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: $0 \leq G \leq \frac{n-1}{n}$

Lorenz-Münzner Coefficient (normed G)

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

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

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)

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

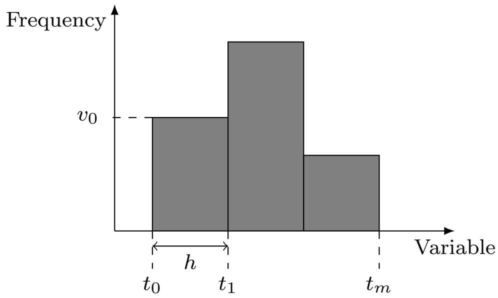
with
$S_{xy} = \sum\limits_{i=1}^{n} (x_i - \bar{x})^2 (y_i - \bar{y})^2$ or $s_{xy} = \frac{S_{xy}}{n}$
$S_{xx} = \sum\limits_{i=1}^{n} (x_i - \bar{x})^2$ or $s_{xx} = \frac{S_{xx}}{n}$
$S_{yy} = \sum\limits_{i=1}^{n} (y_i - \bar{y})^2$ or $s_{yy} = \frac{S_{yy}}{n}$

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) $0 \leq P(A) \leq 1 \qquad \forall A \in \mathcal{A} = \sigma\text{-algebra}(\Omega)$
(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:

- $P(\bar{A}) = 1 - P(A)$
- $P(\emptyset) = 0$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
- $A \subseteq B \Rightarrow P(A) \leq P(B)$

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

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

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

Law of Total Probability

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i) \qquad \text{for } \Omega = \bigcup_{i=1}^{\infty} A_i \text{ and } A_i \cap A_j = \emptyset$$

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 $\Leftrightarrow P(A \cap B) = P(A) \cdot P(B)$

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 $f(\cdot)$** (positive, integrates out to 1):

  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.

  If $Y = g(X)$, then $f_Y(y) = \left|\frac{dg^{-1}(y)}{dy}\right| f_X(g^{-1}(y))$.

- **Cumulative Distribution Function $F(\cdot)$:**

  $$F_Y(y) = P(Y \leq y)$$

  with $\lim_{y\to-\infty} F_Y(y) = 0$ and $\lim_{y\to\infty} F_Y(y) = 1$

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)**:
  $\sigma^2 = Var(Y) = E(\{Y - E(Y)\}^2) = \int (y - E(Y))^2 f_Y(y)dy$
  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**: $E(Y^k) = \int y^k f_Y(y)dy$,
  kth centralized Moment: $E(\{Y - E(Y)\}^k)$

Moment Generating Function

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

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 $\in \mathbb{R}^q$

Definition

$$(Y_1, Y_2, ..., Y_q)$$

with random variables Y_i

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 two-dimensional case

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

Covariance and Correlation

$$Cov(Y_j, Y_k) = E(Y_j Y_k) - E(Y_j)E(Y_k)$$

$$Cor(Y_j, Y_k) = \frac{Cov(Y_j, Y_k)}{\sqrt{Var(Y_j)Var(Y_k)}}$$

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

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

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 sum of squares for 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:

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

with $h(y) \geq 0$, $t(y)$ vector of the canonical statistic, parameter vector θ and $\kappa(\theta)$ as 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 e. g. $\frac{\partial\kappa(\theta)}{\partial\theta_1} = \mathrm{E}(t_1(Y))$

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**
- **Binomial**

2.5 Multivariate Distributions

Multivariate Normal symmetric with μ_i and Σ

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

General Copulas

$F(y_1, .., y_q) = C(F_1(y_1), ..., F_q(y_q))$ with $C : [0,1]^q \to [0,1]$ with C monotonically increasing as a cdf on $[0,1]^q$

Modelled as follows:

1. marginal distributions $F_j(y_j) = C\left(F_j(y_j), 1..., 1\right)$
2. dependence structure $\hat{u}_i = (\hat{u}_{i1}, ..., \hat{u}_{iq}) \overset{iid}{\sim} C(.)$ with $\hat{u}_{ij} := \hat{F}_j(y_{ij})$.

