t) \qquad \substack{x\in[0,1],\, x=F^{-1}(y;\theta) \\ F(F^{-1}(y;\theta);\theta)=y}$$
$$\overset{*}{=} P(\sup_y |\frac{1}{n}\sum_{i=1} \mathbb{1}_{\{U_i \leq y\}} - y| \leq t) \qquad \text{with } U_i \sim U(0,1)$$
$$^{*}F_n(F^{-1}(y;\theta)) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{X_i \leq F^{-1}(y;\theta)\}} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{F(y;\theta) \leq y\}}$$

For an estimated parameter the distribution of $T(X)$ is not independent of F_0: $T(X) \overset{H_0}{\sim} KS$ only holds asymptotically.

Pivotal Statistic

$$g(Y;\theta) \text{ pivotal}$$
$$\Leftrightarrow$$
$$\text{Distribution of } g(Y;\theta) \text{ independent of } \theta$$

Approximative Pivotal Statistic
$H_0\colon\ X_i \sim F$ pivotal $\quad vs. \quad H_1\colon\ X_i \sim F$not pivotal

$$g(\hat\theta;\theta) = \frac{\hat\theta - \theta}{\sqrt{\mathrm{Var}(\hat\theta)}} \overset{\alpha}{\sim} \mathrm{N}(0,1)$$

with $\hat\theta = t(Y) \overset{\alpha}{\sim} \mathrm{N}(\theta, \mathrm{Var}(\hat\theta))$

$$KI = \left[\hat\theta - z_{1-\frac{\alpha}{2}}\sqrt{\mathrm{Var}(\hat\theta)}, \hat\theta + z_{1-\frac{\alpha}{2}}\sqrt{\mathrm{Var}(\hat\theta)}\right]$$

Proof:
$1-\alpha \approx P\left(z_{\frac{\alpha}{2}} \leq \frac{\hat\theta-\theta}{\sqrt{\mathrm{Var}(\hat\theta)}} \leq z_{1-\frac{\alpha}{2}}\right)$

4.4 Multiple Tests

Family-Wise Error Rate (FWER) as *p-value* $\sim U(0,1)$
For m tests:

$$\alpha \leq P\left(\cup_{k=1}^{m}(p_k \leq \alpha)|H_{0k}, k=1,...,m\right) \leq m\alpha$$

$$FWER := P(\exists k : \text{“}H_1 k\text{”} | \forall k :\ H_0 k)$$

Bonferoni Adjustment

$$\alpha_B = \frac{\alpha}{m}$$

Šidák Adjustment only for independent tests

$$\alpha_S = 1 - (1-\alpha)^{1/m}$$

Proof:
$$\alpha \overset{!}{=} P\left(\cup_{k=1}^{m}(p_k \leq \alpha)|H_{0k}, k=1,...,m\right)$$
$$= 1 - (1-\alpha)^{1/m}$$

Holm's Procedure also takes power into account
Order the p-values: $p_{(1)} \leq ... \leq p_{(m)}$
Step $x \in \mathbb{N}^+$: if $p(x) > \frac{\alpha}{m+1-x}$ reject H_{01} to H_{0x} and stop, else move on to step $x+1$.

False Discovery Rate (FDR) balances type I and II errors, especially for $n << m$ problems

$$FDR = \mathrm{E}\left(\frac{\#\text{“}H1\text{”}|H_0}{\#\text{“}H1\text{”}}\right)$$

Order the p-values: $p_{(1)} \leq ... \leq p_{(m)}$, choose $\alpha \in (0,1)$
j is largest index s. t. $p(j) \leq \alpha j/m$, reject all $H_0 i$ for $i \leq j$

It can be shown that $FDR \leq m_0\alpha/m$, with $m_0 = \#H_0$

5 Regression

5.1 Models

5.1.1 Simple Linear Model

Theoretical Model

$$y_i = \beta_0 + \beta_1 x_i + u_i$$

Empirical Model

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + e_i$$

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

Assumptions

- **Independent Observations** $y_1, ...y_n$ are independent
- **Linearity of the Mean** $E(Y|x) = \beta_0 + \beta_1 x$ or $\mathrm{E}(e|x) = 0$
- **Constant Variation** $Var(Y|x) = \sigma^2$

For the normal linear model:

- **Normality** $e|x \sim \mathrm{N}(0, \sigma^2)$; $Y|x \sim \mathrm{N}(\hat{y}, \sigma^2)$

