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FACULTY OF ELECTRICAL ENGINEERING
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LEFT-CENSORED PROBABILITY DISTRIBUTIONS AND THEIR APPLICATIONS

Habilitation thesis

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I hereby declare that the contents of this habilitation thesis is based solely on sources cited in References.

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Contents

Introduction

This thesis is based on author's research during the years 2012-2024. It describes statistical methods that can be used for analyzes of the so-called Type I left-censored data that follow the Weibull distribution and the exponential distribution as its special case.

Chapter 1 describes various types of censoring. A special attention is paid to the Type I left-censored data. Chapter 2 is based on Fusek and Michálek (2019) and describes the Type I multiply left-censored Weibull distribution. The maximum likelihood method is used for estimation of the unknown parameters. In order to describe variability of the parameters' estimates, the expected Fisher information matrix is derived. Behavior of the estimators is analyzed using simulations in Section 2.1. Section 2.2 is based on Fusek and Michálek (2016) and describes confidence intervals for the expected value of the censored Weibull distribution. Confidence intervals based on the maximum likelihood method and the bootstrap are compared using simulations. There are situations when the Weibull distribution is unnecessarily complicated for modelling of real data and the exponential distribution would be a suitable model. Section 2.3 is based on Fusek (2017) and describes statistical tests for testing reduction of the censored Weibull distribution to the exponential submodel. When dealing with real data, there are often situations when we have two independent samples and want to compare, for example, expected values or even distributions of the samples. On that account, we can extend the so-called one-sample model of Chapter 2 to the two-sample model. Chapter 3 is focused on comparison of two independent and identically distributed Type I left-censored Weibull samples. Section 3.1 is based on Fusek and Michálek (2014) and describes statistical tests for testing equality of two left-censored Weibull distributions. Section 3.2 is based on Fusek and Michálek (2015a) and describes statistical tests for testing equality of expectations of two left-censored Weibull distributions. When we want to use the above-mentioned methods for analyzing real data, we need to assume, that our data follow the Weibull distribution. In order to verify such an assumption, we can use a goodness-of-fit test. Chapter 4 is based on Fusek (2023) and describes goodness-of-fit tests for the Type I left-censored Weibull, log-normal and gamma distributions, which are among the most frequently used distributions for modelling of environmental data. Chapter 5 is focused on two applications of the Type I left-censored Weibull distribution. Section 5.1 is based on Fusek and Michálek (2013) and Fusek et al. (2015) and describes the modelling of musk compounds concentrations

in fish caught upstream and downstream the wastewater treatment plant. Section 5.2 is based on Fusek et al. (2020) and describes the modelling of biogenic amines concentrations in various fish species. Another application of the left-censored Weibull distribution can be found in Mbengue et al. (2018) where it was used for modelling of elemental carbon concentrations. In addition, Type I left-censored distributions were also applied in the extreme value theory for estimation of the extremal index (Holešovský and Fusek, 2020, 2022). Brief details can be found in Appendix B.

Chapter 1

Censored Data

Censored data occur frequently in many application areas. When performing an experiment, we can sometimes run into a situation that some of the measured values can be reported only as less than some value, greater than some value, or as an interval. In such cases we talk about left-censored, right-censored and interval-censored data. There are two basic types of censoring, specifically the Type I and the Type II censoring.

The Type I censoring (time censoring) typically occurs in experiments that stop at a prespecified time. The censoring level is known in advance and the number of censored values is a random variable. For example, we have a certain number of light bulbs and study if they fail before a prespecified time. The light bulbs that have not failed are Type I right-censored. Another frequently used application of the Type I censoring is as follows. We measure concentrations of a chemical compound in a sample and our instrument (determination method, respectively) is not able to measure the concentrations below a specified (detection) limit with a stated accuracy and precision. Such observations are called Type I left-censored.

The Type II censoring (failure censoring) typically occurs in experiments that stop when a prespecified number of failures are observed. The number of censored values is known in advance and the censoring level is a random variable. As an example, we can modify our light bulb experiment. Now we have a certain number of light bulbs and study at what time a prespecified number of them fails. The light bulbs that have not failed are Type II right-censored. Another application of the Type II censoring is as follows. We conduct a study where the event of interest, e.g. infection with a sexually transmitted disease, has already taken place at the time when the study starts, but the exact time of occurrence of the event is not known. The exact time when the sickness started is Type II left-censored.

The combination of Type I and Type II censoring is called the hybrid censoring and it is often used in reliability analysis in life testing studies. In the Type I hybrid censoring the experiment is terminated at a random time, specifically it stops either a) when a prespecified number r out of n items fails ($r < n$), or b) when a prespecified time T is

reached. The disadvantage of the Type I hybrid censoring is that there may be very few failures observed up to the prespecified time T, which can have negative influence on the effectiveness of the statistical inference. The Type II hybrid censoring overcomes this issue as it guarantees that at least r failures occurs by the end of the experiment. Specifically, if r out of n items fails before time T, the experiment continues up to time T, which means that there could be more than r failures in total. In case that r failures does not occur before time T, the experiment continues until the time of the r-th failure. The disadvantage of the Type II hybrid censoring is that it may take a long time to observe the required r failures. To overcome disadvantages of both Type I and Type II hybrid censoring schemes, the generalized hybrid censoring schemes can be used.

In case of the generalized Type I hybrid censoring, there is a prespecified time T and two numbers of failures k, r such that $k < r < n$, where k is the minimal number and r is the optimal number of failures required by the experimenter. It means that we would like to observe r failures but k failures are good enough. If the k-th failure occurs before the prespecified time T, the experiment ends either a) when r items fails, or b) when time T is reached. If the k-th failure occurs after time T, the experiment continues until the time of the k-th failure. In other words, the generalized Type I hybrid censoring allows us to continue with the experiment in case very few failures are observed up to time T.

In case of the generalized Type II hybrid censoring, there is a prespecified number of failures r and times T_1, T_2 such that $T_1 < T_2$. If the r-th failure is observed before time T_1, the experiment stops at time T_1. If the r-th failure occurs between times T_1 and T_2, the experiment stops at time of the r-th failure. If the r-th failure is observed after time T_2, the experiment stops at time T_2. In other words, the generalized Type II hybrid censoring guarantees that the experiment stops at time T_2 at the latest. The generalized hybrid censoring also has some drawbacks. For example, in case of the generalized Type I hybrid censoring, there is no guarantee that r failures occur before time T. In case of the generalized Type II hybrid censoring, there is a chance that no failures at all are observed up to the time T_2. To overcome these issues, the unified hybrid censoring, which combines the generalized Type I and Type II hybrid censoring schemes and guarantees that the experiment ends at most in time T_2 with at least k failures, can be used. For more details and additional information about other types of hybrid censoring (e.g., progressive hybrid censoring, adaptive progressive censoring), see Balakrishnan and Kundu (2013).

1.1 Type I Left-Censored Data

When analyzing real data, it is often necessary to work with more than one censoring level. In such case we talk about singly, doubly, or even multiply censored data. This thesis is focused on Type I multiply left-censored data. Standard statistical methods for analyzing such data are usually based on an assumption that the measured

variable has some probability distribution. The log-normal, the Weibull, the exponential, the generalized exponential, and the gamma distribution are usually used as model distributions (Fusek and Michálek, 2015b, 2019; Gupta and Kundu, 1999; Helsel, 2012; Mitra and Kundu, 2008; Schmoyeri et al., 1996; Singh et al., 2002). In order to estimate unknown parameters of the distribution, the maximum likelihood (ML) method (Barndorff-Nielsen and Cox, 1994; Lehmann and Casella, 1998), and the approach based on regression on order statistics (Helsel, 2012; Shoari et al., 2015) are often used. In some cases, it is also possible to convert left-censored data to right-censored, and use nonparametric methods for right-censored samples like the Kaplan-Meier estimator (Shumway et al., 2002). In this thesis, attention is paid to the censored Weibull distribution, which is very flexible and can be used for modelling of various engineering problems. With regards to the terminology that is usually used in applications of these methods, censoring levels will be called detection limits (DLs).