   The copula density is $c(u_{1:q}) = \frac{\partial^q C(u_{1:q})}{\partial u_1 \ldots \partial u_q}$ and $f(y_{1:q}) = c(F_1(y_1), ..., F_q(y_q)) \prod_{j=1}^q f_j(y_j)$.

Tail Dependence

upper: $\lambda_u := \lim\limits_{u\to1} P(Y_1 \geq F_1^{-1}(u)|Y_2 \geq F_2^{-1}(u))$
$= \lim\limits_{u\to1} \frac{1-2u+C(u,u)}{1-u}$
lower: $\lambda_l := \lim\limits_{u\to0} P(Y_1 \leq F_1^{-1}(u)|Y_2 \leq F_2^{-1}(u))$
$= \lim\limits_{u\to0} \frac{C(u,u)}{u}$

Gaussian Copula coefficients for pairwise dependences

$$c(u_{1:q}) = \frac{1}{|R|^{1/2}} \exp\left(-\frac{1}{2}u^T R^{-1} u\right)$$

For $Y_{ij} \sim \mathrm{N}(\mu_j, \sigma_j)$: $f(y_{ij}; \mu_j, \sigma_j^2) = \frac{1}{\sigma_j}\phi(Z_{ij})$ with Z_{ij} the standardized Y_{ij}. With $u_{ij} = \phi^{-1}(Z_{ij})$, R can be estimated.

$\lambda_l = 0$, $\lambda_u = 0$

Archimedean Copulas few parameters even in high dimensions

$$\psi(;\theta) : [0,1] \to [0,\infty)$$

with the parametric generator function $\psi(u,\theta)$ continuous, strictly decreasing, convex, and $\psi(1,\theta) = 0\ \forall\theta$

$$C(u_{1:q};\theta) = \psi^{-1}(\psi(u_1;\theta) + ... + \psi(u_q;\theta);\theta)$$

- **Clayton** $\psi(t;\theta) = \frac{1}{\theta}(\theta^{-1} - 1)$: $\lambda_l = 2^{-1/\theta}$, $\lambda_u = 0$
- **Frank** $\psi(t;\theta) = -\log\frac{\exp(-\theta t)-1}{\exp(-\theta)-1}$: $\lambda_l = 0$, $\lambda_u = 0$
- **Gumbel** $\psi(t;\theta) = (-\log(t))^\theta$: $\lambda_l = 0$, $\lambda_u = 2 - 2^{1/\theta}$

Pair Copulas flexible pairwise dependences

$$f_{123} = c_{12}c_{23}c_{23|1}\prod_{j=1}^3 f_j$$

Generalized Extreme Value Distribution (GEV)
for block maxima $M_n := \max(Y_{1:n})$:
$F_{M_n}(y) = P(M_n \leq y) = P(Y_{1:n} \leq y) = (F_Y(y))^n$

$$\lim_{n\to\infty} f_{M_n}(y) = \begin{cases} 1, & \text{if } F(y) = 1 \\ 0, & \text{otherwise} \end{cases}$$

For $\{a_n\}_{n=1}^\infty$, $\{b_n\}_{n=1}^\infty$ fixed sequences, the standardized maximum $\frac{M_n - a_n}{b_n}$ converges to a GEV as $n \to \infty$.

$$G(x) = \begin{cases} \exp(-(1+\gamma z)^{-1/\gamma}), & \text{for } \gamma \neq 0 \\ \exp(-\exp(-z)), & \text{for } \gamma = 0 \end{cases}$$

with location μ, scale σ, and shape γ and $z = \frac{x-\mu}{\sigma}$

- **Gumbel** $\gamma = 0$
- **Weibull** $\gamma > 0$
- **Frechet-Pareto** $\gamma < 0$

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

$$\begin{aligned}
\left.\frac{\partial K_{Z_n}(t)}{\partial t}\right|_{t=0} &= \frac{n}{\sqrt{n}} \left.\frac{\partial K_Y(t)}{\partial t}\right|_{t=0} = \sqrt{n}\mu \\
\left.\frac{\partial^2 K_{Z_n}(t)}{\partial t^2}\right|_{t=0} &= \frac{n}{n} \left.\frac{\partial^2 K_Y(t)}{\partial t^2}\right|_{t=0} = \sigma^2
\end{aligned}$$

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 quantity. It is also the realisation of a random variable as it depends on a sample.