Attributes of the Regression Line

$$\begin{aligned}
\hat{y}_i &= \hat{\beta}_0 + \hat{\beta}_1 x_i = \bar{y} + \hat{\beta}_1(x_i - \bar{x}) \\
\hat{e}_i &= y_i - \hat{y}_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i) \\
&= y_i - (\bar{y} + \hat{\beta}_1(x_i - \bar{x})) \\
\sum_{i=1}^{n} \hat{e}_i &= \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \bar{y} - \hat{\beta}_1 \sum_{i=1}^{n} (x_i - \bar{x}) \\
&= n\bar{y} - n\bar{y} - \hat{\beta}_1(n\bar{x} - n\bar{x}) = 0 \\
\bar{\hat{y}} &= \frac{1}{n} \sum_{i=1}^{n} \hat{y}_i = \frac{1}{n}(n\bar{y} + \hat{\beta}_1(n\bar{x} - n\bar{x})) = \bar{y}
\end{aligned}$$

Estimates (OLS)

$$\hat{\beta}_1 = \frac{Cov(x,y)}{Var(x)} = \frac{S_{xy}}{S_{xx}} = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}} \cdot \sqrt{\frac{S_{yy}}{S_{xx}}} = r\sqrt{\frac{S_{yy}}{S_{xx}}}$$

Proof:
$Cov(x,y) = Cov(x, \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}) = \hat{\beta}_1 Var(x)$
$\iff \hat{\beta}_1 = \frac{Cov(x,y)}{Var(x)}$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

Proof:
$E[y] = E\left[\hat{\beta}_0 + \hat{\beta}_1 x + \hat{e}\right] \iff \hat{\beta}_0 = E[y] - \hat{\beta}_1 E[x]$

The estimates are the same as for the ML procedure.

Estimates (ML) $Y|x \sim \mathrm{N}(\beta_0 + \beta_1 x, \sigma^2)$

$$\begin{aligned}
\hat{\beta}_0 &= \frac{1}{n}\sum_{i=1}^{n} y_i - \frac{1}{n}\sum_{i=1}^{n} x_i \hat{\beta}_1 \\
\hat{\beta}_1 &= \sum_{i=1}^{n} x_i(y_i - \hat{\beta}_0 / \sum_{i=1}^{n} x_i^2 \\
\hat{\sigma}^2 &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - x_i\hat{\beta}_1)^2
\end{aligned}$$

The β-estimates are the same as for the OLS procedure.

Proof:
$$l(\beta_0, \beta_1, \sigma^2) = \sum_{i=1}^{n}\left\{-\frac{1}{2}\sigma^2 - \frac{1}{2}\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{\sigma^2}\right\}$$

5.1.2 Multivariate Linear Model

Theoretical Model

$$Y = X\beta + u$$

Empirical Model

$$Y = X\hat{\beta} + e$$

$$\hat{Y} = X\hat{\beta}$$

$$y = (y_1, ..., y_n)^T,\ e = (e_1, ..., e_n)^T,\ X = \begin{pmatrix} 1 & x_{11} & \dots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{pmatrix}$$

Assumptions

- **Independent Observations** $y_1, ...y_n$ are independent
- **Linearity of the Mean** $\mathrm{E}(Y|x_{1:p}) = X\beta$ or $\mathrm{E}(e|x_{1:p}) = 0$
- **Constant Variation** $Var(Y|x) = \sigma^2$

For the normal linear model:

- **Normality** $e_i|x_{1:p} \sim \mathrm{N}(0, \sigma^2)$; $Y|x \sim \mathrm{N}(\hat{y}, \sigma^2)$

Estimates (ML) $Y|x_{1:p} \sim \mathrm{N}(X\beta, \sigma^2)$

$$\hat{\beta} = \left(X^T X)^{-1}\right) X^T y$$

$$Var(\hat{\beta}) = \sigma^2(X^T X)^{-1}) = I^{-1}(\beta)$$

Proof:
$l(\beta, \sigma^2) = -\frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(y - X\beta)^T(y - X\beta)$

The estimates are the same as for the OLS procedure.
β is the **B**est **L**inear **U**nbiased **E**stimator

Proof:
Unbiased because of the Gauß-Markov Theorem: $E(\hat{\beta}) = (X^TX)^{-1}X^T E(Y|X) = (X^TX)^{-1}X^TX\beta = \beta$

$$\hat{\sigma}^2 = \frac{1}{n}(y - X\hat{\beta})^T(y - X\hat{\beta}); \quad \hat{\beta} \sim N(\beta, \sigma^2(X^TX)^{-1})$$

The ML-estimate for σ^2 is biased.