In general, it is necessary to be cautious when dealing with censored data. As pointed out by Helsel (2012), an unsuitable approach can influence the results significantly. When the censored values are ignored, a certain amount of information that can be obtained from the data is lost. Moreover, such an approach yields biased estimates of parameters in the model. For example, when censored values are omitted, the mean concentration of a chemical compound is going to be overestimated. A common practice to circumvent this issue is to replace censored values under the detection limits with a constant (e.g., 0, DL/2, $\mathrm{DL}/\sqrt{2}$, $\sqrt{\mathrm{DL}}$, DL), and to analyze data with traditional methods such that the substituted values are assumed to be observed (Guérin et al., 2011; Hoelzer et al., 2014; Munoz et al., 2015; Struciński et al., 2015; Wu et al., 2011). Sometimes, censored values below DLs are replaced by zero in the so-called lower bound scenario, and by the DLs, respectively, in the upper bound scenario (Inthavong et al., 2017; Pardo et al., 2014). Performance of methods based on replacement of censored observations for normally and log-normally distributed data has previously been examined in El-Shaarawi and Esterby (1992), and it was shown that it is not particularly good. Problems can be expected especially in case of skewed data with small sample sizes (Shoari et al., 2015). More information about how substituting values for censored observations can affect the results can be found in Helsel (2006). Other studies (Hewett and Ganser, 2007; Hornung and Reed, 1990) claim that the substitution-based method can perform reasonably well under certain circumstances. For example, when the number of censored values is small (e.g., $< 15\%$), the substitution method can give results similar to other statistical methods for censored data.

Chapter 2

Multiply Left-Censored Weibull Distribution

Let $X_1, \ldots, X_n$ be a random sample from the Weibull distribution with scale parameter $\lambda > 0$, shape parameter $\tau > 0$, cumulative distribution function (cdf)

$$F(x, \lambda, \tau) = \begin{cases} 1 - \exp\left[-\left(\frac{x}{\lambda}\right)^{\tau}\right] & \text{for } x \geq 0, \\ 0 & \text{for } x < 0, \end{cases} \tag{2.1}$$

and probability density function (pdf)

$$f(x, \lambda, \tau) = \begin{cases} \frac{\tau}{\lambda^{\tau}} x^{\tau-1} \exp\left[-\left(\frac{x}{\lambda}\right)^{\tau}\right] & \text{for } x \geq 0, \\ 0 & \text{for } x < 0. \end{cases} \tag{2.2}$$

The expected value μ, the variance σ^2 and the skewness γ are

$$\mu(\lambda, \tau) = \lambda \Gamma\left(1 + \frac{1}{\tau}\right), \tag{2.3}$$

$$\sigma^2(\lambda, \tau) = \lambda^2 \Gamma\left(1 + \frac{2}{\tau}\right) - \mu^2,$$

$$\gamma(\lambda, \tau) = \frac{\lambda^3 \Gamma\left(1 + \frac{3}{\tau}\right) - 3\mu\sigma^2 - \mu^3}{\sigma^3}, \tag{2.4}$$

where Γ is the gamma function.

Let $X_{(1)} \leq \cdots \leq X_{(n)}$ be the ordered sample of $X_1, \ldots, X_n$ which is Type I multiply left-censored with detection limits $d_1, \ldots, d_k$ and we put $d_0 = 0$. Moreover, N_i is the number of observations in the interval $(d_{i-1}, d_i]$, $i = 1, \ldots, k$, and N_0 is the number of uncensored observations $X_{(n-N_0+1)}, \ldots, X_{(n)}$. In order to simplify notation in some formulas, we replace $\log(x)$ by zero in case the natural logarithm is undefined.

Using results from Cohen (1991), the likelihood function of the Type I multiply left-

censored sample can be written as

$$L(\lambda, \tau, N_0, N_1, \ldots, N_k, X_{(n-N_0+1)}, \ldots, X_{(n)}) = \frac{n!}{N_1! \cdots N_k!} \prod_{i=1}^{k} \left[F(d_i, \lambda, \tau) - F(d_{i-1}, \lambda, \tau)\right]^{N_i} \prod_{i=n-N_0+1}^{n} f(X_{(i)}),$$

where we put $\prod_{i=n-N_0+1}^{n} f(X_{(i)}) = 1$ for $N_0 = 0$. The log-likelihood function is

$$l(\lambda, \tau, N_0, \ldots, N_k, X_{(n-N_0+1)}, \ldots, X_{(n)}) = \log\left(\frac{n!}{N_1! \cdots N_k!}\right) + \sum_{i=1}^{k} N_i \log\left[F(d_i, \lambda, \tau) - F(d_{i-1}, \lambda, \tau)\right] + \sum_{i=n-N_0+1}^{n} \log\left[f(X_{(i)})\right], \tag{2.5}$$

and we put $\sum_{i=n-N_0+1}^{n} \log\left[f(X_{(i)})\right] = 0$ for $N_0 = 0$. After the substitution of cdf (2.1) and pdf (2.2) into (2.5) we get the log-likelihood function

$$\begin{aligned} l(\lambda, \tau, N_0, \ldots, N_k, X_{(n-N_0+1)}, \ldots, X_{(n)}) &= \log\left(\frac{n!}{N_1! \cdots N_k!}\right) + \sum_{i=1}^{k} N_i \log\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\} \\ &\quad + N_0 \log\left(\frac{\tau}{\lambda^{\tau}}\right) + (\tau - 1) \sum_{i=n-N_0+1}^{n} \log\left(X_{(i)}\right) - \frac{1}{\lambda^{\tau}} \sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau}. \end{aligned} \tag{2.6}$$

The usual approach to estimation of parameters λ, τ is to derive and solve the likelihood equations

$$\frac{\partial l}{\partial \lambda} = \sum_{i=1}^{k} N_i \frac{\tau\left\{d_{i-1}^{\tau} \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - d_i^{\tau} \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}{\lambda^{\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}} - N_0 \frac{\tau}{\lambda} + \frac{\tau}{\lambda^{\tau+1}} \sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau} = 0,$$

$$\begin{aligned} \frac{\partial l}{\partial \tau} &= \sum_{i=1}^{k} N_i \frac{d_i^{\tau} \log\left(\frac{d_i}{\lambda}\right) \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right] - d_{i-1}^{\tau} \log\left(\frac{d_{i-1}}{\lambda}\right) \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]}{\lambda^{\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}} + N_0 \frac{1 - \tau \log(\lambda)}{\tau} \\ &\quad + \sum_{i=n-N_0+1}^{n} \log\left(X_{(i)}\right) + \frac{\log(\lambda)}{\lambda^{\tau}} \sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau} - \frac{1}{\lambda^{\tau}} \sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau} \log\left(X_{(i)}\right) = 0. \end{aligned}$$

In this case, the system of equations is very complicated and has to be solved numerically using, for example, the Newton-Raphson method. On that account, we decided to maximize the log-likelihood function (2.6) using the Nelder-Mead simplex algorithm (Lagarias et al., 1998) in Matlab (version R2022b), and in that way obtain the ML esti-

mates $\widehat{\lambda}$ and $\widehat{\tau}$. When using this type of algorithm, it is necessary to select initial values of the parameters that need to be estimated. Starting values of the algorithm were selected using the moment estimator of parameters of the Weibull distribution based on samples in which the censored values were replaced by constants lying between the detection limits.

