Statistics

Collection of Formulas

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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

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

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

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

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

Phi-Coefficient

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

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

Cramér's V

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

Range: $0 \le V \le 1$

Contingency Coefficient C

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

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

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 $0 \le C_{corr} \le 1$

Odds-Ratio

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

Range: $0 \le OR < \infty$

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: $-1 \le \gamma \le 1$

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: $-1 \le \tau_b \le 1$

Kendall's/Stuart's τ_c

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

Range: $-1 \le \tau_c \le 1$

Spearman's Rank Correlation Coefficient

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

or

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

Without ties:

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

with

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

Range: $-1 \le \rho \le 1$

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

$S_{xy} = \sum_{i=1}^{n} (x_i - \bar{x})^2 (y_i - \bar{y})^2$ or $s_{xy} = \frac{S_{xy}}{n}$

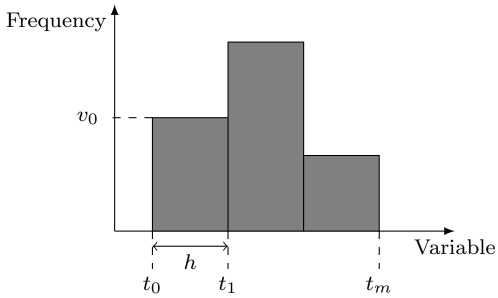
$S_{xx} = \sum_{i=1}^{n} (x_i - \bar{x})^2$ or $s_{xx} = \frac{S_{xx}}{n}$

$S_{yy} = \sum_{i=1}^{n} (y_i - \bar{y})^2$ or $s_{yy} = \frac{S_{yy}}{n}$

Range: $-1 \le r \le 1$

1.2 Diagrams

1.2.1 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) $0 \leq P(A) \leq 1 \quad \forall A \in \mathcal{A} = \sigma\text{-algebra}(\Omega)$
(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 $\Leftrightarrow f_{XY}(x, y) = f_X(x) \cdot f_Y(y) \quad \forall x, y$

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)**: $\mu = E(Y) = \int y f_Y(y)dy$
  with $E(a+bX) = a + bE(X)$ and $E(X\pm Y) = E(X) \pm E(Y)$

- **Variance (2. centralized Moment)**:
  $\sigma^2 = Var(Y) = E(\{Y - E(Y)\}^2) = \int (y - E(Y))^2 f_Y(y)dy$
  with $Var(a + bX) = b^2 Var(X)$ and
  $Var(X\pm Y) = Var(X) + Var(Y) \pm 2Cov(X, Y)$
  Note: $E(\{Y - \mu\}^2) = E(Y^2) - \mu^2$

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

- k**th Moment**: $E(Y^k) = \int y^k f_Y(y)dy$,
  k**th 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).

Chebyshev's Inequality with $E(X) = \mu$ and $Var(X) = \sigma^2$

$$P(|X - \mu| \geq c) \leq \frac{\sigma^2}{c^2}$$

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

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

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

Iterated Expectation

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

Proof:

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

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

Proof:

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

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
with special case Bernoulli: $Y \sim \mathrm{Bin}(1, \pi)$

$$Y \sim \mathrm{Bin}(n, \pi) \text{ with } n \in \mathbb{N}, \pi \in [0, 1]\,,\ y \in \{0, ..., n\}$$

$$P(Y = y|\lambda) = \binom{n}{y}\pi^k(1 - \pi)^{n-y}$$

$$\mathrm{E}(Y|\pi, n) = n\pi,\ \mathrm{Var}(Y|\pi, n) = n\pi(1 - \pi)$$

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 and big n

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

$$Y \sim \mathrm{U}(a, b) \text{ with } \alpha, \beta \in \mathbb{R}, a \leq b,\ y \in [a, b]$$

$$p(y|a, b) = \frac{1}{b - a}$$

$$\mathrm{E}(Y|a, b) = \frac{a + b}{2},\ \mathrm{Var}(Y|a, b) = \frac{(b - a)^2}{12}$$

Exponential Time between Poisson events

$$Y \sim \mathrm{Exp}(\lambda) \text{ with } \lambda > 0,\ y \geq 0$$

$$p(y|\lambda) = \lambda \exp(-\lambda y)$$

$$\mathrm{E}(Y|\lambda) = \frac{1}{\lambda},\ \mathrm{Var}(Y|\lambda) = \frac{1}{\lambda^2}$$