Risk

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

Minimax Approach

The risk still depends on the true parameter θ.
Tentative estimation: Choose θ, s. t. 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 Bound

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

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

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

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 $x = 1$.

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

Proof:

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

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** $J(\theta)$: $-\mathrm{E}_\theta\left(\frac{\partial s(\theta;y)}{\partial\theta}\right)$

Attributes of the Score-Function

first Bartlett-Equation:

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

Proof:

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

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:

$$0 = \frac{\partial 0}{\partial\theta} = \frac{\partial}{\partial\theta}\int \frac{\partial \log f(y;\theta)}{\partial\theta} f(y;\theta)dy \qquad \text{see above}$$
$$= \int \frac{\partial^2 \log f(y;\theta)}{\partial\theta^2} f(y;\theta)dy$$
$$+ \int \frac{\partial \log f(y;\theta)}{\partial\theta}\frac{\partial f(y;\theta)}{\partial\theta}dy$$
$$= \mathrm{E}_\theta\left(\frac{\partial^2 \log f(Y;\theta}{\partial\theta^2})\right)$$
$$+ \int \frac{\partial \log f(y;\theta)}{\partial\theta}\frac{\partial \log f(y;\theta)}{\partial\theta} f(y;\theta)dy$$
$$\Leftrightarrow \mathrm{E}_\theta\left(s(\theta;Y)s(\theta;Y)\right) = \mathrm{E}_\theta\left(-\frac{\partial^2 \log f(Y;\theta)}{\partial\theta^2}\right)$$

Bartlett's second equation holds 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 asymptotically the smallest variance, given by the Cramér-Rao inequality,
$s\left(\hat{\theta}_{ML}; y_1, ..., y_n\right) = 0$
$\hat{\theta} \overset{a}{\sim} \mathrm{N}\left(\theta, I^{-1}(\theta)\right)$
If the true model is unknown, the distribution is
$\hat{\theta} \overset{a}{\sim} \mathrm{N}\left(\theta, I^{-1}(\theta)V(\theta)I^{-1}(\theta)\right)$ with $V(\theta)$ variance of the score function.
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:

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

Then, the Fisher information is $\frac{\partial\theta}{\partial\gamma}I(\theta)\frac{\partial\theta}{\partial\gamma}$

Proof:

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

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

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:

$$0 = s(\hat{\theta}_{ML}; y) \underset{Series}{\overset{Taylor}{\approx}} s(\theta; y) + \frac{\partial s(\theta; y)}{\partial\theta}(\hat{\theta}_{ML} - \theta) \Leftrightarrow$$
$$\hat{\theta}_{ML} \approx \theta - \left(\frac{\partial s(\theta; y)}{\partial\theta}\right)^{-1} s(\theta; y) \approx \theta - I^{-1}(\theta)s(\theta; y)$$

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 $\theta_{(t+1)} := \theta_{(t)} + \widehat{\mathrm{Var}}_{\theta_{(t)}}(t(Y))^{-1}\hat{\mathrm{E}}_{\theta_{(t)}}(t(Y))$ 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:

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

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

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

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

Relation to Kullback-Leibler divergence

$$\hat{\theta}_{ML} = \arg\ \min \mathrm{KL}(g, f)$$

with f distributional model used and g true model

Proof:

$$KL(g, f) = \int \log \frac{g(y)}{f(y)} g(y)dy$$

$$= \int \log(g(y))g(y)dy - \int \log(f(y))g(y)dy$$

To minimize that, the second component needs to be maximized. Its derivative is $\int s(\theta; y)g(y)dy = \mathrm{E}_g(s(\theta; Y)) = 0$

3.4 Consistency and Sufficiency

Statistic

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

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

(Weak) Consistency

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

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

Sufficiency

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:

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

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:

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

Minimal Sufficiency:

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

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.:

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

	"H_0"	"H_1"
H_0	$1-p$ (correct)	p (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

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

The p-value is uniformly distributed on $[0,1]$ under H_0.