In order to calculate variability of the ML estimates $\widehat{\lambda}$ and $\widehat{\tau}$, the Fisher information matrix (FIM) can be used. According to Barndorff-Nielsen and Cox (1994), the sample FIM can be defined (under certain regularity conditions) using formula

$$\widetilde{\boldsymbol{J}}_n(\lambda,\tau) = \begin{bmatrix} -\frac{\partial^2 l}{\partial\lambda^2} & -\frac{\partial^2 l}{\partial\lambda\partial\tau} \\ -\frac{\partial^2 l}{\partial\tau\partial\lambda} & -\frac{\partial^2 l}{\partial\tau^2} \end{bmatrix},$$

which can be rewritten as

$$\widetilde{\boldsymbol{J}}_n(\lambda,\tau) = n\widetilde{\boldsymbol{J}}(\lambda,\tau) = n \begin{bmatrix} \widetilde{J}_{11} & \widetilde{J}_{12} \\ \widetilde{J}_{21} & \widetilde{J}_{22} \end{bmatrix}, \tag{2.7}$$

where

$$\begin{aligned} n\widetilde{J}_{11} = & -\sum_{i=1}^{k} N_i \left\{ \frac{(d_i^\tau\lambda^\tau\tau^2 + d_i^\tau\lambda^\tau\tau - d_i^{2\tau}\tau^2)\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}} \right. \\ & - \frac{\left(d_{i-1}^\tau\lambda^\tau\tau^2 + d_{i-1}^\tau\lambda^\tau\tau - d_{i-1}^{2\tau}\tau^2\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}} \\ & \left. - \frac{\tau^2\left\{d_{i-1}^\tau\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - d_i^\tau\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2} \right\} - \frac{N_0\tau}{\lambda^2} + \frac{\tau^2+\tau}{\lambda^{\tau+2}}\sum_{i=n-N_0+1}^{n} X_{(i)}^\tau, \end{aligned}$$

$$\begin{aligned} n\widetilde{J}_{22} = & -\sum_{i=1}^{k} N_i \left\{ \frac{(d_i^\tau\lambda^\tau - d_i^{2\tau})\left[\log\left(\frac{d_i}{\lambda}\right)\right]^2\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}} \right. \\ & - \frac{\left(d_{i-1}^\tau\lambda^\tau - d_{i-1}^{2\tau}\right)\left[\log\left(\frac{d_{i-1}}{\lambda}\right)\right]^2\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}} \\ & \left. - \frac{\left\{d_{i-1}^\tau\log\left(\frac{d_{i-1}}{\lambda}\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - d_i^\tau\log\left(\frac{d_i}{\lambda}\right)\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2} \right\} \\ & + \frac{N_0}{\tau^2} + \frac{[\log(\lambda)]^2}{\lambda^\tau}\sum_{i=n-N_0+1}^{n} X_{(i)}^\tau - \frac{2\log(\lambda)}{\lambda^\tau}\sum_{i=n-N_0+1}^{n} X_{(i)}^\tau\log\left(X_{(i)}\right) \end{aligned}$$

$$+\frac{1}{\lambda^{\tau}}\sum_{i=n-N_0+1}^{n}X_{(i)}^{\tau}\left[\log\left(X_{(i)}\right)\right]^2,$$

$$n\widetilde{J}_{12}=n\widetilde{J}_{21}=-\sum_{i=1}^{k}N_i\left\{\frac{\left[d_i^{2\tau}\tau\log\left(\frac{d_i}{\lambda}\right)-d_i^{\tau}\lambda^{\tau}\tau\log\left(\frac{d_i}{\lambda}\right)-d_i^{\tau}\lambda^{\tau}\right]\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}\right.$$

$$-\frac{\left[d_{i-1}^{2\tau}\tau\log\left(\frac{d_{i-1}}{\lambda}\right)-d_{i-1}^{\tau}\lambda^{\tau}\tau\log\left(\frac{d_{i-1}}{\lambda}\right)-d_{i-1}^{\tau}\lambda^{\tau}\right]\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}$$

$$+\frac{\tau\left\{d_{i-1}^{\tau}\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-d_i^{\tau}\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}$$

$$\left.\times\frac{\left\{d_{i-1}^{\tau}\log\left(\frac{d_{i-1}}{\lambda}\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-d_i^{\tau}\log\left(\frac{d_i}{\lambda}\right)\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}\right\}$$

$$+\frac{N_0}{\lambda}+\frac{\tau\log(\lambda)-1}{\lambda^{\tau+1}}\sum_{i=n-N_0+1}^{n}X_{(i)}^{\tau}-\frac{\tau}{\lambda^{\tau+1}}\sum_{i=n-N_0+1}^{n}X_{(i)}^{\tau}\log\left(X_{(i)}\right).$$

The sample FIM $\widetilde{\boldsymbol{J}}_n$ is an unbiased estimator of the expected FIM $\boldsymbol{J}_n$ and $\widetilde{\boldsymbol{J}}_n(\lambda,\tau)\to\boldsymbol{J}_n(\lambda,\tau)$ in probability for $n\to\infty$. On that account, in many applications when the exact determination of the expected FIM is complicated, the sample FIM is used instead (Aboueissa and Stoline, 2006; Fahrmeier and Tutz, 2001). One major disadvantage of this approach is the rather extensive variability of the sample FIM. Many authors prefer another approach like bootstrap or Bayesian methods (Joarder et al., 2011) for description of variability of parameters estimates. The expected FIM can be used for statistical inference and more precise description of the asymptotic variability of obtained estimates. On that account, our attention will now be paid to determination of the expected FIM. Similar problems were solved, for example, in Fusek and Michálek (2015b) for exponential distribution, in Mitra and Kundu (2008) for GE distribution or in Zheng (2002) and Gupta and Kundu (2006) using the hazard function according to Efron and Johnstone (1990).

The expected FIM can be calculated using formula

$$\boldsymbol{J}_n(\lambda,\tau)=\mathrm{E}\widetilde{\boldsymbol{J}}_n(\lambda,\tau),$$

which can be rewritten as

$$\boldsymbol{J}_n(\lambda,\tau)=n\boldsymbol{J}(\lambda,\tau)=n\begin{bmatrix}J_{11}&J_{12}\\J_{21}&J_{22}\end{bmatrix},\tag{2.8}$$

where

$$J_{11} = \sum_{i=1}^{k} \frac{\tau^2 \left\{ d_{i-1}^{\tau} \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - d_i^{\tau} \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}^2}{\lambda^{2\tau+2} \left\{ \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}}$$

$$- \frac{(d_k^{\tau}\lambda^{\tau}\tau^2 + d_k^{\tau}\lambda^{\tau}\tau - d_k^{2\tau}\tau^2) \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right]}{\lambda^{2\tau+2}} - \frac{\tau}{\lambda^2} \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right]$$

$$+ \frac{\tau^2 + \tau}{\lambda^2} \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2}$$

$$\times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0},$$

$$J_{22} = \sum_{i=1}^{k} \frac{\left\{ d_{i-1}^{\tau} \log\left(\frac{d_{i-1}}{\lambda}\right) \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - d_{i-1}^{\tau} \log\left(\frac{d_i}{\lambda}\right) \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}^2}{\lambda^{2\tau} \left\{ \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}}$$

$$- \frac{(d_k^{\tau}\lambda^{\tau} - d_k^{2\tau}) \left[\log\left(\frac{d_k}{\lambda}\right) \right]^2 \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right]}{\lambda^{2\tau}} + \frac{1}{\tau^2} \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right]$$

$$+ [\log(\lambda)]^2 \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2}$$

$$\times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0}$$

$$- \frac{2\log(\lambda)}{\tau} \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2}$$

$$\times \left[\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right) + 1 - \gamma_e \right]$$

$$\times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0}$$

$$+ \frac{1}{\tau^2} \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2}$$

$$\times \left\{ \left[\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right) \right]^2 + 2\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right) (1-\gamma_e) \right.$$

$$\left. + \frac{\pi^2}{6} - 2\gamma_e + \gamma_e^2 \right\} \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0},$$

$$
\begin{aligned}
J_{12} = J_{21} = &- \sum_{i=1}^{k} \frac{\tau \left\{ d_{i-1}^{\tau} \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - d_i^{\tau} \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}}{\lambda^{2\tau+1} \left\{ \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\}} \\
&\times \left\{ d_{i-1}^{\tau} \log\left(\frac{d_{i-1}}{\lambda}\right) \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau} \right] - d_i^{\tau} \log\left(\frac{d_i}{\lambda}\right) \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau} \right] \right\} \\
&+ \frac{\left[d_k^{\tau} \tau \lambda^{\tau} \log\left(\frac{d_k}{\lambda}\right) + d_k^{\tau} \lambda^{\tau} - d_k^{2\tau} \tau \log\left(\frac{d_k}{\lambda}\right) \right] \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right]}{\lambda^{2\tau+1}} + \frac{1}{\lambda} \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \\
&+ \frac{\tau \log(\lambda) - 1}{\lambda} \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2} \\
&\times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0} \\
&- \frac{1}{\lambda} \sum_{n_0=0}^{n} \sum_{i=n-n_0+1}^{n} \binom{n-1}{i-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} (n-i+j+1)^{-2} \\
&\times \left[\log\left(\frac{\lambda^{\tau}}{n-i+j+1} \right) + 1 - \gamma_e \right] \\
&\times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau} \right] \left\{ 1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau} \right] \right\}^{n-n_0}.
\end{aligned}
$$