Proof:
$H{:=}X(X^TX)^{-1}X^T$ hat matrix; $HH{=}H{=}H^T$ (idempotent)

$$\begin{aligned} E((Y-X\hat{\beta})^T(Y-X\hat{\beta})) &= E((Y^T(I_n-H)^T((I_n-H)Y) \\ &= E(tr(Y^T(I_n-H)Y) \\ &= E(tr((I_n-H)YY^T) \\ &= tr((I_n-H)E(YY^T)) \\ &= tr((I_n-H)E(X\beta\beta^TX^T + \sigma I_n)) \\ &= \sigma^2 tr((I_n-H)) \\ &= \sigma^2(n-p) \end{aligned}$$

$$s^2 = \frac{1}{n-p}(y - X\hat{\beta})^T(y - X\hat{\beta}); \quad \hat{\beta} \sim t_{n-p}(\beta, s^2(X^TX)^{-1})$$

with s an unbiased estimator

5.1.3 Bayesian Linear Model

Prior flat prior

$$f_{\beta,\sigma^2}(\beta, \sigma^2) = \frac{1}{\sigma^2}$$

Posterior
Resulting posterior:

$$f_{post}(\beta, \sigma^2|y) \propto (\sigma^2)^{-\frac{n}{2}+1} e^{-\frac{1}{2\sigma^2}(y-X\beta)^T(y-X\beta)}$$

Note: $f_{post}(\beta, \sigma^2|y) = f(\beta|\sigma^2, y)f(\sigma^2|y)$

$$\begin{aligned} \beta|\sigma^2, y &\sim N\left(\hat{\beta}, \sigma^2(X^TX)^{-1}\right) \\ \sigma^2|y &\sim IG\left(\frac{n-p}{2}, \frac{s^2(n-p)}{2}\right) \\ \beta|y &\sim t_{n-p}\left(\hat{\beta}, s^2(X^TX)^{-1}\right) \end{aligned}$$

The two distributions for β mirror the results for $\hat{\beta}$ in the linear model.

5.1.4 Quantile Regression

Prediction Interval range of $1-\alpha$ fraction of the data

$$Var(\hat{Y}|x_{1:p}) = Var(X\hat{\beta}) + \sigma^2$$

Determined by estimation variance (usually captured by confidence intervals) plus residual variance.

Quantile

$$Q(\tau) = \inf\{y : F(y) \geq \tau\}$$

If F is invertable: $Q(\tau) = F^{-1}(\tau)$, $\tau \in (0, 1)$

Model

$$Q(\tau|x_{1:p}) = X\beta$$

For median regression: $\hat{\beta} = \arg\ \min \sum_{i=1}^n |y_i - x_i^T\beta|$

In general:

$$\hat{Q}(\tau) = \arg\min_{\beta}\left(\sum_{i=1}^n \delta_\tau(y_i - x_i^T\beta)\right)$$

with check function $\delta_\tau(y) = y\left(\tau - \mathbb{1}_{\{y<0\}}\right)$

Proof:

$$\begin{aligned} Q(\tau) &= \arg\min_q E(\delta_\tau(Y-q)) \\ &= \arg\min_q \left\{(\tau-1)\int_{-\infty}^{q}(y-q)f(y)dy + \tau\int_{q}^{\infty}(y-q)f(y)dy\right\} \end{aligned}$$

Differentiating w.r.t. q gives $(\tau-1)\int_{-\infty}^q f(y)dy - \tau\int_q^\infty f(y)dy$
$= (1-\tau)F(q) - \tau(1-F(q) = F(q) - \tau$

Estimates
The estimates for β can be computed with linear programming and are normally distributed with mean β.