Univariate Normal symmetric with μ and σ^2

$$Y \sim \mathrm{N}(\mu, \sigma^2) \text{ with } \mu \in \mathbb{R}, \sigma^2 > 0,\ y \in \mathbb{R}$$

$$p(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \mu)^2}{2\sigma^2}\right)$$

$$\mathrm{E}(Y|\mu, \sigma^2) = \mu,\ \mathrm{Var}(Y|\mu, \sigma^2) = \sigma^2$$

Approximation of

Binomial for $np(1-p) \geq 9$ with $\mathrm{N}(np, np(1-p))$

Poisson for $\lambda \geq 10$ with $\mathrm{N}(\lambda, \lambda)$

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

Chi-Squared sum of squares for standard normal random variables with ν degrees of freedom

$$Y \sim \chi^2(\nu) \text{ with } \nu > 0,\ y \in \mathbb{R}$$

$$p(y|\nu) = \frac{y^{\frac{\nu}{2}-1} e^{-\frac{y}{2}}}{2^{\frac{\nu}{2}} \Gamma\left(\frac{\nu}{2}\right)}$$

$$\mathrm{E}(Y|\nu) = \nu,\ \mathrm{Var}(Y|\nu) = 2\nu$$

Weibull failure rate is proportional to a power of time

$$Y \sim \mathrm{WB}(\lambda, k) \text{ with } \lambda > 0$$

$$p(y|\lambda, k) = \frac{k}{\lambda} \left(\frac{y}{\lambda}\right)^{k-1} \mathrm{e}^{-(y/\lambda)^k}$$

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: $\lambda_u := \lim_{u \to 1} P(Y_1 \geq F_1^{-1}(u) | Y_2 \geq F_2^{-1}(u))$
$= \lim_{u \to 1} \frac{1-2u+C(u,u)}{1-u}$
lower: $\lambda_l := \lim_{u \to 0} P(Y_1 \leq F_1^{-1}(u) | Y_2 \leq F_2^{-1}(u))$
$= \lim_{u \to 0} \frac{C(u,u)}{u}$

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

$$\lim_{n\to\infty} P\left(\left|\bar{X}_n - \mu\right| < c\right) = 1 \qquad \forall c > 0$$

with X_i i.i.d., $E(X_i) = \mu$, and $\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$

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:

$\mathrm{E}_{\hat{\theta}_{MM}}(Y^k) = m_k(y_1, ..., y_n) = \frac{1}{n}\sum_{i=1}^n y_i^k$

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 minimizing the worst case
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:

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

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

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

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:

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

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 bound,
$s\left(\hat{\theta}_{ML}; y_1, ..., y_n\right) = 0$
$\hat{\theta} \overset{a}{\sim} \mathrm{N}\left(\theta, I^{-1}(\theta)\right)$
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 for a bijective and differentiable function $g(.)$: $\hat{\gamma} = g(\hat{\theta})$ 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 $\hat{\theta}$ gets closer to θ as n grows

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

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:

$t(Y_1,...,Y_n)$ 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

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

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

Binomial Distribution $X_i \overset{iid}{\sim} Bin(1, p)$

Approximate test for p
$H_0\colon\ p = p_0 \quad vs. \quad H_1\colon\ p \neq p_0$

$$T(X) = \frac{\frac{X}{n} - p_0}{\sqrt{p_0(1-p_0)}/\sqrt{n}} \overset{H_0, appr.}{\sim} \mathrm{N}(0,1)$$

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: $P(\varphi(Y)=1|\theta_1) \leq P(\varphi^*(Y)=1|\theta_1)\ \forall\varphi$

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

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:

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

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 $p \sim U(0,1)$

For m tests:

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

$$FWER := P(\exists k : \text{“}H_{1k}\text{”} | \forall k :\ H_{0k})$$

Bonferoni Adjustment

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

Šidák Adjustment only for independent tests

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

Proof:

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

Holm's Procedure also takes power into account
Order the p-values: $p_{(0)} \leq ... \leq p_{(m)}$

Step $x \in \{0, ..., m\}$: if $p_{(x)} > \frac{\alpha}{m-x}$ 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_{0i} 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) $Y|x_{1:p} \sim \mathrm{N}(X\beta, \sigma^2)$

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

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*:

$$\theta = \eta$$

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

6 Survival Analysis

6.1 Basics

Time-to-Event Data outcome tuple (t_i, δ_i) is observed with time $0 < t < \infty$ and event/censoring indicator δ_i

typically: $\delta_i = \begin{cases} 1, & i \text{ experienced event} \\ 0, & i \text{ is (right-)censored} \end{cases}$

Censoring $T_i \sim F$ times to event & $C_i \sim G$ censoring times

- **right-censoring:** observe $t_i = \min(T_i, C_i)$
- **left-censoring:** observe $t_i = \max(T_i, C_i)$
- **interval-censoring:** only known $t_i \in \left[C_i^l, C_i^r\right]$