Details of the derivation can be found in Appendix A. Considering the asymptotic properties of ML estimator $\widehat{\lambda}$ ($\widehat{\tau}$ respectively), according to Lehmann and Casella (1998), $\sqrt{n}(\widehat{\lambda} - \lambda)$ ($\sqrt{n}(\widehat{\tau} - \tau)$ respectively) has asymptotically normal distribution $\mathrm{N}(0, J^{11})$ ($\mathrm{N}(0, J^{22})$ respectively), where J^{11}, J^{22} are diagonal elements of the variance matrix

$$
\boldsymbol{J}^{-1}(\lambda, \tau) = \begin{bmatrix} J^{11} & J^{12} \\ J^{21} & J^{22} \end{bmatrix}.
$$

A similar notation can be used in case of the sample FIM, i.e.

$$
\widetilde{\boldsymbol{J}}^{-1}(\lambda, \tau) = \begin{bmatrix} \widetilde{J}^{11} & \widetilde{J}^{12} \\ \widetilde{J}^{21} & \widetilde{J}^{22} \end{bmatrix}.
$$

The properties of estimators $\widehat{\lambda}$, $\widehat{\tau}$ considering various sample sizes n, various number of detection limits k and various censoring schemes will be analyzed using simulations in the next section.

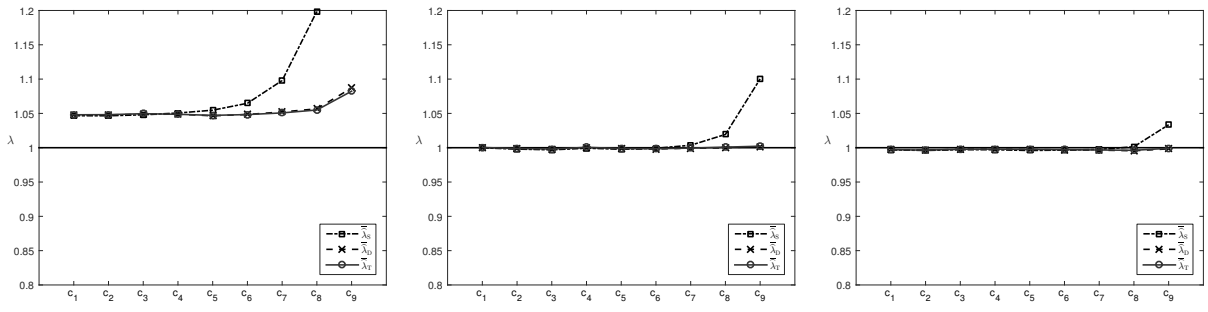
2.1 Estimators Behavior Based on Simulations

In order to analyze the estimates of parameters and parametric functions, 20,000 Type I singly, doubly and triply left-censored random samples with size $n = 10, 20, 30, 50, 100$

Table 2.1: Quantiles for determination of detection limits considering single, double and triple censoring and various censoring schemes.

	Single	Double		Triple		
Censoring	q_1	q_1	q_2	q_1	q_2	q_3
c_1	0.10	0.05	0.10	0.03	0.07	0.10
c_2	0.20	0.10	0.20	0.07	0.13	0.20
c_3	0.30	0.15	0.30	0.10	0.20	0.30
c_4	0.40	0.20	0.40	0.13	0.27	0.40
c_5	0.50	0.25	0.50	0.17	0.33	0.50
c_6	0.60	0.30	0.60	0.20	0.40	0.60
c_7	0.70	0.35	0.70	0.23	0.47	0.70
c_8	0.80	0.40	0.80	0.27	0.53	0.80
c_9	0.90	0.45	0.90	0.30	0.60	0.90

from the Weibull distribution were generated. Since λ is the scale parameter, and the ML estimators are scale invariant, we take $\lambda = 1$ without the loss of generality. In order to describe various shapes of the Weibull distribution, we take $\tau = 0.5, 1.5, 3$, which corresponds to skewnesses $\gamma = 6.62, 1.07, 0.17$. Limits of detection d_i, $i = 1, \ldots, k$, $k = 1, 2, 3$, were selected as quantiles of the Weibull distribution using equations $q_i = F(d_i, \lambda, \tau)$, where q_i are given in Table 2.1. The individual censoring schemes are denoted as $c_1, \ldots, c_9$, and correspond to various quantiles which determine detection limits for $k = 1, 2, 3$. For example, q_1 given in column "Double" in Table 2.1 denotes the proportion of doubly censored values, and describes the given censoring scheme. The censoring scheme c_1 represents the smallest proportion (10%) of censored data, and the censoring scheme c_9 represents the largest proportion (90%) of censored data.



(a) $\tau = 0.5$ (b) $\tau = 1.5$ (c) $\tau = 3$

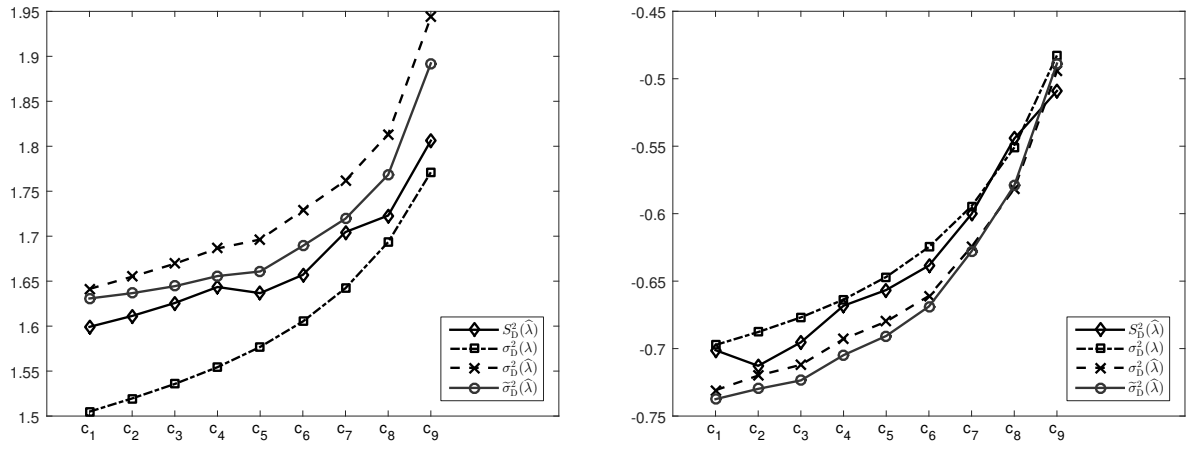
Figure 2.1: The average ML estimates of parameter λ considering various values of τ and single (index S), double (index D), triple (index T) censoring; sample size $n = 30$.

