# **Statistics**

Collection of Formulas

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#### **Descriptive Statistics** 1

#### 1.1 **Summary Statistics**

#### Location 1.1.1

**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

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

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

Minimum/Maximum

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

#### 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:

$$\star Var(aX + b) = a^2 \cdot Var(X)$$

## Arithmetic Mean

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

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

$$\star E(a+b\cdot X) = a+b\cdot E(X)$$

$$\star E(X \pm Y) = E(X) \pm E(Y)$$

Geometric Mean

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

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

Harmonic Mean

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

## $\star \ Var(X \pm Y) = Var(X) + Var(Y) + 2Cov(X, Y)$

(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

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

These are also the values for the Lorenz curve.

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

Lorenz-Münzner Coefficient (normed G)  $G^+ = \frac{n}{n-1}G$ 

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

Range:  $0 < G^+ < 1$ 

#### Shape 1.1.4

(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

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

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

Spearman's Rank Correlation Coefficient

Kendall's/Stuart's  $\tau_c$ 

Without ties:

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

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

#### Excess

$$\gamma = k - 3$$

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

 $T_X = \sum_{i=m} \sum_{j < n} n_{ij} n_{mn}$  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

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

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

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

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

# 1.1.5Dependence

# for two nominal variables

 $\chi^2$ -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

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

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 metric variables

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

# Correlation Coefficient (Bravais-Pearson)

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

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

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

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

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

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

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

# for two ordinal variables

# Gamma (Goodman and Kruskal)

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

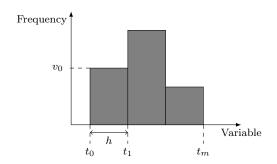
$$K = \sum_{i < m} \sum_{j < n} n_{ij} n_{mn}$$
 Number of concordant pairs 
$$D = \sum_{i < m} \sum_{j > n} n_{ij} n_{mn}$$
 Number of reversed pairs

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

# 1.2 Tables

# 1.3 Diagrams

# 1.3.1 Histogram



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

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

with:  

$$n! = n \cdot (n-1) \cdot \dots \cdot 1$$

$$\binom{n}{m} = \frac{n!}{m!(n-m)!}$$

# 2.2 Probability Theory

Laplace

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

Kolmogorov Axioms mathematical definition of probability

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

Implications:

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

Probability (Mises) frequentist definition of probability

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

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

Conditional Probability

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

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

Law of Total Probability

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

Bayes' Theorem

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

Stochastic Independence

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

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

# 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  $f(\cdot)$ :

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:

$$\int_{-\infty}^{y} f_Y(\tilde{y}) d\tilde{y} := \sum_{k:k \le y} P(Y = k)$$
. This notation is used.

• Cumulative Distribution Function  $F(\cdot)$ :

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

Relationship:

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

Moments

- Expectation (1. Moment):  $\mu = E(Y) = \int y f_Y(y) dy$
- Variance (2. centralized Moment):

$$\sigma^2 = Var(Y) = E(\{Y - E(Y)\}^2) = \int (y - E(Y))^2 f(y) dy$$
  
Note:  $E(\{Y - \mu\}^2) = E(Y^2) - \mu^2$ 

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

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

#### Moment Generating Function

$$\begin{aligned} M_Y(t) &= \mathbf{E}(e^{tY}) \\ \text{with} \ \frac{\partial^k M_Y(t)}{\partial t^k} \bigg|_{t=0} &= \mathbf{E}(Y^k) \\ \text{Cumulant Generating Function} \ K_Y(t) &= \log M_Y(t) \end{aligned}$$

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

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

#### Density and Cumulative Distribution Function

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

Marginal Density

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

Conditional Density

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

Iterated Expectation

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

#### Proof:

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

$$Var(Y) = E_X(Var(Y|X)) + Var_X(E(Y|X))$$

Proof:

$$Var(Y) = \int (y - \mu_Y)^2 f(y) dy$$

$$= \int (y - \mu_Y)^2 f(y|x) f(x) dy dx$$

$$= \int (y - \mu_Y|_x + \mu_Y|_x - \mu_Y)^2 f(y|x) f(x) dy dx$$

$$= \int (y - \mu_Y|_x)^2 f(y|x) f(x) dy dx +$$

$$\int (\mu_Y|_x - \mu_Y)^2 f(y|x) f(x) dy dx +$$

$$2 \int (y - \mu_Y|_x) (\mu_Y|_x - \mu_Y) f(y|x) f(x) dy dx$$

$$= \int Var(Y|x) f(x) dx + \int (\mu_Y|_x - \mu_Y)^2 f(x) dx$$

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

#### 2.4 **Probability Distributions**

#### Discrete Distributions 2.4.1

## Discrete Uniform

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

Binomial Successes in independent trials

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

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

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

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

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

# Geometric

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

# **Negative Binomial**

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

# 2.4.2 Continuous Distributions

#### Continuous Uniform

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

Univariate Normal symmetric with  $\mu$  and  $\sigma^2$ 

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

#### Log-Normal

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

non-standardized Student's t  $\,$  statistical Tests for  $\mu$  with unknown (estimated) variance and  $\nu$  degrees of freedom