Censoring and event distributions need to be independent given explanatory variables for models to be unbiased

Truncation a form of sampling bias

- **left-truncation:** observations with $t_i < a$ excluded
- **right-truncation:** observations with $t_i > a$ excluded

Description of the Distribution

- **survival function**
$$S(t) := P(T > t) = 1 - F(t)$$
- **hazard rate**
$$h(t) := \lim_{\delta \to 0} \frac{P(T \in [t, t+\delta] | T \geq t)}{\delta} = \frac{f(t)}{S(t)}$$
- **cumulative hazard rate**
$$H(t) := \int_0^t h(u) du = -\log(S(t))$$

6.2 Modelling

Kaplan-Meier non-parametric estimate for $S(t)$
For ordered event times $t_{(1)}, ..., t_{(f)}$:
$$\hat{S}\left(t_{(f)}\right) = \prod_{i=1}^{f} \hat{P}\left(T > t_{(i)} | T \geq t_{(i)}\right)$$
$\hat{P}\left(T > t_{(i)} | T \geq t_{(i)}\right) = 1 - \frac{d_i}{n_i}$, with d_i number of events at $t_{(i)}$ and n_i number of observations under risk at $t_{(i)}$

- also called product-limit estimator
- formula closely related to path rule
- assumes piecewise constant survival (step function)

Greenwoods' Formula basis for confidence intervals
$$\widehat{Var}\left(\hat{S}(t)\right) = \hat{S}(t)^2 \sum_{t_{(k)} \leq t} \frac{d_k}{n_k(n_k - d_k)}$$

Nelson-Aalen non-parametric estimate for $H(t)$
$$H(t) = \sum_{k: t_{(k)} \leq t} \hat{h}_k^d$$
with h_k^d discrete time hazard rate for k-th interval $\left[t_{(k-1)}, t_{(k)}\right]$

- results in piecewise constant estimate (step function)
- $\exp\left(-\hat{H}(t)\right)$ gives Breslow estimate for $S(t)$

Accelerated Failure Time parametric modelling of T

$T \sim \text{WB}(\lambda, k)$: leads to proportional hazards
$T \sim \text{Exp}(\lambda) = \text{WB}(\lambda, 1)$: results in constant hazard rate

Location-Scale-Model (with $\lambda = \exp(-\eta)$ and $k = \frac{1}{\sigma}$):
$$\log(T) = x^T\beta + \sigma\epsilon \iff$$
$$T = \exp(\beta_0)\exp(\beta_1 x_1) ... \exp(\beta_p x_p)\exp(\sigma\epsilon)$$
incrementing x_1 means survival time stretches by $\exp(\beta_1)$, c. p.

Diagnostics

- $\ln(-\ln S(t)) = \ln(\lambda) + \sigma \ln(t)$, use $\hat{S}_{KM}$ for graphical check (for single categorical x only)
- Distribution assumption (for Weibull): $\epsilon \sim \text{Gumbel}\left(\frac{y-\eta}{\sigma}\right)$

ML estimation under right-censoring
$$L(\theta) = \prod_{i=1}^{n} \left(f(t_i|\theta, x_i)\right)^{\delta_i} \left(S(t_i|\theta, x_i)\right)^{1-\delta_i}$$
standard likelihood theory applies

Cox Proportional Hazards semi-parametric
$$h(t, x) = h_0(t) \cdot \exp(x^T\beta)$$
with non-parametric baseline hazard rate $h_0(t)$ independent of x, but can depend on (part of) x in stratified models

Proportional Hazards incrementing x_1 means hazard rate multiplies by $\exp(\beta_1)$, ceteris paribus

Proof: $\dfrac{h(t|x^{(a)})}{h(t|x^{(b)})} = \exp((x^{(a)} - x^{(b)})^T\beta)$

Diagnostics

- **Proportional Hazard:** Schoenfeld residuals ($E(r_i) = 0$) and corresponding test (H_0 : proportional hazards)
- **Overall Fit:** Cox Snell residuals $\sim$ Exp(1)
- **Functional Form:** Martingale residuals ($E(r_i) = 0$)
- **Outliers:** Deviance residuals ($E(r_i) = 0$)
- **Leverage:** Jack-Knife residuals

Partial Likelihood consider risk sets $R_i = R(t_{(i)})$ for ordered event times $t_{(1)}, ..., t_{(f)}$:
$$PL(\beta) = \prod_{i=1}^{m} P(t_i = t_{(i)} | \exists j \in R_i : t_j = t_{(j)})$$
$$= \prod_{i=1}^{m} \frac{\exp\left(x_{(i)}^T\beta\right)}{\sum_{j \in R_i} \exp\left(x_j^T\beta\right)}$$

Random Survival Forests Machine Learning method

1. draw B Bootstrap samples from the data
2. grow binary decision tree for each sample finding splits with log rank tests out of p randomly drawn splitting candidates
3. stopping: minimum $d_0 > 0$ deaths per node
4. calculate $\hat{H}(t)$ via Nelson-Aalen and average for samples
5. get prediction error using Out-Of-Bag samples

6.3 Model Comparison

General Some measures (e. g. AIC) require equal likelihood estimation and are typically only valid within a model class. Other methods (presented below) should be used on test data.