The ML estimates of parameters λ, τ from 20,000 samples were calculated and their

Table 2.2: The average ML estimates $\overline{\widehat{\lambda}}$, $\overline{\widehat{\tau}}$ and their average MSE (in the parenthesis) considering single (S), double (D) and triple (T) censoring and sample size n.

	$\lambda = 1$								
	$n = 10$			$n = 30$			$n = 100$		
Censoring	S	D	T	S	D	T	S	D	T
c_1	1.00 (0.050)	1.00 (0.050)	1.00 (0.049)	1.00 (0.017)	1.00 (0.017)	1.00 (0.017)	1.00 (0.005)	1.00 (0.005)	1.00 (0.005)
c_2	0.99 (0.051)	1.00 (0.050)	1.00 (0.050)	1.00 (0.017)	1.00 (0.016)	1.00 (0.016)	1.00 (0.005)	1.00 (0.005)	1.00 (0.005)
c_3	0.99 (0.052)	1.00 (0.050)	1.00 (0.049)	1.00 (0.017)	1.00 (0.017)	1.00 (0.016)	1.00 (0.005)	1.00 (0.005)	1.00 (0.005)
c_4	0.99 (0.054)	0.99 (0.050)	1.00 (0.049)	1.00 (0.019)	1.00 (0.017)	1.00 (0.017)	1.00 (0.005)	1.00 (0.005)	1.00 (0.005)
c_5	0.99 (0.058)	0.99 (0.051)	1.00 (0.050)	1.00 (0.020)	1.00 (0.017)	1.00 (0.017)	1.00 (0.006)	1.00 (0.005)	1.00 (0.005)
c_6	1.01 (0.063)	1.00 (0.051)	1.00 (0.049)	1.00 (0.023)	1.00 (0.018)	1.00 (0.017)	1.00 (0.007)	1.00 (0.005)	1.00 (0.005)
c_7	1.03 (0.071)	1.00 (0.053)	1.00 (0.049)	1.00 (0.029)	1.00 (0.018)	1.00 (0.017)	1.00 (0.009)	1.00 (0.005)	1.00 (0.005)
c_8	1.11 (0.095)	1.02 (0.055)	1.02 (0.050)	1.02 (0.046)	1.00 (0.019)	1.00 (0.018)	1.00 (0.014)	1.00 (0.006)	1.00 (0.005)
c_9	1.33 (0.214)	1.07 (0.066)	1.07 (0.055)	1.10 (0.112)	1.00 (0.020)	1.00 (0.018)	1.02 (0.038)	1.00 (0.006)	1.00 (0.005)
	$\tau = 1.5$								
	$n = 10$			$n = 30$			$n = 100$		
	S	D	T	S	D	T	S	D	T
c_1	1.75 (0.355)	1.75 (0.350)	1.75 (0.349)	1.57 (0.067)	1.57 (0.065)	1.57 (0.064)	1.52 (0.016)	1.52 (0.016)	1.52 (0.016)
c_2	1.76 (0.384)	1.75 (0.359)	1.75 (0.354)	1.57 (0.071)	1.57 (0.066)	1.57 (0.064)	1.52 (0.018)	1.52 (0.016)	1.52 (0.016)
c_3	1.78 (0.446)	1.76 (0.382)	1.76 (0.371)	1.58 (0.081)	1.57 (0.069)	1.57 (0.066)	1.52 (0.019)	1.52 (0.016)	1.52 (0.016)
c_4	1.82 (0.607)	1.77 (0.395)	1.76 (0.369)	1.59 (0.096)	1.58 (0.073)	1.57 (0.068)	1.52 (0.023)	1.52 (0.018)	1.52 (0.016)
c_5	1.96 (58.58)	1.77 (0.408)	1.76 (0.370)	1.60 (0.119)	1.58 (0.076)	1.57 (0.069)	1.53 (0.028)	1.52 (0.019)	1.52 (0.017)
c_6	2.29 (252.0)	1.78 (0.442)	1.76 (0.377)	1.63 (0.162)	1.58 (0.083)	1.58 (0.074)	1.54 (0.036)	1.52 (0.020)	1.52 (0.018)
c_7	2.76 (161.9)	1.77 (0.442)	1.75 (0.365)	1.67 (0.273)	1.59 (0.091)	1.58 (0.076)	1.54 (0.051)	1.52 (0.022)	1.52 (0.018)
c_8	3.85 (259.8)	1.74 (0.477)	1.71 (0.362)	1.84 (4.263)	1.59 (0.097)	1.58 (0.080)	1.57 (0.089)	1.52 (0.024)	1.52 (0.020)
c_9	6.59 (558.9)	1.62 (0.418)	1.60 (0.237)	2.84 (80.11)	1.58 (0.095)	1.57 (0.076)	1.66 (0.278)	1.53 (0.026)	1.53 (0.021)

mean values $\overline{\widehat{\lambda}}$, $\overline{\widehat{\tau}}$ were determined. It was found out (see Figure 2.1) that the estimates of parameter λ have lower bias for higher values of parameter τ (i.e. for a lower skewness of the sample distribution) considering various censoring schemes. The estimates of parameter τ are similar bias-wise for various values of τ (not shown in figures). Table 2.2 shows the average ML estimates $\overline{\widehat{\lambda}}$, $\overline{\widehat{\tau}}$ and their mean squared errors (MSE). It can be seen that the ML estimate $\overline{\widehat{\lambda}}$ is rather satisfying until the censoring scheme c_7 even when the sample size is small ($n = 10$). For $n > 10$, the bias of $\overline{\widehat{\lambda}}$ is very small, and from the practical point of view negligible for the censoring scheme c_7 and lower. The effect of multiplicity of censoring on the estimation of parameter λ is noticeable only for higher detection limits depending on the sample size. For $n \geq 30$, the differences among the single, double and triple censoring are almost negligible until scheme c_8 when, in accordance with expectations, the highest bias of the estimate is present in case of single censoring. The ML estimate $\overline{\widehat{\tau}}$ is significantly biased even when the censoring is low, and sample size $n = 100$.



(a) $\tau = 0.5$ (b) $\tau = 1.5$

Figure 2.2: Comparison of the estimates of variance $S^2(\widehat{\lambda})$, $\sigma^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\lambda})$ and the asymptotic variance $\sigma^2(\lambda)$ considering double censoring and sample size $n = 30$; logarithmic scale on the y-axis.

Variances of the ML estimators $\widehat{\lambda}$, $\widehat{\tau}$ of parameters λ, τ were estimated by means of sample variances $s^2(\widehat{\lambda})$, $s^2(\widehat{\tau})$ from the simulated values. Furthermore, the asymptotic variances $\sigma^2(\lambda) = J^{11}(\lambda, \tau)$, $\sigma^2(\tau) = J^{22}(\lambda, \tau)$ were compared with their estimates $\sigma^2(\widehat{\lambda}) = J^{11}(\widehat{\lambda}, \widehat{\tau})$, $\sigma^2(\widehat{\tau}) = J^{22}(\widehat{\lambda}, \widehat{\tau})$ based on the expected FIM (2.8) and $\widetilde{\sigma}^2(\widehat{\lambda}) = \widetilde{J}^{11}(\widehat{\lambda}, \widehat{\tau})$, $\widetilde{\sigma}^2(\widehat{\tau}) = \widetilde{J}^{22}(\widehat{\lambda}, \widehat{\tau})$ based on the sample FIM (2.7) using simulations. The estimates $\sigma^2(\widehat{\lambda})$, $\sigma^2(\widehat{\tau})$ and $\widetilde{\sigma}^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\tau})$ were averaged over 20,000 repetitions, and from now on when speaking about the estimates $\sigma^2(\widehat{\lambda})$, $\sigma^2(\widehat{\tau})$, $\widetilde{\sigma}^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\tau})$ of the asymptotic variances $\sigma^2(\lambda)$, $\sigma^2(\tau)$, we have in mind the estimates averaged over 20,000 repetitions, i.e. $\sigma^2(\widehat{\lambda}) = \overline{J^{11}(\widehat{\lambda}, \widehat{\tau})}$, $\sigma^2(\widehat{\tau}) = \overline{J^{22}(\widehat{\lambda}, \widehat{\tau})}$, $\widetilde{\sigma}^2(\widehat{\lambda}) = \overline{\widetilde{J}^{11}(\widehat{\lambda}, \widehat{\tau})}$, $\widetilde{\sigma}^2(\widehat{\tau}) = \overline{\widetilde{J}^{22}(\widehat{\lambda}, \widehat{\tau})}$. These

Table 2.3: Comparison of the estimates of variance $S^2(\widehat{\lambda})$, $\sigma^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\lambda})$ and the asymptotic variance $\sigma^2(\lambda)$ considering double censoring and sample size n.