Confidence Interval

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

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

Corresponding Test

$$\theta_0 \notin [t_l(y_{1:n}), t_r(y_{1:n})] \Leftrightarrow \text{“}H_1\text{”}$$

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)
$H_0\colon\ \mu = \mu_0 \quad vs. \quad H_1\colon\ \mu \neq \mu_0$

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

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

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

$$T(X) = 2(l(\hat{\theta}) - l(\theta_0)) \overset{H_0}{\sim} \chi^2_1$$

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: $\varphi^* = \begin{cases} 1 & \text{if } \frac{f(y;\theta_0)}{f(y;\theta_1)} \leq \mathrm{e}^c \\ 0 & \text{otherwise} \end{cases}$

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)
$H_0\colon\ X_i \sim F_0 \quad vs. \quad H_1\colon\ X_i \sim F \neq F_0$

$$T(X) = \sup_x |F_n(x) - F_0(x;\theta)| \overset{H_0}{\sim} KS$$

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:

$$P(\sup_x |F_n(x) - F(x;\theta)| \leq t) =$$

$$= P(\sup_y |F^{-1}(y;\theta) - x| \leq t) \qquad \substack{x\in[0,1],\ x=F^{-1}(y;\theta) \\ F(F^{-1}(y;\theta);\theta)=y}$$

$$\overset{*}{=} P(\sup_y |\frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{U_i \leq y\}} - y| \leq t) \qquad \text{with } U_i \sim U(0,1)$$

$$^*F_n(F^{-1}(y;\theta)) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{X_i \leq F^{-1}(y;\theta)\}} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{F(y;\theta) \leq y\}}$$

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 $p \sim U(0,1)$
For m tests:

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

$$FWER := P(\exists k : \text{“}H_1k\text{”}|\forall k :\ H_0k)$$

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 $x \in \{1,...,m\}$: 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: $\mathrm{E}(\hat\beta) = (X^TX)^{-1}X^T\mathrm{E}(Y|X) = (X^TX)^{-1}X^TX\beta = \beta$

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

The ML-estimate for σ^2 is biased.

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

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

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

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:

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

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

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

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

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:

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

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

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

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

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

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

with z_i indicating group affiliation

5.2 Goodness of Fit

5.2.1 Coefficient of Determination

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

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

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:

$$\begin{aligned} f_{post}(\theta|X) &= \frac{f(X|\theta)\cdot f_\theta(\theta)}{\int f(X|\tilde\theta) f_\theta(\tilde\theta)d\tilde\theta} \\ &= C\cdot f(X|\theta)\cdot f_\theta(\theta) \quad \text{choose C s.t.} \int f_{post}(\theta|X) = 1 \\ &\propto f(X|\theta)\cdot f_\theta(\theta) \end{aligned}$$

Point Estimates

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

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:
$R_{postBayes}(t(.)|y) = \int \mathcal{L}(t(y),\vartheta) f_\theta(\vartheta|y)d\vartheta = \mathrm{E}_{\theta|y}(\mathcal{L}(t(y),\theta)|y)$

For squared loss: $\hat\theta_{postBayesrisk} = \hat\theta_{postmean}$

Credibility Interval

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

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

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

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-dimensional $J_P := -\frac{\partial^2 l_{(n)}(\theta,y)}{\partial\theta^2} - \frac{\partial^2 \log f\theta(\theta)}{\partial\theta^2}$ 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: $\int e^{\{\sum_{i=1}^n \log f(y_i|\theta)+\log f_\theta(\theta)\}}d\theta =$