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

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

Beta

$$\begin{split} Y \sim \mathrm{Be}(a,b) \text{ with } a,b > 0, \ y \in [0,1] \\ p(y|a,b) &= \frac{\Gamma\left(a+b\right)}{\Gamma(a)\Gamma(b)} y^{a-1} (1-y)^{b-1} \end{split}$$

# 2.4.3 Exponential Family

## Definition

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

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

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

#### Normalising Constant

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

$$\begin{split} & \mathrm{E}(Y|a,b) = \frac{a}{a+b}, \\ & \mathrm{Var}(Y|a,b) = \frac{ab}{(a+b)^2 \left(a+b+1\right)}, \\ & \mathrm{mod}(Y|a,b) = \frac{a-1}{a+b-2} \text{ for } a,b > 1 \end{split}$$

#### Gamma

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

#### Inverse-Gamma

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

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

Exponential Time between Poisson events

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

Chi-Squared squared standard normal random variables with  $\nu$  degrees of freedom

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

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

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

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

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

#### Members

- Poisson
- Geometric
- Exponential

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

- Chi-Squared
- Beta

# 2.5 Multivariate Distributions

Multivariate Normal symmetric with  $\mu_i$  and  $\Sigma$ 

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

## 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  $F_j(y_j) = C(F_j(y_j), 1..., 1)$
- 2. dependence structure  $\hat{u}_i = (\hat{u}_{i1}, ..., \hat{u}_{iq}) \stackrel{iid}{\sim} C(.)$  with  $\hat{u}_{ij} := \hat{F}_j(y_{ij})$ .

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

#### Tail Dependence

$$\begin{split} & \text{upper: } \lambda_u := \lim_{u \to 1} P(Y_1 \ge F_1^{-1}(u) | Y_2 \ge F_2^{-1}(u)) \\ &= \lim_{u \to 1} \frac{1 - 2u + C(u, u)}{1 - u} \\ & \text{lower: } \lambda_l := \lim_{u \to 0} P(Y_1 \le F_1^{-1}(u) | Y_2 \le F_2^{-1}(u)) \\ &= \lim_{u \to 0} \frac{C(u, u)}{u} \end{split}$$

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  $Y_{ij} \sim N(\mu_j, \sigma_j)$ :  $f(y_{ij}; \mu_j, \sigma_j^2) = \frac{1}{\sigma_j} \phi(Z_{ij})$  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  $\psi(1,\theta)=0 \ \forall \theta$ 

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

- 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  $M_n := \max(Y_{1:n})$ :

$$F_{M_n}(y) = P(M_n \le y) = P(Y_{1:n} \le y) = (F_Y(y))^n$$

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

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  $\mu$ , scale  $\sigma$ , and shape  $\gamma$  and  $z = \frac{x-\mu}{\sigma}$ 

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

# 2.6 Limit Theorems

Law of Large Numbers

# Central Limit Theorem

$$Z_n \stackrel{d}{\longrightarrow} N(0, \sigma^2)$$

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

#### Proof

9

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  $\mu$  and  $\sigma$ . All other moments are zero.

For 
$$Z_n = (Y_1 + Y_2 + ... + Y_n)/\sqrt{n}$$
:

$$\begin{split} M_{Z_n}(t) &= \mathbf{E} \left( e^{t(Y_1 + Y_2 + \ldots + Y_n)/\sqrt{n}} \right) \\ &= \mathbf{E} \left( e^{tY_1/\sqrt{n}} \cdot e^{tY_2/\sqrt{n}} \cdot \ldots \cdot e^{tY_n/\sqrt{n}} \right) \\ &= \mathbf{E} \left( e^{tY_1/\sqrt{n}} \right) \mathbf{E} \left( e^{tY_2/\sqrt{n}} \right) \ldots \mathbf{E} \left( e^{tY_n/\sqrt{n}} \right) \\ &= M_V^n(t/\sqrt{n}) \end{split}$$

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

$$\frac{\partial K_{Z_n}(t)}{\partial t}\bigg|_{t=0} = \frac{n}{\sqrt{n}} \frac{\partial K_Y(t)}{\partial t}\bigg|_{t=0} = \sqrt{n}$$

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

Using the Taylor Expansion, we can write  $K_{Z_n}(t) = 0 +$ 

# 3 Inference

# 3.1 Method of Moments

The theoretical moments are estimated by their empirical counterparts:

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

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

# 3.2 Loss Functions

Loss

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

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

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

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

Risiko

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

#### Minimax Approach

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

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

Mean Squared Error (MSE)

$$MSE(t(.), \theta) = \mathcal{E}_{\theta} \left( \{ t(Y) - \theta \}^2 \right)$$
$$= \operatorname{Var}_{\theta} \left( t(Y_1, ..., Y_n) \right) + Bias^2((t(.); \theta))$$
with  $Bias(t(.); \theta) = \mathcal{E}_{\theta} \left( t(Y_1, ..., Y_n) \right) - \theta$ 

Proof:  
Let 
$$\mathcal{L}(t,\theta) = (t-\theta)^2$$
  
 $R(t(.),\theta) = \mathcal{E}_{\theta}(\{t(Y) - \theta\}^2)$   
 $= \mathcal{E}_{\theta}(\{t(Y) - \mathcal{E}_{\theta}(t(Y)) + \mathcal{E}_{\theta}(t(Y)) - \theta\}^2)$   
 $= \mathcal{E}_{\theta}(\{t(Y) - \mathcal{E}_{\theta}(t(Y))\}^2) + \mathcal{E}_{\theta}(\{\mathcal{E}_{\theta}(t(Y)) - \theta\}^2)$   
 $+ 2\mathcal{E}_{\theta}(\{t(Y) - \mathcal{E}_{\theta}(t(Y))\}\{\mathcal{E}_{\theta}(t(Y)) - \theta\})$   
 $= \mathcal{V}_{\theta}(t(Y_1, ..., Y_n)) + Bias^2((t(.); \theta) + 0)$ 

Cramér-Rao Inequality

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

Proof: For unbiased estimates:  $\theta = E_{\theta}(\hat{\theta}) = \int t(y)f(y;\theta)dy$   $1 = \int t(y)\frac{\partial f(y;\theta)}{\partial \theta}dy$   $= \int t(y)\frac{\partial \log f(y;\theta)}{\partial \theta}f(y;\theta)dy$   $= \int t(y)s(y;\theta)f(y;\theta)dy$   $= \int (t(y)-\theta)(s(\theta;y)-0)f(y;\theta)dy \qquad \text{1. Bartlett equation } E_{\theta}(s(\theta;y))=0$   $= \text{Cov}_{\theta}(t(Y);s(\theta;Y))$   $\geq \sqrt{\text{Var}_{\theta}(t(Y))}\sqrt{\text{Var}_{\theta}(s(\theta;Y))} \qquad \text{Cauchy-Schwarz}$   $= \sqrt{MSE(t(Y);\theta)}\sqrt{I(\theta)}$ 

Kullback-Leibler Divergence Comparing distributions

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

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

Proof:

Follows from  $\log(x) \le x - 1 \forall x \ge 0$ , with equality for x = 1.

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

Proof:  

$$R_{KL}(t(.),\theta) =$$

$$= \int_{-\infty}^{\infty} \mathcal{L}_{KL}(t(Y_1,...,Y_n),\theta) \prod_{i=1}^{n} f(y_i;\theta) dy_i$$

$$= \int \int \log \frac{f(\tilde{y};\theta)}{f(\tilde{y};t)} f(\tilde{y};\theta) d\tilde{y} \prod_{i=1}^{n} f(y_i;\theta) dy_i$$

$$= \int \int (\log f(\tilde{y};\theta) - \log f(\tilde{y};t)) f(\tilde{y};\theta) d\tilde{y} - \prod_{i=1}^{n} f(y_i;\theta) dy_i$$

$$\approx -\int \underbrace{\left(\int \frac{\partial \log f(\tilde{y};\theta)}{\partial \theta} f(\tilde{y};\theta) d\tilde{y}\right)}_{0} (t-\theta) \prod_{i=1}^{n} f(y_i;\theta) dy_i$$

$$+ \frac{1}{2} \int \underbrace{\left(-\int \frac{\partial^2 \log f(\tilde{y};\theta)}{\partial \theta^2} f(\tilde{y};\theta) d\tilde{y}\right)}_{I(\theta)} (t-\theta)^2 \prod_{i=1}^{n} f(y_i;\theta) dy_i$$

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  $\theta$
  - Parameter space  $\Theta$  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  $I(\theta)$ :  $-\mathbb{E}_{\theta}\left(\frac{\partial s(\theta;Y)}{\partial \theta}\right)$
- observed Fisher-Information  $I_{obs}(\theta)$ :  $-\mathrm{E}_{\theta}\left(\frac{\partial s(\theta;y)}{\partial \theta}\right)$

## Attributes of the Score-Function

first Bartlett-Equation:

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

Proof:  

$$1 = \int f(y;\theta)dy$$

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

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

second Bartlett-Equation:

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

Proof:  

$$0 = \frac{\partial 0}{\partial \theta} = \frac{\partial}{\partial \theta} \int \frac{\partial}{\partial \theta} \log f(y; \theta) f(y; \theta) dy \qquad \text{see above}$$

$$= \int \left( \frac{\partial^2}{\partial \theta^2} \log f(y; \theta) \right) f(y; \theta) dy$$

$$+ \int \frac{\partial \log f(y; \theta)}{\partial \theta} \frac{\partial f(y; \theta)}{\partial \theta} dy$$

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

$$+ \int \frac{\partial \log f(y; \theta)}{\partial \theta} \frac{\partial \log f(y; \theta)}{\partial \theta} f(y; \theta) dy$$

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

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 ay smptotically the smallest variance, given by the Cramér-Rao inequality,

$$s\left(\hat{\theta}_{ML}; y_1, ..., y_n\right) = 0$$
$$\hat{\theta} \stackrel{a}{\sim} N\left(\theta, I^{-1}(\theta)\right)$$

If the true model is unknown, the distribution is  $\hat{\theta} \stackrel{\sim}{\sim} \mathcal{N}\left(\theta, I^{-1}(\theta)V(\theta)I^{-1}(\theta)\right)$  with  $V(\theta)$  variance of the score function.

The ML-estimate is invariant:  $\hat{\gamma} = g(\hat{\theta})$  if  $\gamma = g(\theta)$ .

Proof

$$\gamma = g(\theta) \Leftrightarrow \theta = g^{-1}(\gamma)$$

For the log-likelihood of  $\gamma$  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:  

$$I_{\gamma}(\gamma) = -E\left(\frac{\partial^{2}l(g^{-1}(\hat{\gamma}))}{\partial \gamma^{2}}\right) = -E\left(\frac{\partial}{\partial \gamma}\left(\frac{\partial g^{-1}(\gamma)}{\partial \gamma}\frac{\partial l(\theta)}{\partial \theta}\right)\right)$$

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

$$= \frac{\partial g^{-1}(\gamma)}{\partial \gamma}I(\theta)\frac{\partial g^{-1}(\gamma)}{\partial \gamma} = \frac{\partial \theta}{\partial \gamma}I(\theta)\frac{\partial \theta}{\partial \gamma}$$

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

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

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

Proof: 
$$0 = s(\hat{\theta}_{ML}; y) \overset{Taylor}{\underset{Series}{\approx}} s(\theta; y) + \frac{\partial s(\theta; y)}{\partial \theta} (\hat{\theta}_{ML} - \theta) \Leftrightarrow$$
 
$$\hat{\theta}_{ML} \approx \theta - \left(\frac{\partial s(\theta; y)}{\partial \theta}\right)^{-1} s(\theta; y) \approx \theta - I^{-1}(\theta) s(\theta; y)$$
 As  $\frac{\partial s(\theta; y)}{\partial \theta}$  is often complicated, its expectation  $I(\theta)$  is used.

The second part in 2 can be weighted with a step size  $\delta$  or  $\delta(t) \in (0,1)$ , e. g. to ensure convergence.

If  $I(\theta)$  can't be analytically derived, simulation from  $f(y;\theta_{(t)})$  can be used. For the exponential family, step 2 then changes to  $\theta_{(t+1)} := \theta_{(t)} + \hat{\mathrm{Var}}_{\theta_{(t)}}(t(Y))^{-1} \mathrm{E}_{\theta_{(t)}}(t(Y))$  as the ML estimate is the expectation.

## Log Likelihood Ratio

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

with  $2 \cdot lr(\theta, \hat{\theta}) \stackrel{a}{\sim} \chi_1^2$ 

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

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

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

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

## Relation to Kullback-Leibler divergence

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

with f distributional model used and g true model

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

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

#### Consistency and Sufficiency 3.4

(Weak) Consistency

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

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

Statistic

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

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

#### Suffizienz

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

## Neyman criterion:

$$t(Y_1, ..., Y_n)$$
 suffizient  $\Leftrightarrow f(y; \theta) = h(y)g(t(y); \theta)$ 

Proof:

"⇒":

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

': 
$$f_t(t;\theta) = \int_{t=t(y)} f(y;\theta) dy = \int_{t=t(y)} h(y) g(t;\theta) dy$$
 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  $\forall \tilde{t}(.) \exists h(.) \text{ s.t. } t(y) = h(\tilde{t}(y))$ 

# 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.:

$$P("H_1"|H_0) \le \alpha$$

$$\frac{"H_0"}{H_0} \frac{"H_1"}{A}$$

$$\frac{H_0}{H_0} \frac{1 - \alpha \text{ (correct)}}{A} \frac{\alpha \text{ (type I error)}}{1 - \beta \text{ (correct)}}$$