	$\tau = 0.5$							
	$n = 10$				$n = 100$			
Censoring	$S^2(\widehat{\lambda})$	$\sigma^2(\lambda)$	$\sigma^2(\widehat{\lambda})$	$\widetilde{\sigma}^2(\widehat{\lambda})$	$S^2(\widehat{\lambda})$	$\sigma^2(\lambda)$	$\sigma^2(\widehat{\lambda})$	$\widetilde{\sigma}^2(\widehat{\lambda})$
c_1	6.270	4.602	6.804	6.623	4.494	4.468	4.657	4.642
c_2	6.159	4.756	6.880	6.561	4.667	4.507	4.706	4.679
c_3	6.083	4.915	6.929	6.481	4.599	4.556	4.749	4.712
c_4	5.992	5.086	7.128	6.548	4.737	4.620	4.807	4.761
c_5	6.037	5.279	7.298	6.586	4.826	4.707	4.937	4.883
c_6	6.328	5.504	7.829	6.955	4.863	4.827	4.986	4.928
c_7	6.303	5.780	8.204	7.178	5.109	4.998	5.165	5.101
c_8	6.878	6.137	9.493	8.192	5.397	5.249	5.431	5.362
c_9	8.764	6.600	13.072	11.098	5.789	5.653	5.859	5.775
	$\tau = 1.5$							
	$n = 10$				$n = 100$			
	$S^2(\widehat{\lambda})$	$\sigma^2(\lambda)$	$\sigma^2(\widehat{\lambda})$	$\widetilde{\sigma}^2(\widehat{\lambda})$	$S^2(\widehat{\lambda})$	$\sigma^2(\lambda)$	$\sigma^2(\widehat{\lambda})$	$\widetilde{\sigma}^2(\widehat{\lambda})$
c_1	0.495	0.504	0.456	0.447	0.500	0.496	0.490	0.489
c_2	0.504	0.512	0.463	0.450	0.498	0.499	0.495	0.493
c_3	0.498	0.521	0.471	0.455	0.496	0.504	0.499	0.497
c_4	0.503	0.529	0.476	0.460	0.505	0.510	0.506	0.504
c_5	0.509	0.539	0.488	0.472	0.519	0.519	0.514	0.512
c_6	0.511	0.551	0.504	0.491	0.532	0.531	0.526	0.525
c_7	0.526	0.566	0.524	0.514	0.548	0.549	0.543	0.543
c_8	0.547	0.589	0.581	0.577	0.585	0.575	0.570	0.571
c_9	0.606	0.627	0.725	0.723	0.616	0.618	0.610	0.612

estimates together with the corresponding empirical sample variances $S^2(\widehat{\lambda}) = ns^2(\widehat{\lambda})$, $S^2(\widehat{\tau}) = ns^2(\widehat{\tau})$ were compared with the asymptotic variances considering various sample sizes n. Due to a rather large number of samples, the estimators $S^2(\widehat{\lambda})$, $S^2(\widehat{\tau})$ allow us to assess the bias of estimators $\sigma^2(\widehat{\lambda})$, $\sigma^2(\widehat{\tau})$, $\widetilde{\sigma}^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\tau})$, and the bias of asymptotic variances $\sigma^2(\lambda)$, $\sigma^2(\tau)$ from the true (simulation-based) variances $S^2(\widehat{\lambda})$, $S^2(\widehat{\tau})$ of the estimates.

Figure 2.2 shows that behavior of estimates $\sigma^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\lambda})$ is significantly influenced by values of parameter τ. In case $\tau < 1$, i.e. the skewness of the sample distribution is high (> 2), both estimates are higher than the asymptotic variance $\sigma^2(\lambda)$. When $\tau > 1$, i.e. the skewness of the sample distribution is low (< 2), both estimates are lower than the asymptotic variance $\sigma^2(\lambda)$. The comparison of above mentioned characteristics of variance (see Table 2.3 in case of double censoring) shows that the anticipated bias of estimator $\sigma^2(\widehat{\lambda})$ is substantial for small sample sizes. Furthermore, the estimator $S^2(\widehat{\lambda})$ is of lower

Table 2.4: The asymptotic variance $\sigma^2(\lambda)$ considering single (S), double (D) and triple (T) censoring and sample size n.

	$\tau = 0.5$								
	$n = 10$			$n = 30$			$n = 100$		
Censoring	S	D	T	S	D	T	S	D	T
c_1	4.625	4.602	4.750	4.527	4.504	4.647	4.491	4.468	4.609
c_2	4.832	4.756	4.874	4.643	4.570	4.682	4.579	4.507	4.616
c_3	5.088	4.915	4.937	4.814	4.645	4.665	4.723	4.556	4.575
c_4	5.437	5.086	5.001	5.081	4.732	4.647	4.969	4.620	4.536
c_5	5.963	5.279	5.103	5.532	4.840	4.665	5.404	4.707	4.532
c_6	6.854	5.504	5.237	6.362	4.979	4.711	6.231	4.827	4.559
c_7	8.626	5.780	5.434	8.103	5.166	4.821	7.997	4.998	4.652
c_8	13.234	6.137	5.696	12.667	5.438	5.018	12.653	5.249	4.835
c_9	36.457	6.600	5.976	33.361	5.877	5.338	32.729	5.653	5.138
	$\tau = 1.5$								
	$n = 10$			$n = 30$			$n = 100$		
	S	D	T	S	D	T	S	D	T
c_1	0.506	0.504	0.520	0.500	0.498	0.514	0.498	0.496	0.511
c_2	0.520	0.512	0.525	0.511	0.503	0.515	0.507	0.499	0.511
c_3	0.538	0.521	0.523	0.526	0.508	0.510	0.522	0.504	0.506
c_4	0.563	0.529	0.521	0.552	0.515	0.506	0.548	0.510	0.501
c_5	0.603	0.539	0.523	0.596	0.524	0.505	0.595	0.519	0.500
c_6	0.670	0.551	0.527	0.678	0.535	0.507	0.684	0.531	0.502
c_7	0.799	0.566	0.536	0.847	0.552	0.516	0.872	0.549	0.511
c_8	1.096	0.589	0.552	1.265	0.576	0.534	1.360	0.575	0.530
c_9	2.093	0.627	0.576	2.786	0.617	0.563	3.311	0.618	0.562

Table 2.5: Comparison of the estimates of variance $S^2(\widehat{\tau})$, $\sigma^2(\widehat{\tau})$, $\widetilde{\sigma}^2(\widehat{\tau})$ and the asymptotic variance $\sigma^2(\tau)$ considering double censoring and sample size n; $\tau = 1.5$.