C-Index compare predictions if censor times allow it

$$C = \frac{\#\text{concordant pairs}}{\#\text{comparable pairs}}$$

with $0 \leq C \leq 1$ and $C = 0.5$ for random guessing

Brier Score equivalent to the MSE for predicted probabilities

$$\widehat{BS}(t, \hat{S}) = \frac{1}{n} \sum_{i=1}^{n} (\tilde{Y}_i(t) - \hat{S}(t|x_i))^2$$

with $\tilde{Y}_i(t) = \mathbb{1}(t_i > t)$ and $t_i = \min(T_i, C_i)$

the arithmetic mean above is often weighted using Inverse Probability of Censoring Weights

Integrated Brier Score as the Brier Score depends on t

$$IBS(\tau) = \frac{1}{\tau} \int_0^\tau \widehat{BS}(u, \hat{S}) du$$

can also be shown graphically as the Brier Score over different time points in so-called prediction error curves (PEC)

7 Spatial Statistics

7.1 Markov Random Field

Lattice Data observations from a random process observed over spatial regions, supplemented by a neighborhood structure

Random Field synonymous to stochastic process

$$(X_1, ..., X_n)$$

realisations of random variable X_i for locations $D = \{1, ..., n\}$

Markov Properties extend the temporal $X_{t+1}|X_t \perp X_{1,...,t-1}$

- **pairwise:** $X_i|X_{-ij} \perp X_j$ for $i \neq j$ and $i \not\sim j$
- **local:** $X_i|X_{-\{i,n\in\partial(i)\}} \perp X_{n\in\partial(i)}$ with $\partial(i) := \{j : j \sim i\}$
- **global:** $X_A|X_B \perp X_C$ for C separating A and B

global implies local implies pairwise; equivalent in a GMRF

Neighbourhood System set of neighbourhoods

$$\partial = \{\partial(s) : s \in D\}$$

if $s \notin \partial(s)$ (antireflexive) and $v \in \partial(s) \Leftrightarrow s \in \partial(v)$ (symmetric)

GMRF Gauss Markov Random Field

$$f(x) = (2\pi)^{-\frac{n}{2}} |P|^{\frac{1}{2}} \exp\left(-\frac{1}{2}(x-\mu)^T P(x-\mu)\right)$$

with precision matrix $P := \Sigma^{-1} > 0$ and $p_{ij} \neq 0 \Leftrightarrow i \sim j$
p_{ij} define neighbourhoods with $X_i|X_{-ij} \perp X_j \Leftrightarrow p_{ij}$=0 for $i \neq j$
GMRFs fulfill the pairwise, local, and global Markov property

canonical representation:

$$X \sim N^k(m, P) := N(P^{-1}m, P^{-1})$$

$$\Leftrightarrow f(x) \propto |P|^{\frac{1}{2}} \exp\left(-\frac{1}{2}x^T Px + m^T x\right)$$

get m via completing the square

improper GMRFs: P s.p.d. with $\text{rk}(P) = r < n$

$$f(x) = (2\pi)^{-\frac{r}{2}} \det{}^*(P)^{\frac{1}{2}} \exp\left(-\frac{1}{2}(x-\mu)^T P(x-\mu)\right)$$

with $\det^*(P) = \prod_{j=1}^r \lambda_j$ with $\lambda_1, ..., \lambda_r$ non-zero eigenvalues
intrinsic GMRFs ($\sum_{j=1}^n p_{ij} = 0 \;\; \forall i = 1, ..., n$) with irregular grids: rank decline is number of independent areas
models:

- Conditional Autoregressive (**CAR**):
  $\text{E}(X_i|X_{-i}) = \mu_i + \sum_{j:i\sim j} c_{ij}(X_j - \mu_j)$, resulting in a GMRF with $p_{ij} = \begin{cases} -c_{ij}/(\sigma_i\sigma_j), & i \neq j \\ 1/\sigma_i, & i = j \end{cases}$
  Weights c_{ij} are symmetric and often correspond to distance
- Intrinsic Autoregressive (**ICAR**)
  $p_{ij} = \begin{cases} -1/(\sigma_i\sigma_j), & i \sim j \\ |\partial(i)|/\sigma_i, & i = j \\ 0, & \text{else} \end{cases}$
- Simultaneous Autoregressive (**SAR**)
  $\text{E}(X_i|X_{-i}, Z) = Z_i\beta + \sum_{j:i\sim j} b_{ij}X_j$ with covariates Z