Power concerns the type II error

$$power = P("H_1"|H_1) = 1 - \beta$$

**p-Value** measures the amount of evidence against  $H_0$ 

$$p-value \leq \alpha \Leftrightarrow "H_0"$$

# 4.2 Tests for One Sample

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

Test for  $\mu$ , known  $\sigma^2$  (Simple Gauss-Test)

 $H_0$ :  $\mu = \mu_0$  vs.  $H_1$ :  $\mu \neq \mu_0$ 

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

Test for  $\mu$ , unknown  $\sigma^2$  (Simple t-Test)

 $H_0$ :  $\mu = \mu_0$  vs.  $H_1$ :  $\mu \neq \mu_0$ 

$$T(X) = \frac{\bar{X} - \mu_0}{\hat{\sigma}/\sqrt{n}} \stackrel{H_0}{\sim} t_{n-1}$$
 with  $\hat{\sigma} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (Y_i - \bar{Y})^2}$ 

# **ML** Estimate $\hat{\theta} \stackrel{a}{\sim} N(\theta, I^{-1}(\theta))$

Wald Test

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

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

As  $\hat{\theta}$  converges to  $\theta_0$  under  $H_0$ , it can also be used to calculate the variance:  $I^{-1}(\hat{\theta})$ .

Score Test

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

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

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

#### Confidence Interval

 $[t_l(Y), t_r(Y)]$  Confidence Interval

 $\Leftrightarrow$ 

$$P_{\theta}\left(\left(t_{l}(Y) \leq \theta \leq t_{r}(Y)\right) \geq 1 - \alpha\right)$$

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

Corresponding Test

$$\theta \notin [t_l(y), t_r(y)] \Leftrightarrow "H_1"$$

**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)

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

## Likelihood Ratio Test

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

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

#### Neyman-Pearson Test

 $H_0: \theta = \theta_0 \quad vs. \quad H_1: \theta = \theta_1$ 

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

For a given significance level  $\alpha$ , the Neyman Pearson Test is the most powerful test for comparing two estimates for  $\theta$ .

Proof:

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

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

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

# 4.3 Tests for Goodness of Fit

Discrete (Chi-Squared)

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

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

with the following contingency table:

 $l_k > 5$  and  $l_k > n-5$  for the  $\chi^2_{K-1-p}$ -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)

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

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

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

Proof:

$$\begin{split} P(\sup_{x} |F_{n}(x) - F(x;\theta)| &\leq t) = \\ &= P(\sup_{y} |F^{-1}(y;\theta) - x| \leq t) & \sum_{\substack{x \in [0,1], \ x = F^{-1}(y;\theta) \\ F(F^{-1}(y;\theta);\theta) = y}}^{x \in [0,1], \ x = F^{-1}(y;\theta)} \\ &\stackrel{*}{=} P(\sup_{y} |\frac{1}{n} \sum_{i=1} \mathbbm{1}_{\{U_{i} \leq y\}} - y| \leq t) & \text{with } U_{i} \sim U(0,1) \\ &^{*}F_{n}(F^{-1}(y;\theta)) = \frac{1}{n} \sum_{i=1}^{n} \mathbbm{1}_{\{X_{i} \leq F^{-1}(y;\theta)\}} = \frac{1}{n} \sum_{i=1}^{n} \mathbbm{1}_{\{F(y;\theta) \leq y\}} \end{split}$$

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

Pivotal Statistic

$$g(Y;\theta)$$
 pivotal

Distribution of  $g(Y;\theta)$  independent of  $\theta$ 

Approximative Pivotal Statistic

 $H_0: X_i \sim F$  pivotal vs.  $H_1: X_i \sim F$  not pivotal

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

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

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

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

# 4.4 Multiple Tests

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

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

$$FWER := P(\exists k : "H_1k" | \forall k : H_0k)$$

Bonferoni Adjustment

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

Šidák Adjustment only for independent tests

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

$$\alpha \stackrel{!}{=} P(\bigcup_{k=1}^{m} (p_k \le \alpha) | H_{0k}, k = 1, ..., m)$$
$$= 1 - (1 - \alpha)^{1/m}$$

Holm's Procedure also takes power into account

Order the p-values:  $p_{(1)} \leq ... \leq p_{(m)}$ 

Step  $x \in \mathbb{N}^+$ : if  $p(x) > \frac{\alpha}{m+1-x}$  reject  $H_{01}$  to  $H_{0x}$  and stop, else move on to step x+1.

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

$$FDR = \mathbf{E}\left(\frac{\#"H1"|H_0}{\#"H1"}\right)$$

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  $m_0 = \#H_0$ 

#### Regression 5

#### 5.1 Models

#### Simple Linear Model 5.1.1

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 E(e|x) = 0
- Constant Variation  $Var(Y|x) = \sigma^2$

For the normal linear model:

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

Attributes of the Regression Line

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

# 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:

Proof:  

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

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

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

The estimates are the same as for the ML procedure.