5.1.5 Flexible Regression

Assumptions

- **Independent Observations** $y_1, ...y_n$ are independent
- **Constant Variation** $Var(Y|x) = \sigma^2$
- **Normality** $e_i|x_{1:p} \sim N(0, \sigma^2)$; $Y|x \sim N(\hat{y}, \sigma^2)$

Knot Placement

- equidistant
- based on quantiles (more structure where data is dense)
- all data points plus penalization

Penalized Regression Splines

$$||y-X\beta||^2 + \lambda \int_{x_1}^{x_n} \left[f''(x)\right]^2 dx = ||y-X\beta||^2 \lambda \beta^T D\beta$$

$l_p(\beta, \sigma^2, \lambda) = l(\beta, \sigma^2) - \frac{\lambda}{2\sigma_\epsilon^2}\beta^T D\beta$
$\hat{\beta} = (X^T X + \lambda D)^{-1} X^T y$

Difference Penalty

- first order: $\beta^T D\beta = \sum_{j=1}^{p}(\beta_{j+1} - \beta_j)^2$
- second order: $\beta^T D\beta = \sum_{j=1}^{p}(\beta_{j+1} - 2\beta_j + \beta_{j-1})^2$

Choosing $\boldsymbol{\lambda}$ Model complexity

$$\dim(\lambda) = tr\left\{(X^T X + \lambda D)^{-1}(X^T X)\right\}$$

$AIC(\lambda) = fit(\lambda) + 2\dim(\lambda)$

Numerically complex. Alternative: **Bayes**

$\beta \sim \mathrm{N}(0, \sigma_\beta^2 D^-)$ with $(D^-)^- = D$ (generalized inverse)

$$\log f(\beta, \sigma^2; \sigma_\beta^2|y) \propto l(\beta, \sigma^2) - \frac{rk(D^-)}{2}\log(\sigma_\beta^2) - \frac{1}{2\sigma_\beta^2}\beta^T D^- \beta$$

As $\lambda = \frac{1}{\sigma_\beta^2}$, marginal posterior for σ_β^2 can be derived. E.g. set λ to the posterior mode estimate.

5.1.6 Generalized Regression

Assumptions

- **Independent Observations** $y_1, ...y_n$ are independent
- **Linearity of the Mean** $\mathrm{E}(Y|x_{1:p}) = X\beta$ or $\mathrm{E}(e|x_{1:p}) = 0$
- **Exponential Family** $Y|x \sim \exp\{t(y)\theta(x) - \kappa(\theta(x))\}\, h(y)$

Link Function
Linear predictor $\eta = X\beta$; $\mu = \frac{\partial\kappa(\theta)}{\partial\theta} = \mathrm{E}(t(Y);\theta)$

$$\mu = g^{-1}(\eta)$$

If $\lambda = 0$, *canonical link*:

$$g(\theta) = \eta$$

- score function: $s(\beta) = X^T\,(t(y) - \mathrm{E}(t(Y);\eta))$
- estimate $\hat{\beta} = X^T \mathrm{E}(t(Y);\hat{\eta}) = X^T t(y)$
- Fisher matrix $I(\beta) = X^T W X$
with W diagonal and $W_{ii} = \frac{\partial^2\kappa(\eta_i)}{\partial\eta^2} = Var(t(Y_i), \eta_i)$

Examples:

- **Logistic**: $\mathrm{logit}P(Y_i{=}1|x_i) = \log\frac{P(Y_i=1|x_i)}{1-P(Y_i=1|x_i)} = \eta$
$Var(Y_i|x_i) = P(Y_i{=}1|x_i)\cdot(1{-}P(Y_i{=}1|x_i))$
- **Poisson**: $log\mathrm{E}(Y_i|x_i) = \eta$
$Var(Y_i|x_i) = \mathrm{E}(Y_i|x_i) = e^\eta$

5.1.7 Weighted Regression

Different Precision variance heterogeneity: $e_i \sim \mathrm{N}(0, \sigma_i^2)$

$$l(\beta, \sigma^2) = -\frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2(y - X\beta)^T(y - X\beta)}$$

with $W = diag(\frac{1}{a_1}, ..., \frac{1}{a_n})$ and $a_i = \frac{\sigma_i^2}{\sigma^2}$

$$\hat{\beta}_{ML} = (X^T W X)^{-1}(X^T W y)$$

$$Var(\hat{\beta}_{ML}) = \sigma^2(X^T W X)^{-1}$$

Different Group Representation

$$Y_i|x_{i,1:p}, z_i \sim \mathrm{N}(x_{i,1:p}\beta_{z_i}, \sigma^2)$$

with z_i indicating group affiliation

5.2 Analysis of Variances (ANOVA)

$$SS_{Total} = SS_{Explained} + SS_{Residual}$$

with

$$SS_{Total} = \sum_{i=1}^{n}(y_i - \bar{y})^2$$

$$SS_{Explained} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$$

$$SS_{Residual} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} e_i^2 = S_{yy} - \hat{\beta}^2 S_{xx}$$