GMRF Regression Bayesian prior equals likelihood penalty

$$Y = X\beta + Z\eta + \epsilon$$

with $\epsilon_i \sim \text{N}(0, \sigma^2)$; $\eta \sim \text{N}(0, (\tau Q)^{-1})$; $\beta_k \sim N(0, \kappa_k)$
get hyperparameters: cross validation, empirical Bayes, or Bayes
Gamma is non-informative, semi-conjugated prior on τ, $\frac{1}{\sigma^2}$, & $\frac{1}{\kappa_k}$

Drawing from a GMRF Rue algorithm

1. perform Cholesky decomposition: $P = LL'$
2. calculate w and u with $Lw = m$ and $L'u = w$
3. draw $z \sim \text{N}(0, I_n)$ and calculate v with $L'v = z$
4. calculate result $y = u + v$

Proof:
$u = P^{-1}m$, as $m = Lw = LL'u = Pu$
$E(v) = E(L'^{-1}z) = L'^{-1}E(z) = 0$
$Var(v) = Var(L'^{-1}z)$=$(L'^{-1})^2 Var(z)$=$(L''L')^{-1}I = P^{-1}$
Therefore $y = u + v \sim \text{N}(mP^{-1}, P^{-1})$.

latent GMRF solution if target is not Gaussian
hierarchical model with τ as smoothing parameter:

$$Y_i|\eta_i \overset{iid}{\sim} F(\eta_i) \quad \text{e. g. Poisson for count data}$$

$$\eta \sim GMRF(\tau Q)$$

Inference with MCMC, with a penalized Likelihood, or with INLA (fully Bayesian using approximations)

Ising Model $X_i \sim \text{B}(1, \pi_i)$, $x_i \in \{-1, 1\}$, e. g. black/white
Minimize:

$$H(f, x) = -c\sum_{i\in I} f_i x_i - \beta \sum_{i\sim j} f_i f_i - h\sum_{i\in I} f_i$$

- $-\sum_{i\in I} f_i x_i \propto$ Hamming distance
- $\sum_{i\sim j} f_i f_i$ penalty for differing neighbors
- $\sum_{i\in I} f_i$ to achieve a balance between values (optional)

Bayesian View

- $-\sum_{i\in I} f_i x_i = -l(f|x)$ for multiplicative noise ($x_i = f_i\eta_i$, with η_i flip indicator), the rest of the formula is the prior
- **Perfect Sampling:** Do MCMC from all possible start values. Combine paths with same status. Once all paths are combined, distribution is independent of starting value.

Potts Model as extension to categorical data

7.2 Geostatistics

Spatially Continuous Random Field random variables Y_S

$$Y_S : (\mathbb{R}^d, \mathcal{B}^d, \mathbb{P}) \to (Z, \mathcal{F})$$

i. e. probability space $\to$ status space (including σ-Algebra)

Variogram typically plot over distance $|s - s'|$

$$\gamma(s, s') := \frac{1}{2}\mathrm{Var}(Y(s) - Y(s'))$$

Covariogram $c(s, s') := \mathrm{Cov}(Y(s), Y(s'))$ (= covariance)
It holds: $\gamma(s, s') = \frac{1}{2}\mathrm{Var}(Y(s)) + \frac{1}{2}\mathrm{Var}(Y(s')) - c(s, s')$

Gauss Random Field $Y = \{Y(s), s \in D \subseteq \mathbb{R}^d\}$

$\forall s_1, ..., s_n : (Y(s_1), ..., Y(s_n))^T$ multivariate normal
uniquely defined by $\mu(s)$ and $c(s, s')$

Stationarity strong $\Rightarrow$ weak $\Rightarrow$ intrinsic

intrinsic $\mathrm{E}(Y(s)) =$ const. and $\gamma(s, s') = \gamma(\Delta s)$
weak $\mathrm{E}(Y(s)) =$ const. and $c(s, s') = c(\Delta s)\, \forall s, s' \in S$
strong all n-dimensional distributions translation invariant