$\int e^{\{l(\theta;y)+\log f_\theta(\theta)\}}d\theta \overset{TS}{\approx} \int e^{(l_P(\hat\theta_P)-\frac{1}{2}J_P(\hat\theta_P)(\vartheta-\hat\theta_P)^2)}d\vartheta$

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:

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

- **Rejection Sampling**

  An umbrella distribution $g(x)$ can be found s. t. $\frac{f(x)}{g(x)} \leq M \; \forall x$ 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 $u \leq \alpha$, else: step 1

Proof:

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

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

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

- **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:

$$\theta^*_{t+1,i} \sim f_{\theta_i|y,\theta\backslash\theta_i}\left(\theta_i^*|y, \theta_{t^*,i}\right)$$

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 $\int_{-\infty}^{\infty} |t|^p dF(t) < \infty$; $(X, Y) \sim T \in \mathcal{T}_{XY}$ 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: $G_n(t, H_n) \to G_\infty(t, F)$

8 Model Selection

AIC (Akaike Information Criterion)

$$AIC = -2\sum_{i=1}^{n} \log f(y_i; \hat{\theta}) + 2p$$

The AIC estimates $2\mathrm{E}_Y\left\{\mathrm{KL}(g,f)\right\} - 2\int \log(g(y))g(y)dy$. The latter component is unknown, so the absolute value of the AIC is not informative. The AIC favours complex models.

For regressions: $AIC = 2n\log(\hat{\sigma}^2) + 2(p+2)$

The AIC as theoretical cross validation

The AIC minimizes $\mathrm{E}_{Y_{1:n}}\left\{\mathrm{E}_Y\left[Y-\hat{\mu}\right]^2\right\}$ if we use the MSE instead of the Kullback-Leibler divergence. This can be estimated via cross validation.

Bias Corrected AIC

$$AIC_{corr} = -2\sum_{i=1}^{n} \log f(y_i; \hat{\theta}) + 2p\left(\frac{n}{n-p-1}\right)$$

should be preferred if $\frac{n}{p} < 40$

BIC (Bayesian Information Criterion)

$$BIC = -2\sum_{i=1}^{n} \log f(y_i; \hat{\theta}) + \log(n)p$$

approximately maximizes the posterior probability of a model and selects less complex models as the AIC

DIC (Deviance Information Criterion) Bayesian AIC

$$DIC = D(y, \hat{\theta}_{postmean}) + 2p_D = \int D(y,\vartheta)f_{post}(\vartheta|y)d\vartheta + p_D$$

with deviance $D(y;\theta) := -2l(\theta)$ the difference in likelihood compared to the full model and $\Delta D(y;\theta,\hat{\theta}) = 2\left\{l(\hat{\theta}) - l(\theta)\right\} \overset{a}{\sim} \chi^2_p$ the difference in deviance

$p_D := \mathrm{E}(\Delta D(y;\theta,\hat{\theta}_{\substack{post\\mean}}|y) = \int D(y,\vartheta)f_{post}(\vartheta|y)d\vartheta - D(y,\hat{\theta}_{\substack{post\\mean}})$

The integral can be approximated using MCMC.

Model Averaging Using probabilities as weights

$$P(M_k|y) := \frac{\exp(-\frac{1}{2}\Delta IC_k)}{\sum_{k'=1}^{K}\exp(-\frac{1}{2}\Delta IC'_k)}$$

with $\Delta IC_k = IC_k - min(IC)$

For regressions: $P(\text{covariate } x|y) = \sum_{k=1}^{K} \mathbb{1}_{\{x \text{ in } M_k\}} P(M_k|y)$

Inference After Model Selection neglect is a quiet scandal

$$\begin{aligned} Var(\hat{\theta}) &= \mathrm{E}_{model}(Var(\hat{\theta}|model)) + Var_{model}(E(\hat{\theta}|model)) \\ &= \sum_{k=1}^{K} \pi_k Var_k(\hat{\theta}) + \sum_{k=1}^{K} \pi_k(\theta_k - \bar{\theta})^2 \end{aligned}$$

The last component depends on the true parameter and will be biased if the estimates are used.