	$n = 10$				$n = 100$			
Censoring	$S^2(\widehat{\tau})$	$\sigma^2(\tau)$	$\sigma^2(\widehat{\tau})$	$\widetilde{\sigma}^2(\widehat{\tau})$	$S^2(\widehat{\tau})$	$\sigma^2(\tau)$	$\sigma^2(\widehat{\tau})$	$\widetilde{\sigma}^2(\widehat{\tau})$
c_1	2.884	1.420	2.084	2.199	1.524	1.419	1.467	1.476
c_2	2.951	1.462	2.152	2.310	1.574	1.478	1.524	1.539
c_3	3.144	1.511	2.240	2.452	1.600	1.549	1.598	1.617
c_4	3.237	1.572	2.347	2.627	1.725	1.632	1.685	1.710
c_5	3.359	1.651	2.482	2.828	1.840	1.732	1.790	1.821
c_6	3.632	1.757	2.711	3.105	1.949	1.848	1.913	1.950
c_7	3.667	1.900	2.920	3.297	2.114	1.983	2.057	2.098
c_8	4.213	2.108	3.166	3.571	2.302	2.139	2.224	2.265
c_9	4.030	2.456	3.186	3.611	2.554	2.338	2.462	2.488

(higher respectively) values than asymptotic variance $\sigma^2(\lambda)$ for $\tau > 1$ ($\tau < 1$ respectively). All estimators of the variance almost coincide for $\tau > 1$ and the sample size $n \geq 100$. In addition, the asymptotic variance $\sigma^2(\lambda)$ (obtained from the expected FIM) was analyzed considering various sample sizes and censoring schemes (see Table 2.4). With the exception of schemes c_1–c_3, variability of the estimators is, as expected, the lowest for triple censoring for an arbitrary sample size.

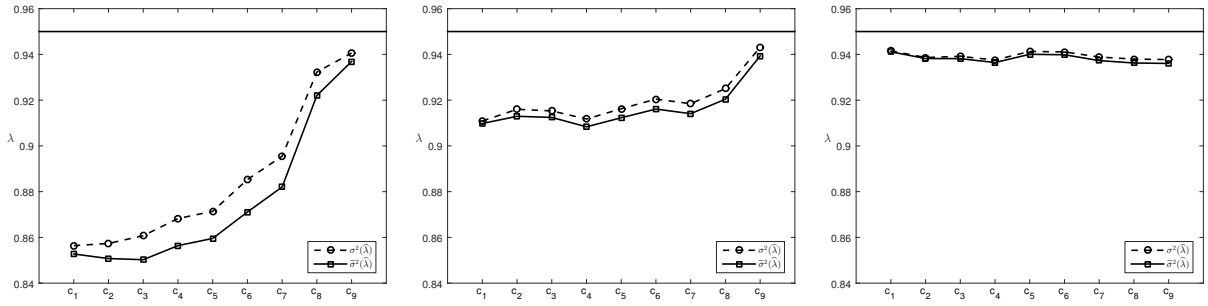
In case of $\widehat{\tau}$, behavior of the variance estimators is similar for various values of τ. The comparison of the characteristics of variance (see Table 2.5 in case of double censoring) shows that the anticipated bias of estimator $\sigma^2(\widehat{\tau})$ is substantial for small sample sizes. Moreover, the estimator $S^2(\widehat{\tau})$ is of higher values than asymptotic variance $\sigma^2(\tau)$ for all sample sizes and censoring schemes. Furthermore, the asymptotic variance $\sigma^2(\tau)$ (obtained from the expected FIM) was analyzed considering various sample sizes and censoring schemes (see Table 2.6). With the exception of schemes c_1–c_2, the variability of the estimators is, as expected, the lowest for triple censoring for arbitrary sample size.

Finally, using the variance estimators $\sigma^2(\widehat{\lambda})$, $\sigma^2(\widehat{\tau})$, $\widetilde{\sigma}^2(\widehat{\lambda})$, $\widetilde{\sigma}^2(\widehat{\tau})$, the lower and the upper confidence limits of the estimate of parameters λ and τ can be obtained. The coverage probability of 95% confidence interval, computed as the proportion of the number of times, out of 20,000 replications, the estimated 95% confidence interval contains the true parameter value, is calculated.

In general, the coverage probability of λ is better with higher values of τ, because the estimator of parameter λ performs better for higher values of parameter τ. When $\tau < 1$, i.e. the skewness of the sample distribution is high (> 2), the estimator based on expected FIM (2.8) performs better than the estimator based on sample FIM (2.7) for all censoring schemes, especially for small sample sizes (see Figure 2.3 in case of double censoring). For $\tau > 1$, coverage probabilities of both estimators almost coincide. The results showed that

Table 2.6: The asymptotic variance $\sigma^2(\tau)$ considering single (S), double (D) and triple (T) censoring and sample size n; $\tau = 1.5$.

	$n = 10$			$n = 30$			$n = 100$		
Censoring	S	D	T	S	D	T	S	D	T
c_1	1.476	1.420	1.513	1.476	1.420	1.512	1.474	1.419	1.511
c_2	1.602	1.462	1.500	1.616	1.474	1.513	1.621	1.478	1.517
c_3	1.770	1.510	1.473	1.808	1.538	1.499	1.823	1.548	1.509
c_4	2.004	1.572	1.478	2.078	1.615	1.514	2.109	1.632	1.530
c_5	2.341	1.651	1.532	2.469	1.707	1.576	2.525	1.731	1.596
c_6	2.848	1.756	1.629	3.067	1.818	1.671	3.171	1.848	1.693
c_7	3.675	1.900	1.787	4.068	1.951	1.813	4.276	1.983	1.834
c_8	5.202	2.108	2.022	6.017	2.116	2.001	6.520	2.139	2.013
c_9	8.804	2.456	2.328	11.216	2.357	2.217	13.138	2.338	2.191



(a) $n = 10$ (b) $n = 30$ (c) $n = 100$

Figure 2.3: Coverage probabilities for parameter $\widehat{\lambda}$ considering various estimates of variance and double censoring.

the coverage probabilities of λ are very similar considering double and triple censoring for all sample sizes and various values of τ (see Table 2.7 for $\tau = 1.5$). The coverage probability gets higher with a higher censoring scheme for small sample sizes ($n < 50$). In case of single censoring, the behavior is similar until censoring scheme c_7.

The coverage probability of τ is similar considering double and triple censoring for all values of τ (see Table 2.8 for $\tau = 1.5$), because all the estimates of τ are similar bias-wise. The coverage probabilities are quite close to the prescribed significance level for both estimators (based on the expected and the sample FIM) and practically coincide for $n > 50$.

Table 2.7: Coverage probabilities for parameter $\widehat{\lambda}$ based on expected FIM (2.8) considering single (S), double (D) and triple (T) censoring and sample size n; $\tau = 1.5$. The average lower (LCL) and upper (UCL) confidence limits are included.

	$n = 10$								
	S			D			T		
Censoring	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	0.593	1.398	0.888	0.596	1.398	0.887	0.592	1.403	0.890
c_2	0.588	1.401	0.887	0.593	1.399	0.888	0.588	1.405	0.890
c_3	0.580	1.406	0.896	0.589	1.402	0.894	0.588	1.406	0.898
c_4	0.572	1.412	0.901	0.585	1.403	0.895	0.587	1.404	0.897
c_5	0.562	1.428	0.909	0.580	1.408	0.898	0.584	1.407	0.901
c_6	0.555	1.460	0.930	0.579	1.420	0.907	0.584	1.415	0.909
c_7	0.549	1.515	0.912	0.572	1.432	0.918	0.581	1.425	0.923
c_8	0.581	1.643	0.782	0.566	1.479	0.943	0.580	1.467	0.951
c_9	0.729	1.926	0.599	0.554	1.588	0.942	0.576	1.565	0.955
	$n = 30$								
	S			D			T		
	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	0.754	1.245	0.930	0.755	1.245	0.931	0.752	1.249	0.935
c_2	0.750	1.246	0.934	0.752	1.245	0.933	0.750	1.248	0.937
c_3	0.745	1.248	0.935	0.750	1.245	0.932	0.750	1.246	0.934
c_4	0.741	1.257	0.936	0.751	1.250	0.933	0.753	1.249	0.934
c_5	0.730	1.266	0.939	0.747	1.250	0.933	0.751	1.246	0.933
c_6	0.714	1.284	0.947	0.745	1.252	0.933	0.751	1.246	0.932
c_7	0.685	1.322	0.940	0.741	1.257	0.935	0.749	1.250	0.934
c_8	0.635	1.404	0.897	0.736	1.264	0.934	0.746	1.255	0.940
c_9	0.570	1.631	0.791	0.725	1.278	0.949	0.739	1.266	0.947
	$n = 100$								
	S			D			T		
	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	0.863	1.137	0.944	0.863	1.137	0.944	0.861	1.139	0.947
c_2	0.861	1.138	0.945	0.862	1.137	0.945	0.861	1.139	0.948
c_3	0.859	1.140	0.947	0.862	1.137	0.945	0.861	1.138	0.947
c_4	0.856	1.143	0.948	0.861	1.139	0.946	0.862	1.137	0.946
c_5	0.850	1.149	0.947	0.860	1.140	0.943	0.862	1.137	0.942
c_6	0.840	1.161	0.949	0.858	1.141	0.944	0.862	1.138	0.943
c_7	0.819	1.182	0.948	0.856	1.143	0.946	0.860	1.139	0.944
c_8	0.777	1.230	0.936	0.851	1.146	0.944	0.858	1.141	0.946
c_9	0.671	1.371	0.899	0.846	1.151	0.944	0.854	1.145	0.949