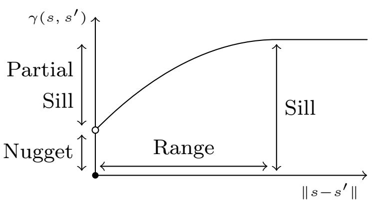
For stationary processes: **Correlogram** $\rho(\Delta s) := \frac{c(\Delta s)}{\sigma^2}$,
$c(0) = \sigma^2 = \mathrm{Var}(Y(s))$ nugget effect, and γ, c, ρ symmetric;
$\gamma(\Delta s) = c(0) - c(\Delta s) = \sigma^2(1 - \rho(\Delta s))$

Isotropy compare directional variograms

$$c(s, s') = c(\|s - s'\|) \Leftrightarrow Y \text{ isotrop}$$

- **geometric anisotropy** same sill, different range
- **zonal anisotropy** different sill

Empirical Variogram estimated via kernel functions and nearest neighbours (similar to gliding histograms)



Parametric Models for Correlograms

- **Exponential** $\rho(h) = \exp(-(h/\phi))$
- **Gauss** $\rho(h) = \exp(-(h/\phi)^2)$
- **Spherical** $\rho(h) = \begin{cases} 1 - \frac{2}{3}(h/\phi) + \frac{1}{2}(h/\phi)^3, & 0 \le h \le \phi \\ 0, & h \ge \phi \end{cases}$
- **Matérn** $\frac{1}{2^{\kappa-1}\Gamma(\kappa)}(h/\phi)^\kappa K_\kappa(h/\phi)$ with K_κ Bessel function

Simple Kriging assumes known expectation and $c(s, s')$

$$Y(s_i) = Z(s_i) + \epsilon(s_i)$$

with random field Z with $\mu(s)$ and $c(s, s') = \sigma^2\rho(s, s')$
and $\epsilon(s_i)$ i.i.d. with expectation 0 and variance σ^2_ϵ
minimizing MSPE $\min \sigma^2_Y(s_0) = c(s_0, s_0) - c(s_0)' C_Y^{-1} c(s_0)$:

$$\hat{Z}(s_0) = \mu(s_0) + c(s_0)' C_Y^{-1}(Y - \mu_Y)$$

ordinary constant unknown mean $\mu(s) = \mu$
universal known beta in $\mu(s) = x(s)'\beta$

Gauss Model Kriging same estimates as for simple kriging
Equivalent Approaches:
additive: $Y(s) = \mu(s) + Z(s) + \epsilon(s)$, with $Z(s)$ as $\mathrm{GRF}(0, \tau^2)$
hierarchical: $Y(s)|Z(s), \sigma^2 \sim \mathrm{N}(Z(s), \sigma^2)$, $Z(s)$ as $\mathrm{GRF}(\mu(s), \tau^2)$

Inference:

- ML: via profile-log-likelihood, but biased
- REML: via restricted (or marginal) likelihood, less biased
- fully Bayesian: MCMC but how to choose priors

Kriging Procedure

1. variogram
2. fit correlation function
3. test stationarity/isotropy
4. if so, transform for isotropy
5. Kriging
6. residual variogram
7. geoadditive regression
8. maybe generalized Kriging

Geoadditive Regression

$$Y_i = x_i\beta + \sum_{j=1}^{p} f_j(z_{ij}) + f_{geo}(s_i) + \epsilon_i$$

Modelling $f_{geo}(s) = z_{geo}\gamma_{geo}$ with $\gamma_{geo} \sim \mathrm{N}\left(0, (\tau_{geo}K_{geo})^{-1}\right)$:

- **lattice data:** $f_{geo} = \phi_K$ for $s_i = K$ and GMRF pior
- **geostatistical data:** $f_{geo} = Z\gamma_{geo}$ using radial basis functions or 2D-splines

$$Y = X\beta + \sum_{j=1}^{p,geo} Z_j\gamma_j + \epsilon \quad \text{with } \gamma_j \sim \mathrm{N}\left(0, (\tau_j K_j)^{-1}\right)$$

with inference via REML, cross validation or fully Bayesian
INLA (Integrated Nested Laplace Approximation):
2 Laplace approximations for fully Bayesian procedure
AIC is impossible for spatial, but DIC works

7.3 Point Processes

Spatial Point Process countable set of locations of events

$$N = s_1, ..., s_n, ... \subset S \subseteq \mathbb{R}^d$$

equivalent to $P(s_1 \in B_1, ..., s_n \in B_n)$ for any Borel sets $B_i \subseteq S$ or as counting process $P(N(B_1) = n_1, ..., N(B_k) = n_k)$ with $N(B) < \infty$ and bounded B for any k

k-dimensional distributions are determined by void probabilities:

$$P(N(B) = 0)$$

Intensity first (λ) and second (λ_2) order

$$\lambda(s) := \lim_{|ds| \to 0} \frac{\mathrm{E}(N(ds))}{|ds|}$$

with ds Borel set around s; similar to hazard rate

$$\lambda_2(s, u) := \lim_{|ds|, |du| \to 0} \frac{\mathrm{E}(N(ds) \cdot N(du))}{|ds| \cdot |du|}$$