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

$$\hat{\beta}_0 = \frac{1}{n} \sum_{i=1}^n y_i - \frac{1}{n} \sum_{i=1}^n x_i \hat{\beta}_1$$

$$\hat{\beta}_1 = \sum_{i=1}^n x_i (y_i - \hat{\beta}_0 / \sum_{i=1}^n x_i^2)$$

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

The  $\beta$ -estimates are the same as for the OLS procedure.

Proof:

oor:  

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

#### Multivariate Linear Model 5.1.2

Theoretical Model

$$Y = X\beta + u$$

**Empirical Model** 

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

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

Assumptions

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

For the normal linear model:

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

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

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

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

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

The estimates are the same as for the OLS procedure.

 $\beta$  is the Best Linear Unbiased Estimator

Proof:

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

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

The ML-estimate for  $\sigma^2$  is biased.

#### Proof

$$\begin{split} H &:= X(X^TX)^{-1}X^T \text{ hat matrix; } HH = H = H^T \text{ (idempotent)} \\ & \mathbb{E}((Y - X\hat{\beta})^T(Y - X\hat{\beta})) = \mathbb{E}((Y^T(I_n - H)^T((I_n - H)Y) \\ & = \mathbb{E}(tr(Y^T(I_n - H)Y) \\ & = \mathbb{E}(tr((I_n - H)YY^T) \\ & = tr((I_n - H)\mathbb{E}(YY^T)) \\ & = tr((I_n - H)\mathbb{E}(X\beta\beta^TX^T + \sigma I_n)) \\ & = \sigma^2 tr((I_n - H)) \\ & = \sigma^2 (n - p) \end{split}$$

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

$$\begin{split} f_{post}(\beta,\sigma^2|y) \propto (\sigma^2)^{-\frac{n}{2}+1} \mathrm{e}^{-\frac{1}{2\sigma^2}(y-X\beta)^T(y-X\beta)} \end{split}$$
 Note: 
$$f_{post}(\beta,\sigma^2|y) = f(\beta|\sigma^2,y) f(\sigma^2|y)$$

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

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

# 5.1.4 Quantile Regression

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

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

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

Quantile

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

Model

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

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

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

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

Proof:

$$Q(\tau) = \arg\min_{q} E(\delta_{\tau}(Y - q))$$

$$= \arg\min_{q} \left\{ (\tau - 1) \int_{-\infty}^{q} (y - q) f(y) dy + \tau \int_{q}^{\infty} (y - q) f(y) dy \right\}$$
Differentiation of the state of t

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  $\beta$  can be computed with linear programming and are normally distributed with mean  $\beta$ .

# 5.1.5 Flexible Regression

## Assumptions

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

## Knot Placement

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

## Penalized Regression Splines

$$\begin{split} ||y-X\beta||^2 + \lambda \int_{x_1}^{x_n} \left[f''(x)\right]^2 dx &= ||y-X\beta||^2 \lambda \beta^T D\beta \\ l_p(\beta,\sigma^2,\lambda) &= l(\beta,\sigma^2) - \frac{\lambda}{2\sigma_\ell^2} \beta^T D\beta \\ \hat{\beta} &= (X^TX + \lambda D)^{-1} X^T y \end{split}$$

#### 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  $\lambda$  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:  ${\bf Bayes}$ 

 $\beta \sim {\rm N}(0,\sigma_\beta^2 D^-)$  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  $\sigma_{\beta}^2$  can be derived. E. g. set  $\lambda$  to the posterior mode estimate.

# 5.1.6 Generalized Regression

# Assumptions

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

#### Link Function

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

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

If  $\lambda = 0$ , canonical link:

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

- score function:  $s(\beta) = X^T (t(y) E(t(Y); \eta))$
- estimate  $\hat{\beta} = X^T E(t(Y); \hat{\eta}) = X^T t(y)$
- 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: 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:  $log E(Y_i|x_i) = \eta$  $Var(Y_i|x_i) = E(Y_i|x_i) = e^{\eta}$

# 5.1.7 Weighted Regression

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

$$\begin{split} l(\beta,\sigma^2) &= -\frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2(y-X\beta)^T(y-X\beta)} \end{split}$$
 with  $W = diag(\frac{1}{a_1},...,\frac{1}{a_n})$  and  $a_i = \frac{\sigma_i^2}{\sigma^2}$  
$$\hat{\beta}_{ML} = (X^TWX)^{-1}(X^TWy) \end{split}$$