5.3 Goodness of Fit

5.3.1 Coefficient of Determination

$$R^2 = \frac{SS_{Explained}}{SS_{Total}} = 1 - \frac{SS_{Residual}}{SS_{Total}} = r^2$$

Range: $0 \leq R^2 \leq 1$

6 Bayesian Statistics

6.1 Basics

Bayes Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \qquad \text{für } P(A), P(B) > 0$$

or more general:

$$f_{post}(\theta|X) = \frac{f(X|\theta) \cdot f_\theta(\theta)}{\int f(X|\tilde{\theta}) f_\theta(\tilde{\theta}) d\tilde{\theta}}$$
$$= C \cdot f(X|\theta) \cdot f_\theta(\theta) \quad \text{choose C so that} \int f(\theta|X) = 1$$
$$\propto f(X|\theta) \cdot f_\theta(\theta)$$

Point Estimates

$$\hat{\theta}_{postmean} = E_0(\vartheta|x) = \int_{\vartheta \in \Theta} \vartheta f_\theta(\vartheta|x) d\vartheta$$
$$\hat{\theta}_{postmode} = \underset{\vartheta}{\operatorname{argmax}} f_\theta(\vartheta, x)$$
$$\hat{\theta}_{Bayesrisk} = \underset{t(.)}{\operatorname{argmin}} R_{Bayes}(t(.))$$

with Bayes risk: $R_{Bayes}(t(.)) = \int_\Theta R(t(.), \vartheta) f_\theta(\vartheta) d\vartheta$

$$\hat{\theta}_{postBayesrisk} = \underset{t(.)}{\operatorname{argmin}} R_{postBayes}(t(.)|y)$$

with posterior Bayes risk:
$R_{postBayes}(t(.)|y) = \int L(t(y), \vartheta) f_\theta(\vartheta|y) = \mathrm{E}_{\theta|y}(L(t(y), \theta)|y$

Credibility Interval

$$P_\theta(\theta \in [t_l(y), t_r(y)] \,|y) = \int_{t_l(y)}^{t_r(y)} f_\theta(\vartheta|y) d\vartheta = 1 - \alpha$$

- symmetric: $\int_{-\infty}^{t_l(y)} f_\theta(\vartheta|y) d\vartheta = \int_{t_r(y)}^{\infty} f_\theta(\vartheta|y) d\vartheta = \frac{\alpha}{2}$
- highest density: $HDI = \theta | f_\theta(\theta|y) \geq c$, choose c s. t. $\int_{\vartheta \in HDI(y)} f_\theta(\vartheta|y) d\vartheta = 1 - \alpha$

Bayes Factor evidence contained in data for M_1 vs. M_2

$$\frac{P(M_1|y)}{P(M_0|y)} = \underbrace{\frac{f(y|M_1)}{f(y|M_0)}}_{\text{Bayes Factor}} \frac{P(M_1)}{P(M_0)}$$

with marginal likelihood $f(y|M_i) = \int f(y|\vartheta) f_\theta(\vartheta|M_i) d\vartheta$

Priors

Flat (uninformative) Prior

$f_\theta(\theta) = const.$ for $\theta > 0$, therefore: $f(\theta|X) = C \cdot f(X|\theta)$
As $\int f_\theta(\theta) = 1$ not possible like this, this is not a real density.
Changes for transformations of the parameter.

Proof: For $\gamma = g(\theta)$: $f_\gamma(\gamma) = f_\theta(g^{-1}(\gamma)) \left| \frac{\partial g^{-1}(\gamma)}{\partial \gamma} \right|$

No prior is truly uninformative.