λ and λ_2 determine the first two moments of $N(B) \forall B \subseteq \mathbb{R}^d$

Stationarity

weak $\lambda(s) = \text{const.}$ and $\lambda_2(s,u) = \lambda_2(s+\Delta, u+\Delta) \forall \Delta$

strong distributions are translation invariant

Isotropy

weak $\lambda_2(s,u) = \lambda_2(\|s-u\|)$ rotation invariant

strong distributions are rotation invariant

Point Patterns

- complete spatial randomness (CSR)
- aggregated/clustering
- regular/grid

Can be tested via χ^2-Goodness-of-fit for discretized S

Binomial Process overlay of n Bernoulli Processes

$$P(s_1 \in B_1, ..., s_n \in B_n) = \frac{|B_1| \cdot ... \cdot |B_n|}{|S|^n}$$

with Bernoulli Processes: $N = \{s\}$, with $P(s \in B) = \frac{|B|}{|S|}$
As $\lambda(s) = \lambda$, the Binomial Process is homogeneous.

Proof:
$$\lambda(s) = \lim_{|ds| \to 0} \frac{\mathrm{E}(N(ds))}{|ds|} = \lim_{|ds| \to 0} \frac{n|ds|/|S|}{|ds|} = \frac{n}{|S|} = \lambda$$

However, $N(B)$ and $N(S \setminus B)$ are dependent

Poisson Process

homogeneous if: $N(B) \sim \mathrm{Po}(\lambda \cdot |B|)$ with $0 < \lambda < \infty$
results in CSR and void probability $P(N(K) = 0) = \exp(-\lambda|K|)$
inhomogeneous if $\lambda(s)$ varies:
$N(B) \sim \mathrm{Po}(\mu(B))$ with $\mu(B) = \int_B \lambda(s) ds$
Both have independent scattering: $N(B_1) \perp N(B_2)$ for $B_1 \cap B_2 = \emptyset$.

Estimating Intensity $\boldsymbol{\lambda}$

parametric step function: ML estimate $\hat{\lambda}_B = \frac{N(B)}{|B|}$
parametric and likelihood based: $\lambda(s|\theta) := \exp(z'\theta)$
$l(\theta)$ can be approximated by a weighted Poisson-log-likelihood
univariate kernel density estimation:

$$\hat{\lambda}(s) = \frac{1}{\nu(W) b_x b_y} \sum_{i=1}^{n} K\left(\frac{x_i - x}{b_x}\right) K\left(\frac{y_i - y}{b_y}\right)$$

with $\nu(W)$ size of window W, $s = (x,y)$ and bandwidths b_x, b_y
bivariate kernel density estimation with edge correction:

$$\hat{\lambda}(s) = \frac{1}{\int_W \frac{1}{b^2} K\left(\frac{s-u}{b}\right) du} \sum_{i=1}^{n} \frac{1}{b^2} K\left(\frac{s_i - s}{b}\right)$$

The bandwidths can be estimated via cross validation.

K-Function for stationary and isotrope processes

$$K(h) := \frac{\mathrm{E}\left[\sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} \frac{\mathbb{1}(\|s_i - s_j\| \leq h)}{\nu(W_{s_i} \cap W_{s_j})}\right]}{n(n-1)/\nu(W)^2}$$

with W window of observation, W_{s_i} window of shape W with center s_i, and $\nu(W)$ volume of W
$\lambda \cdot K(h) = \mathrm{E}(h)$: expected number of events around an event
$K(h)$ determines $\lambda_2(h)$, e.g. for $d = 2$: $\lambda_2(h) = \frac{\lambda^2}{2\pi h} \frac{dK(h)}{dh}$

Ripley's $\boldsymbol{\hat{K}(h)}$ $= \frac{1}{\hat{\lambda}} \hat{\mathrm{E}}(h)$, with $\hat{\lambda} = \frac{N(B)}{|B|}$ and

$$\hat{\mathrm{E}}(h) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} \frac{\mathbb{1}(\|s_i - s_j\| \leq h)}{\nu(W_{s_i} \cap W_{s_j})}$$

for $d = 2$ and CSR: $K(h) = \pi h^2$ is quadratic

L-Function scales $K(h)$ to linear

$$L(h) = \sqrt{K(h)/\pi}$$

Pair Correlation Function first derivative of $K(h)$

$$g(s,u) = \frac{\lambda_2(s,u)}{\lambda(s)\lambda(u)} =: g(\|s-u\|)$$

For tests on CSR an envelope of $\hat{K}$, $\hat{L}$ or $\hat{g}$ can be calculated.