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

## Different Group Representation

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

with  $z_i$  indicating group affiliation

# 5.2 Analysis of Variances (ANOVA)

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

with

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

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

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

# 5.3 Goodness of Fit

# 5.3.1 Coefficient of Determination

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

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

# 6 Bayesian Statistics

# 6.1 Basics

Bayes Theorem

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

or more general:

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

Point Estimates

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

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

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

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

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

with posterior Bayes risk:

$$R_{postBayes}(t(.)|y) = \int L(t(y), \vartheta) f_{\theta}(\vartheta|y) = E_{\theta|y}(L(t(y), \theta)|y)$$

Credibility Interval

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

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

**Bayes Factor** evidence contained in data for  $M_1$  vs.  $M_2$ 

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

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

# Priors

Flat (uninformative) Prior

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

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

No prior is truly uninformative.

## Jeffrey's Prior

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

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

$$= \sqrt{I_{\gamma}(\gamma)}$$

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

#### **Empirical Bayes**

Let the prior depend on a hyper-parameter:  $f_{\theta}(\theta, \gamma)$  Choose  $\gamma$  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
$\pi \sim \mathrm{Be}(\alpha, \beta)$	$\operatorname{Bin}(n,\pi)$	$Be(\alpha+k,\beta+n-k)$
$\mu \sim N(\gamma, \tau^2)$	$N(\mu, \sigma^2)$	$N(.,.) \stackrel{n \to \infty}{\longrightarrow} N(\bar{y}, \frac{\sigma^2}{n})$
$\sigma^2 \sim \mathrm{IG}(\alpha, \beta)$	$N(\mu, \sigma^2)$	$IG(\alpha + \frac{n}{2}, \beta + \frac{1}{2} \sum_{i=1}^{n} (y_i - \mu)^2)$
$\lambda \sim \mathrm{Ga}(\alpha, \beta)$	$Po(\lambda)$	$Ga(\alpha+n\bar{y},\beta+n)$

# 6.2 Numerical Methods for the Posterior

Numerical Integration here: trapezoid approximation

$$\int_{\Theta} f(y|\vartheta) f_{\theta}(\vartheta) d\vartheta \approx$$

$$\sum_{k=1}^{K} \frac{f(y;\theta_{k}) f_{\theta}(\theta_{k}) + f(y;\theta_{k-1}) f_{\theta}(\theta_{k-1})}{2} (\theta_{k} - \theta_{k-1})$$

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

Laplace Approximation

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

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

Proof:

For n independent samples:

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

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

$$\int \mathrm{e}^{\{l(\theta;y) + \log f_{\theta}(\theta)\}} d\theta \overset{TS}{\approx} \int \mathrm{e}^{(l_{P}(\hat{\theta}_{P}) - \frac{1}{2}J_{P}(\hat{\theta}_{P})(\vartheta - \hat{\theta}_{P})^{2})} d\vartheta$$

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

#### • Inverse CDF

F(X) known. Since F(x) = u,  $F^{-1}(u) = x$ ,  $u \sim U(0, 1)$ 

- 1. Draw  $u \sim U(0,1)$
- 2. Compute  $F^{-1}(u)$  to get a value x

Proof:

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

#### • Rejection Sampling

An umbrella distribution g(x) can be found s. t.  $\frac{f(x)}{g(x)} \le M \ \forall x \ \text{with} \ f(x) > 0 \ \text{when} \ g(x) > 0$ 

- 1. Draw candidate  $y \sim g(x)$
- 2. Acceptance probability  $\alpha$  for y:  $\alpha = \frac{f(x)}{Ma(x)}$
- 3. Draw  $u \sim U(0,1)$  and accept if  $u \leq \alpha$ , else: step 1

Proof:

$$\begin{split} P\left(Y \leq x | U \leq \frac{f(Y)}{Mg(Y)}\right) &= \frac{P\left(Y \leq x, U \leq \frac{f(Y)}{Mg(Y)}\right)}{P\left(U \leq \frac{f(Y)}{Mg(Y)}\right)} \\ &= \frac{\int_{-\infty}^{x} \int_{0}^{\frac{f(y)}{g(x)}} du \ g(y) dy}{\int_{-\infty}^{\infty} \int_{0}^{x} \frac{f(y)}{g(x)} g(y) dy} \\ &= \frac{\int_{-\infty}^{x} \int_{0}^{x} du \ g(y) dy}{\int_{-\infty}^{\infty} \frac{f(y)}{g(x)} g(y) dy} \\ &= \frac{\int_{-\infty}^{x} f(y) dy}{\int_{-\infty}^{\infty} f(y) dy} = P(X \leq x) \end{split}$$

#### • Importance Sampling

Directly estimate  $E_{\theta}(f(y;\theta))$ .