Jeffrey's Prior

Remains unchanged for transformations of the parameter.
For Fisher-regular distributions: $f(\theta) \propto \sqrt{I_\theta(\theta)}$

Proof:
For $\gamma = g(\theta)$ and $f_\theta(\theta) = \sqrt{I_\theta(\theta)}$:

$$f_\gamma(\gamma) \propto f_\theta(g^{-1}(\gamma)) \left| \frac{\partial g^{-1}(\gamma)}{\partial \gamma} \right| \propto \sqrt{\frac{\partial g^{-1}(\gamma)}{\partial \gamma} I_\theta(g^{-1}(\gamma)) \frac{\partial g^{-1}(\gamma)}{\partial \gamma}} = \sqrt{I_\gamma(\gamma)}$$

Maximizes the information gained from the data (under appropriate regulatory conditions), i. e. maximizes $\mathrm{E}(KL(f_\theta(.), f_{post}(., x))$

Empirical Bayes

Let the prior depend on a hyper-parameter: $f_\theta(\theta, \gamma)$
Choose γ s. t. $L(\gamma) = f(x; \gamma) = \int f(x; \vartheta) f_\theta(\vartheta, \gamma) d\vartheta$ is maximal.
Using the data to find the prior contradicts the Bayes approach of incorporating prior knowledge.

Hierarchical Prior

$$x|\theta \sim f(x; \theta); \quad \theta|\gamma \sim f_\theta(\theta, \gamma); \quad \gamma \sim f_\gamma(\gamma)$$

Conjugate Priors

If Prior and Posterior belong to the same family of distributions for a given likelihood function, they are called conjugate.

Examples:

Prior	Likelihood	Posterior
$\pi \sim \mathrm{Be}(\alpha, \beta)$	$\mathrm{Bin}(n, \pi)$	$\mathrm{Be}(\alpha{+}k, \beta{+}n{-}k)$
$\mu \sim \mathrm{N}(\gamma, \tau^2)$	$\mathrm{N}(\mu, \sigma^2)$	$\mathrm{N}(.,.) \overset{n\to\infty}{\longrightarrow} \mathrm{N}(\bar{y}, \frac{\sigma^2}{n})$
$\sigma^2 \sim \mathrm{IG}(\alpha, \beta)$	$\mathrm{N}(\mu, \sigma^2)$	$\mathrm{IG}(\alpha{+}\frac{n}{2}, \beta{+}\frac{1}{2}\sum_{i=1}^n (y_i{-}\mu)^2)$
$\lambda \sim \mathrm{Ga}(\alpha, \beta)$	$\mathrm{Po}(\lambda)$	$\mathrm{Ga}(\alpha{+}n\bar{y}, \beta{+}n)$

6.2 Numerical Methods for the Posterior

Numerical Integration here: trapezoid approximation

$$\int_\Theta f(y|\vartheta) f_\theta(\vartheta) d\vartheta \approx$$
$$\sum_{k=1}^K \frac{f(y; \theta_k) f_\theta(\theta_k) + f(y; \theta_{k-1}) f_\theta(\theta_{k-1})}{2} (\theta_k - \theta_{k-1})$$

only normalisation constant unknown, works well for one-dimensional integrals

Laplace Approximation

$$\int_\Theta f(y|\vartheta) f_\theta(\vartheta) d\vartheta \approx f(y; \hat{\theta}_P) f_\theta(\hat{\theta}_P) (2\pi)^{p/2} \left| J_P(\hat{\theta}_P) \right|^{\frac{1}{2}}$$

with the one-dimenional $J_P := -\frac{\partial^2 l_{(n)}(\theta, y)}{\partial \theta^2} - \frac{\partial^2 \log f\theta(\theta)}{\partial \theta^2}$ Fisher information considering the prior, $\hat{\theta}_P$ posterior mode estimate s. t. $s_{P,\theta}(\hat{\theta}_P) = 0$

Proof:
For n independent samples:

$$f_{post}(\theta|y) = \frac{\prod_{i=1}^{n} f(y_i|\theta) f_\theta(\theta)}{\int \prod_{i=1}^{n} f(y_i|\theta) f_\theta(\theta) d\theta}$$

Denominator: $\int \mathrm{e}^{\{\sum_{i=1}^{n} \log f(y_i|\theta) + \log f_\theta(\theta)\}} d\theta =$
$\int \mathrm{e}^{\{l(\theta;y) + \log f_\theta(\theta)\}} d\theta \overset{TS}{\approx} \int \mathrm{e}^{(l_P(\hat{\theta}_P) - \frac{1}{2} J_P(\hat{\theta}_P)(\vartheta - \hat{\theta}_P)^2)} d\vartheta$

Resembles the normal distribution, therefore the inverse of the normalisation constant can be calculated, which gives the inverse of the Laplace approximation in the univariate case.

Works well for large n and is numerically simple also for big p.