Marked Point Processes discrete or continuous

discrete with 2 types (A, B) or more:

- **Clark-Evans aggregation index:** $CE_{AB} = \bar{d}_{AB} \cdot 2\sqrt{\lambda_B}$ with $\bar{d}_{AB}$ average distance of A points to nearest B point; $CE_{AB} > 1$ shows repulsion, $CE_{AB} < 1$ attraction
- **Segregation coefficient:** $S = 1 - \frac{p_{AB} + p_{BA}}{p_{A\cdot} p_{\cdot B} + p_{\cdot A} p_{B\cdot}}$ with p_{xy} number of pairs where type x's nearest neighbor is type y; $S < 0$ is mixing, $S > 0$ segregation, and $S = 0$ independence
- **Mingling index:** $M_k = \frac{1}{k} \mathrm{E}\left[\sum_{i=1}^{k} \mathbb{1}\left(m(o) \neq m(n_i(o))\right)\right]$ with point o, its k nearest neighbors $n_i(o)$, and mark $m(o)$
- **Bivariate $\boldsymbol{K}$, $\boldsymbol{L}$, and $\boldsymbol{g}$:** expected y points around x point
- **Mark correlation function:** $K_t(r) = \frac{C_t(r)}{C_t(\infty)}$ with radius $r > 0$, $C_t(r) = \mathrm{E}_{or}\left[t(m(o), m(r))\right]$ and test function $t(\cdot)$; $K > 1$ signals mutual stimulation, $K < 1$ inhibition

continuous leading to weighted measures:

$$K_{mm}(r) = \frac{c_{mm}(r)}{\lim_{r\to\infty} c_{mm}(r)}$$

with $c_{mm}(r) = \mathrm{E}(m(o) \cdot m(r))$

Poisson Cluster Process The parent is an inhomogeneous poisson process. Each parent event creates a random amount of $n(s)$ children according to a 2D density function.

- **Neyman-Scott:** $\mathrm{P}(n(s) = k) = p_k$ and i.i.d. densities
- **Matérn:** stationary parent and $f(s) \propto$ const. for $\|s\| < R$

Non-stationarity and Pairwise Interaction

$$f(s_1, ..., s_n|\theta) = \overbrace{a(\theta)}^{\text{normalising}} \prod_{i=1}^{n} \overbrace{b(s_i|\theta)}^{\text{trend}} \prod_{i<j} \overbrace{h(s_i, s_j|\theta)}^{\text{interaction}}$$

8 Bayesian Statistics

8.1 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

$$\hat\theta_{postmean} = E_0(\vartheta|x) = \int_{\vartheta\in\Theta} \vartheta f_\theta(\vartheta|x) d\vartheta$$

$$\hat\theta_{postmode} = \underset{\vartheta}{\operatorname{argmax}} f_\theta(\vartheta, x)$$

$$\hat\theta_{Bayesrisk} = \underset{t(.)}{\operatorname{argmin}} R_{Bayes}(t(.))$$

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

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

Credibility Interval

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

- 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 $f_\theta(\theta) = \sqrt{I_\theta(\theta)}$:

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

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

8.2 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: $\int \mathrm{e}^{\{\sum_{i=1}^{n} \log f(y_i|\theta) + \log f_\theta(\theta)\}} d\theta =$

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

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

- **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.

9 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 version $\hat{F}_n(y) = \frac{1}{n}\sum_{i=1}^n \mathbb{1}_{(y_i \le y)}$ 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 $= \frac{1}{B}\sum_{b=1}^B \mathbb{1}_{\{t(x_b^*, y_b^*) \ge t(x,y)\}}$

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 $e_i \sim \mathrm{N}(0, \hat{\sigma}^2_{ML})$, 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 $F_n(y) = \frac{1}{n}\sum_{i=1}^n \mathbb{1}_{\{Y_i \le y\}}$ empirical distribution function, $G_n(t, F) = P(T_n \le t)$ exact finite sample distribution of $T_n = t(Y_1, ..., Y_n)$, 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: $G_n(t, H_n) \to G_\infty(t, F)$

10 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)

11 Dimensionality Reduction

Covariance Matrix Σ

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

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 $Y^T Y$ respectively
4. explained variance $\sum_{i=1}^{r} \lambda_i / \sum_{i=1}^{q} \lambda_i$

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

12 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:

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

Iterate over E and M step until convergence

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), $\mathrm{Var}(U)$ (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)

13 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