For sampling distribution g(x),

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

is a consistent estimator

Proof:

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

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  $\theta^*$  from proposal distribution  $q\left(\theta|\theta_{(t)}^*\right)$
- 2. Accept  $\theta_{(t+1)}^* = \theta^*$  with probability

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

This sequence has a stationary distribution for  $n \to \infty$ .

Choice of q: trade-off between exploring  $\Theta$  and reaching a high  $\alpha$ . Burn-in and thinning out give i.i.d. samples from  $f_{post}(\theta|X)$ .

**Gibbs Sampling**: For high dimensions  $\alpha$  is close to zero.

Sample from the marginal distributions seperately:

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

with  $\theta_{t^*,i}$  most recent estimates without  $\theta_i$ 

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  $q_{\theta}$  to independence:  $q_{\theta}(\theta) = \prod_{k=1}^{p} q_{k}(\theta_{k})$ 

Update each component iteratively. Works well for big p.

# 7 Sampling

#### Bootstrap

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

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

### **Bootstrap Probability**

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

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

# Consistency of a Bootstrap Estimator

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

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

The bootstrap estimate is inconsistent for the maximum of a sample or if the  $\theta$  lies on the boundary of  $\Theta$ .

#### Mallow's Metric

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

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

## Theorem of Beran and Ducharme

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

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

# 8 Model Selection

## AIC (Akaike Information Criterion)

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

The AIC estimates  $2E_Y \{KL(g,f)\} - 2 \int \log(g(y))g(y)dy$ . 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  $E_Y \left\{ E_Y \left[ Y - \hat{\mu} \right]^2 \right\}$  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  $\frac{n}{n} < 40$ 

# 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 mode and  $\Delta D(y;\theta,\hat{\theta})=2\left\{l(\hat{\theta})-l(\theta)\right\}\stackrel{a}{\sim}\chi_p^2$  the difference in deviance

$$\begin{split} p_D := \mathrm{E}(\Delta D(y;\theta,\hat{\theta}_{post} \mid y) = \int & D(y,\vartheta) f_{post}(\vartheta \mid y) d\vartheta - D(y,\hat{\theta}_{post}) \\ & \text{The integral can be approximated using MCMC.} \end{split}$$

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 regression covariates:  $P(x_i|y) = \sum_{k=1}^{K} \mathbb{1}_{\{x_i \text{ in } M_k\}} P(M_k|y)$ 

Inference After Model Selection neglect is a quiet scandal

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

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

Solutions:

• 
$$\widehat{Var}(\hat{\theta}) = \left[ \sum_{k=1}^{K} \pi_k \sqrt{\widehat{Var}_k(\hat{\theta}_k) + (\hat{\theta}_k - \hat{\hat{\theta}})^2} \right]^2$$

- 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:  $f_{\theta_j}(\theta_j) \propto \exp(-|\theta_j|) \text{ (Laplace prior)}$ 

# 9 Dimensionality Reduction

#### Covariance Matrix $\Sigma$

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

## Marginal Independence

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

# Conditional Independence

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

Proof.

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

# 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  $\Sigma$
- 2. Prune smallest k=q-r eigenvalues in  $\tilde{\Lambda}$
- 3. Simplify model with spectral decomposition  $\tilde{Y} = \tilde{V}\tilde{\Lambda}^{1/2}\tilde{U}^T$  with  $\tilde{V}$ ,  $\tilde{U}$  first r eigenvectors of  $YY^T$  and  $Y^TY$  respectively
- 4. explained variance  $\sum_{i=1}^{r} \lambda_i / \sum_{i=1}^{q} \lambda_i$

#### Proof:

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

# 10 Missing/Deficient Data

Missing Completely at Random (MCAR) independent

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

A complete case analysis will lead to unbiased results

Missing at Random (MAR) depends on observed variables

$$P(R_i|Y_i) = P(R_i|Y_{iO_i})$$
 with  $O_i = \{j: R_{ij} = 1\}$  and  $M_i = \{j: R_{ij} = 0\}$  Complete case analysis  $P(Y|X,Z)$ :

- $\bullet\,$ only response  $Y_i$  MAR: unbiased
- ullet 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

Expectation Step:

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

Maximization Step:

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

Proof:

$$l_i(\theta) = l_{iO_i} + \log f(y_{iM_i}|y_{iO_i}; \theta)$$
$$l_O(\theta) = l(\theta) - \sum_{i=1}^n \log f(y_{iM_i}|y_{iO_i}; \theta)$$

$$l_O(\theta) = Q(\theta|\theta_{(t)}) - H(\theta, \theta_{(t)})$$

$$l_O(\theta_{(t+1)} \ge l_O(\theta_{(t)})$$

$$l_O(\theta) = \sum_{i=1}^n l_{iO}(\theta) = \sum_{i=1}^n \int f(y_i; \theta) dy_{iM}$$