Solutions:

- $\widehat{Var}(\hat{\theta}) = \left[\sum_{k=1}^{K} \pi_k \sqrt{\widehat{Var}_k(\hat{\theta}_k) + (\hat{\theta}_k - \hat{\bar{\theta}})^2}\right]^2$
- Use the Variance of the full (saturated) model
- Use bootstrap for confidence intervals

Lasso least absolute shrinkage and selection operator

$$l_p(\theta,\lambda) = l(\theta) - \lambda\sum_{j=1}^{p}|\theta_j|$$

This penalized log likelihood can be solved with iterative quadratic programming using a Taylor expansion.

Using Bayesian view the penalty corresponds to a prior: $f_{\theta_j}(\theta_j) \propto \exp(-|\theta_j|)$ (Laplace prior)

9 Dimensionality Reduction

Covariance Matrix $\boldsymbol{\Sigma}$

- symmetric, $\in \mathbb{R}^{n\times n}$ therefore $\frac{q(q+1)}{2}$ parameters
- positive definite, i. e. $\forall a \in \mathbb{R}^q : a^T \Sigma a \geq 0$

Marginal Independence

$$\Sigma_{jk} = 0 \Leftrightarrow Y_{ij} \text{ and } Y_{ik} \text{ are independent}$$

Conditional Independence

$\Omega = \Sigma^{-1}_{jk} = 0 \Leftrightarrow Y_{ij}$ and Y_{ik} are independent given all other Y with concentration matrix Ω

Proof:
$$f(y_{\cdot j}, y_{\cdot k}|y_{\cdot\overline{j,k}}) = \frac{f(y)}{f_{\cdot\overline{j,k}}} \propto f(y) \overset{\mathrm{N}(\mu,\Sigma)}{\propto} \exp\left\{-\frac{1}{2}y^T\Sigma^{-1}y\right\}$$

Graphical Models
visualize conditional dependences in a graph

Principal Component Analysis (PCA)

1. Use singular value decomposition $\Sigma = U\Lambda U^T$ with U matrix of orthonomal eigenvectors and $\Lambda = diag(\lambda_1, ..., \lambda_q)$ matrix of sorted eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_q$ of Σ
2. Prune smallest $k = q - r$ eigenvalues in $\tilde{\Lambda}$
3. Simplify model with spectral decomposition $\tilde{Y} = \tilde{V}\tilde{\Lambda}^{1/2}\tilde{U}^T$ with $\tilde{V}$, $\tilde{U}$ first r eigenvectors of YY^T and Y^TY respectively
4. explained variance $\sum_{i=1}^{r} \lambda_i / \sum_{i=1}^{q} \lambda_i$

Proof:
Karhunen-Loève expansion: $U\Lambda^{\frac{1}{2}}Z_{\cdot} \sim \mathrm{N}(0, U\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}}U^T) = \mathrm{N}(0,\Sigma)$ with $Z_{\cdot} \sim \mathrm{N}(0, \mathbb{1})$, therefore $\tilde{Y}_{\cdot} = \tilde{V}\tilde{\Lambda}^{\frac{1}{2}}\tilde{Z}_{\cdot}$
With spectral decomposition: $Y = V\Lambda^{\frac{1}{2}}U^T$ (for column-centered Y)

10 Missing/Deficient Data

Missing Completely at Random (MCAR) independent

$$P(R_i|Y_i) = P(R_i)$$

with $R_{ij} = \begin{cases} 0 & \text{if } Y_{ij} \text{ missing} \\ 1 & \text{otherwise} \end{cases}$ and $R_i = (R_{i1}, ..., R_{iq})$

A complete case analysis will lead to unbiased results.