Monte Carlo Approximations
The denominator can be written as $\mathrm{E}_\theta(f(y;\theta)) = \int_\Theta f(y|\vartheta) f_\theta(\vartheta) d\vartheta$, which can be estimated by the arithmetic mean for a sample of $\theta_1, ..., \theta_N$, which needs to be drawn from the prior. The following methods to draw from non-standard distributions can be used for that.

- **Inverse CDF**
  $F(X)$ known. Since $F(x) = u$, $F^{-1}(u) = x$, $u \sim U(0,1)$
  1. Draw $u \sim U(0,1)$
  2. Compute $F^{-1}(u)$ to get a value x

Proof:

$$P(x \le y) = P(F^{-1}(u) \le y) = P(u \le F(y)) = F(y)$$

- **Rejection Sampling**
  An umbrella distribution $g(x)$ can be found s.t. $\frac{f(x)}{g(x)} \le M \; \forall x$ with $f(x) > 0$ when $g(x) > 0$
  1. Draw candidate $y \sim g(x)$
  2. Acceptance probability α for y: $\alpha = \frac{f(x)}{Mg(x)}$
  3. Draw $u \sim U(0,1)$ and accept if $u \le \alpha$, else: step 1

Proof:

$$P\left(Y \le x | U \le \frac{f(Y)}{Mg(Y)}\right) = \frac{P\left(Y \le x, U \le \frac{f(Y)}{Mg(Y)}\right)}{P\left(U \le \frac{f(Y)}{Mg(Y)}\right)}$$

$$= \frac{\int_{-\infty}^{x} \int_0^{\frac{f(y)}{g(x)}} du \, g(y) dy}{\int_{-\infty}^{\infty} \int_0^{\frac{f(y)}{g(x)}} du \, g(y) dy} = \frac{\int_{-\infty}^{x} \frac{f(y)}{g(x)} g(y) dy}{\int_{-\infty}^{\infty} \frac{f(y)}{g(x)} g(y) dy}$$

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

- **Importance Sampling**
  Directly estimate $\mathrm{E}_\theta(f(y;\theta))$.

  For sampling distribution $g(x)$,

$$\frac{1}{N} \sum_{i=1}^{n} \frac{f(x)}{g(x)}$$

  is a consistent estimator.

Proof:

$$\mathrm{E}_g\left(\frac{1}{N} \sum_{i=1}^{n} \frac{f(x)}{g(x)}\right) = \int \frac{f(x)}{g(x)} g(x) dx = \int f(x) dx = f(x)$$

Markov Chain Monte Carlo sample from $f_{post}(\theta|X)$
$f(y)$ unknown, however:

$$\frac{f_{post}(\theta|x)}{f_{post}(\tilde{\theta}|x)} = \frac{f(x|\theta) f_\theta(\theta)}{f(y)} \frac{f(y)}{f(x|\tilde{\theta}) f_\theta(\tilde{\theta})} = \frac{f(x|\theta) f_\theta(\theta)}{f(x|\tilde{\theta}) f_\theta(\tilde{\theta})}$$

Metropolis-Hastings: Draw Markov Chain $\theta_1^*, ..., \theta_n^*$:

1. Draw candidate θ^* from proposal distribution $q\left(\theta|\theta_{(t)}^*\right)$

2. Accept $\theta_{(t+1)}^* = \theta^*$ with probability

$$\alpha(\theta_{(t)}|\theta^*) = \min\left\{1, \frac{f_{post}(\theta^*|y) \, q\left(\theta_{(t)}^*|\theta^*\right)}{f_{post}\left(\theta_{(t)}^*|y\right) q\left(\theta^*|\theta_{(t)}^*\right)}\right\}$$

   else choose $\theta_{(t+1)}^* = \theta_{(t)}^*$

This sequence has a stationary distribution for $n \to \infty$.
Choice of q: trade-off between exploring Θ and reaching a high α.
Burn-in and thinning out give $i.i.d.$ samples from $f_{post}(\theta|X)$.

Gibbs Sampling: For high dimensions α is close to zero.
Sample from the marginal distributions seperately:

$$\theta_i^* \sim f_{\theta_i|y,\theta\backslash\theta_i}\left(\theta_i^*|y, \theta_{t^*,i}\right)$$

with $\theta_{t^*,i}$ most recent estimates without θ_i
A Gibbs sampled sequence converges to $f_{post}(\theta|X)$ as stationary.
Can also be used on its own, if marginal densities are known.