Missing at Random (MAR) depends on observed variables

$$P(R_i|Y_i) = P(R_i|Y_{iO_i})$$

with $O_i = \{j : R_{ij} = 1\}$ and $M_i = \{j : R_{ij} = 0\}$

Complete case analysis $P(Y|X, Z)$:

- only response Y_i MAR: unbiased
- only covariate X_i MAR: biased
  Asymptotically unbiased with *inverse probability weighting*:
  1. Estimate $\pi(y_i, z_i) = P(R_{X_i}{=}1|y_i, z_i)$
  2. Use weighted score function $\hat{s}_w(\theta) = \sum_{i=1}^n \frac{R_{X_i}}{\hat{\pi}} s_i(\theta)$
- both MAR: biased and $\pi(y_i, z_i)$ can not be estimated due to missing Y_i

Missing Not at Random (MNAR)

$$P(R_i|Y_i) \neq P(R_i|Y_{iO_i})$$

Can not be corrected to be unbiased.

EM Algorithm replace y_{iM} by $E(Y_{iM}|y_{iO})$

Expectation Step:

$$Q(\theta, \theta_{(t)}) = \sum_{i=1}^n \int l_i(\theta) f(y_{iM}|y_{iO}; \theta_{(t)}) dy_{iM}$$

Maximization Step:

$$\frac{\partial Q(\theta, \theta_{(t)})}{\partial \theta} = s(\theta, \theta_{(t)}) \stackrel{!}{=} 0$$

Louis' Formula for Variance Estimates in EM Settings

$$J_O(\theta) = \sum_{i=1}^n \{\mathrm{E}(J_i(\theta)|y_{iO}) - \mathrm{E}(s_i(\theta)s_i(\theta)|y_{iO}) + s_{iO}(\theta)s_{iO}(\theta)\}$$

Multiple Imputation EM but considers estimation variability

1. Create K complete datasets by simulating missing data $\sim f_{post}(y_{iM}|y_{iO})$
2. Fit K models $Y_i \sim f(y|\theta)$
3. Rubin's Rule: $\hat{\theta}_{MI} = \frac{1}{K}\sum_{k=1}^K \hat{\theta}^*_{(k)}$;
   $\widehat{\mathrm{Var}}(\hat{\theta}_{MI}) = \hat{V} + (1+\frac{1}{K})\bar{B}$ with $\hat{V} = \frac{1}{K}\sum_{k=1}^K I^{-1}(\hat{\theta}^*_{(k)})$ and
   $\bar{B} = \frac{1}{K-1}\sum_{k=1}^K (\hat{\theta}^*_{(k)} - \hat{\theta}_{MI})(\hat{\theta}^*_{(k)} - \hat{\theta}_{MI})^T$

Estimate Accuracy

$$\hat{\mu}_g - \mu_g = \rho_{R_g} \times \sigma_g \times \sqrt{\frac{N-n}{n}}$$

with ρ_{R_g} data quality (correlation between R_j and $g(Y_j)$), σ_g variability, and $\sqrt{\frac{N-n}{n}}$ data quantity; g some known function

- MCAR: $MSE(\hat{\mu}_g) = \frac{1}{N-1} \times \sigma_g^2 \times \frac{N-n}{n}$
- MNAR: $MSE(\hat{\mu}_g) = \mathrm{E}(\rho^2_{R_g}) \times \sigma_g^2 \times \frac{N-n}{n}$
  $n_{eff} = \frac{\frac{n}{N}}{1-\frac{n}{N}} \frac{1}{\mathrm{E}(\rho^2_{R_g})}$

Measurement Error

$$U = X - X_m \text{ with } \mathrm{E}(U) = \mu_U \text{ and } \mathrm{Var}(U) = \sigma_U^2$$

with μ_U systematic error (bias/validity), Var(U) (reliability)

In Regression Settings:

- **error in Y**: $Y_m = \beta_0 + \beta_1 X + \epsilon + U$ and $\mathrm{E}(Y_m|X) = \beta_0 + \mu_U + \beta_1 X$ leads to biased $\hat{\beta}_0$
- **error in X**: $Y = \beta_0 + \beta_1 X + \epsilon$ and $X_m = X + U$ leads to biased $\hat{\beta}_0$ and $\hat{\beta}_1$, the latter is attenuated by the inverse of reliability ratio $rr = \frac{\sigma_X^2}{\sigma_X^2+\sigma_U^2} = \frac{\sigma^2_{X_m}-\sigma_U^2}{\sigma^2_{X_m}}$
  Getting information about σ_U^2:
  - **Validation Data** with both X and X_m observed
  - **Replication Data** repeated measures of X_m
  - **Assumptions** e. g. $\sigma_U^2 = 0$ (naive estimator)

11 Experiment Design

Omitted Variables

Regression setting ignoring omitted Variables:

$$\int f_{Y|X,Z,U} f_{Z,U} dzdu = \int \frac{f_{Y,X,Z,U}}{f_{X|Z,U}} dzdu \neq f_{Y|X}$$

with Z observable and U unobservable quantities influencing Y

Solutions:

- *Randomization*: randomly assign X and then observe Y
- *Balancing*: make X independent of Z

Analysis of Variances (ANOVA) of one categorical variable
Linear constraint: $\sum_{k=1}^{K} n_k \beta_k = 0$ (usually controlled over β_K)

$$\hat{\beta}_{0,ML} = \hat{\mu}_{ML} = \sum_{k=1}^{K} \sum_{j=1}^{n_k} \frac{y_{kj}}{n} = \bar{y}_{..}$$

$$\hat{\beta}_{k,ML} = \sum_{j=1}^{n_k} \frac{y_{kj} - \bar{y}_{..}}{n_k} = \bar{y}_{k.} - \bar{y}_{..}$$

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

with

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

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

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

F-Test

$$F = \frac{SS_{Explained}/(df_0 - df_X)}{SS_{Residual}/df_X} \sim \mathcal{F}_{df_0 - df_X, df_X}$$

with $df_0 = n-1$ and $df_X = n-K$

Block Design account for block effects

$$Y_{kbj} = \mu + \beta_k + \alpha_k + \epsilon_{kbj}$$

Linear constraints: $\sum_{k=1}^{K} n_{k.} \beta_k = 0$ and $\sum_{b=1}^{B} n_{.b} \alpha_b = 0$

For the F-Test: $df_0 = df_Z = n-B$ and $df_{X+Z} = n-K-B+1$

Latin Squares Sodoku pattern for more variables

Instrumental Variable

$$Y = \beta_0 + X\beta_X + \overbrace{U\beta_U + \epsilon}^{\tilde{\epsilon}} \Rightarrow \frac{\partial Y}{\partial X} = \beta_X + \frac{\partial \tilde{\epsilon}}{\partial X}$$

Construct instrumental variable Z: $Cov(Z,\epsilon)$=0, $Cov(Z,X)$≠0:

$$\frac{\partial Y}{\partial X}|(U{=}u) = \frac{\partial Y/\partial Z}{\partial X/\partial Z}$$

i. e. fit two regressions $Y|Z$ and $X|Z$ and set $\hat{\beta}_X = \frac{\hat{\beta}_{YZ}}{\hat{\beta}_{XZ}}$

Propensity Score

$$\tau = \mathrm{E}(Y(1)|D{=}1) - \mathrm{E}(Y(0)|D{=}1)$$

with τ average treatment effect on the treated, $Y(1)$ response if treated, $Y(0)$ analogous; D_i indicator if i is influenced by the treatment

$$\mathrm{E}(Y(1)|D{=}1) - \mathrm{E}(Y(0)|D{=}0) = \tau + \underbrace{\mathrm{E}(Y(0)|D{=}1) - \mathrm{E}(Y(0)|D{=}0)}_{\text{selection bias}}$$

If the selection bias is zero, D and X are unconfounded.

$$\hat{\tau} = \sum_{i=1}^{n} (Y_i(1) - Y_{j(i)}(0))$$

after matching treated individual i with individual $j(i)$ from non-treatment group