Variational Bayes Principles
Approximate $f_{post}(\theta|X)$ by $q_\theta = \min_{q_\theta \in Q} KL(f_{post}(.|X), q_\theta(.))$
Restrict q_θ to independence: $q_\theta(\theta) = \prod_{k=1}^{p} q_k(\theta_k)$
Update each component iteratively. Works well for big p.

7 Sampling

Bootstrap

1. Draw y_i^*: n samples with replacement from y
2. Calculate the statistic of interest $t(y_i^*)$
3. Repeat this B times
4. *Plug-in Principle*: Whenever the distribution function is involved in estimating a statistic, use the empirical bootstrapped version instead.

In a **Parametric Bootstrap** the parameter is first estimated from the data and then Bootstrap samples are drawn from the resulting distribution.

Bootstrap Probability

$$P(Y_i \in Y^*) = 1 - (1 - \frac{1}{n})^n \overset{n\to\infty}{\to} 1 - e^{-1} \approx 0.632$$

Subsampling

- **replacement** m-out-of-n bootstrap
- **non-replacement** subsampling directly from true F

Permutation Test for two variables

1. Calculate $t(x, y)$, e. g. differences in mean, correlation...
2. Draw samples x^*, y^* of size n from x and y without replacement ("shuffel")
3. Calculate $t(x^*, y^*)$
4. $p - value = \frac{1}{B}\sum_{b=1}^{B} \mathbb{1}_{\{t(x_b^*, y_b^*) \geq t(x,y)\}}$

For a **Boostrap Test** do step 2 with replacement.

Bootstrap in Regression

- **Residual based**: 1. Get Bootstrap sample e_i^* from fitted residuals $\hat{e} = y - X\hat{\beta}$, 2. Calculate new response $y_i^* = x_i\hat{\beta} + e_i^*$, 3. Calculate $\hat{\beta}^*$
- **Model based** 1. Draw a sample from $e_i \sim \mathrm{N}(0, \hat{\sigma}^2)$, 2. Calculate new response $y_i^* = x_i\hat{\beta} + e_i^*$, 3. Calculate $\hat{\beta}^*$
- **Pairwise** 1. Draw (y_i^*, x_i^*) from the original sample for $i = 1, .., n$, 2. Calculate $\hat{\beta}^*$
- **Wild** Set $\hat{e}_i^* = V_i^*\hat{e}_i$, with V_i^* from the 2-point distribution $P(V_i^* {=} \frac{\sqrt{5}+1}{2}) = \frac{\sqrt{5}-1}{2\sqrt{5}}$ and $P(V_i^* {=} {-}\frac{\sqrt{5}-1}{2}) = \frac{\sqrt{5}+1}{2\sqrt{5}}$, chosen as $\mathrm{E}(V_i^*) = 0$, $Var(V_i^*) = 1$, $\mathrm{E}(V_i^{*3}) = 1$

Consistency of a Bootstrap Estimator

$$\lim_{n\to\infty} P_n \left\{ \sup_t |G_n(t, F_n) - G_\infty(t, F)| > \epsilon \right\} = 0 \ \ \forall\epsilon$$

with $F_n(y) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{Y_i \leq y\}}$ empirical distribution function, $G_n(t, F) = P(T_n \leq t)$ exact finite sample distribution, and P_n joint probability of the sample

The bootstrap estimate is inconsistent for the maximum of a sample or if the θ lies on the boundary of Θ.

Mallow's Metric

$$\rho_p(F, G) = \inf_{\mathcal{T}_{XY}} \{E(|X - Y|)^p\}^{\frac{1}{p}}$$

for F, G in the set of distributions where $\inf_{-\infty}^{\infty} |t|^p dF(t) < \infty$; $(X, Y) \sim T \in \mathcal{T}_{XY}$ with $X \sim F$ and $Y \sim G$

Theorem of Beran and Ducharme

$G_n(., F_n)$ is consistent if $\forall\epsilon > 0, F$ the following holds:

1. $\lim_{n\to\infty} P_n(\rho(F_n, F) > \epsilon) = 0$
2. $G_\infty(t, F)$ is a continuous function of t
3. $\forall t$ and sequences $\{H_n\}$ s. t. $\lim_{n\to\infty} \rho(H_n, F) = 0$ holds: $G_n(t, H_n) \to G_\infty(t, F)$