Table 2.8: Coverage probabilities for parameter $\widehat{\tau}$ based on expected FIM (2.8) considering single (S), double (D) and triple (T) censoring and sample size n; $\tau = 1.5$. The average lower (LCL) and upper (UCL) confidence limits are included.

	$n = 10$								
	S			D			T		
Censoring	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	0.876	2.620	0.942	0.889	2.605	0.942	0.861	2.637	0.949
c_2	0.848	2.673	0.944	0.881	2.626	0.942	0.855	2.648	0.953
c_3	0.813	2.751	0.937	0.870	2.650	0.939	0.855	2.660	0.957
c_4	0.764	2.882	0.937	0.855	2.679	0.943	0.851	2.666	0.962
c_5	0.688	3.233	0.933	0.831	2.706	0.943	0.835	2.676	0.960
c_6	0.564	4.018	0.935	0.804	2.756	0.943	0.813	2.703	0.961
c_7	0.384	5.137	0.937	0.760	2.789	0.950	0.772	2.719	0.967
c_8	0.081	7.616	0.945	0.698	2.776	0.955	0.714	2.705	0.968
c_9	0.000	13.689	0.967	0.605	2.642	0.961	0.632	2.577	0.976
	$n = 30$								
	S			D			T		
	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	1.119	2.029	0.946	1.126	2.020	0.946	1.111	2.036	0.954
c_2	1.097	2.048	0.946	1.117	2.025	0.947	1.107	2.033	0.957
c_3	1.075	2.085	0.946	1.109	2.038	0.947	1.110	2.036	0.954
c_4	1.044	2.131	0.941	1.099	2.052	0.943	1.108	2.038	0.953
c_5	1.003	2.200	0.944	1.087	2.069	0.948	1.100	2.049	0.953
c_6	0.949	2.308	0.944	1.075	2.092	0.946	1.090	2.067	0.952
c_7	0.864	2.483	0.938	1.058	2.114	0.945	1.071	2.085	0.954
c_8	0.724	2.959	0.934	1.038	2.144	0.947	1.051	2.115	0.960
c_9	0.391	5.290	0.953	0.996	2.166	0.958	1.014	2.121	0.971
	$n = 100$								
	S			D			T		
	LCL	UCL	CP	LCL	UCL	CP	LCL	UCL	CP
c_1	1.280	1.763	0.950	1.285	1.758	0.951	1.277	1.766	0.958
c_2	1.268	1.773	0.949	1.279	1.761	0.948	1.275	1.765	0.954
c_3	1.254	1.790	0.949	1.274	1.768	0.951	1.275	1.765	0.956
c_4	1.236	1.813	0.949	1.267	1.775	0.950	1.274	1.767	0.955
c_5	1.212	1.846	0.948	1.261	1.784	0.950	1.270	1.773	0.954
c_6	1.179	1.893	0.948	1.253	1.794	0.952	1.263	1.781	0.954
c_7	1.127	1.963	0.947	1.244	1.805	0.948	1.253	1.792	0.957
c_8	1.043	2.096	0.946	1.233	1.816	0.948	1.241	1.805	0.961
c_9	0.861	2.467	0.942	1.223	1.836	0.947	1.231	1.820	0.964

2.2 Confidence Intervals for Expectation

In general, in order to estimate a statistic (e.g., mean, standard deviation) of a population, a random sample from the population is taken, and the individual statistics are calculated. In the field of environmental sciences or chemistry, it is often of interest to estimate the expected concentration of a chemical compound. In case the concentration can be modeled using the Weibull distribution, the expected value $\mu = \mu(\lambda, \tau)$ can be calculated using formula (2.3). In order to calculate the estimate $\widehat{\mu}$ of the expected value μ, we can replace λ, τ in (2.3) by their ML estimates $\widehat{\lambda}$, $\widehat{\tau}$.

However, it is always an issue to assess how well the sample statistic estimates the underlying population value. For this purpose, a confidence interval is used because it provides a range of values which is likely to contain the population parameter of interest. In this section, two methods of confidence interval construction are described and compared.

2.2.1 Maximum Likelihood Method

Considering the asymptotic normality of ML estimates, the expected value has the asymptotically normal distribution (Likeš and Machek, 1988), specifically

$$\mu(\lambda, \tau) \overset{A}{\sim} \mathrm{N}\left(\mu(\lambda, \tau), \mathrm{Var}\left(\mu(\lambda, \tau)\right)\right),$$

where

$$\begin{aligned}
\mathrm{Var}\left(\mu(\lambda, \tau)\right) &= \left[\frac{\partial \mu(\lambda, \tau)}{\partial \lambda}, \frac{\partial \mu(\lambda, \tau)}{\partial \tau}\right] \boldsymbol{J}_n^{-1}(\lambda, \tau) \left[\frac{\partial \mu(\lambda, \tau)}{\partial \lambda}, \frac{\partial \mu(\lambda, \tau)}{\partial \tau}\right]^{\mathrm{T}} \\
&= \left[\Gamma\left(1 + \frac{1}{\tau}\right), -\frac{\lambda \Psi\left(1 + \frac{1}{\tau}\right) \Gamma\left(1 + \frac{1}{\tau}\right)}{\tau^2}\right] \boldsymbol{J}_n^{-1}(\lambda, \tau) \\
&\quad \times \left[\Gamma\left(1 + \frac{1}{\tau}\right), -\frac{\lambda \Psi\left(1 + \frac{1}{\tau}\right) \Gamma\left(1 + \frac{1}{\tau}\right)}{\tau^2}\right]^{\mathrm{T}}
\end{aligned} \tag{2.9}$$

and $\Psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function.

Considering $\widehat{\mu} = \mu(\widehat{\lambda}, \widehat{\tau})$ and $\widehat{\mathrm{Var}}\left(\widehat{\mu}\right) = \mathrm{Var}\left(\mu(\widehat{\lambda}, \widehat{\tau})\right)$, the asymptotic $(1 - \alpha)\%$ confidence interval for μ can be calculated as

$$\left(\widehat{\mu} - z_{1-\frac{\alpha}{2}} \sqrt{\widehat{\mathrm{Var}}\left(\widehat{\mu}\right)}, \widehat{\mu} + z_{1-\frac{\alpha}{2}} \sqrt{\widehat{\mathrm{Var}}\left(\widehat{\mu}\right)}\right), \tag{$\mathrm{CI_{ML}}$}$$

where $z_{1-\alpha/2}$ is the $1 - \alpha/2$ quantile of the standard normal distribution $\mathrm{N}(0, 1)$.

2.2.2 Bootstrap Methods

Bootstrap procedure was proposed by Efron (1979), and it is an alternative method for obtaining unbiased nonparametric estimates of parameters and their confidence intervals. Bootstrap estimates are produced by computing statistics on repeated random samples taken with replacement from the observed data. The repeated samples have the same number of observations as in the observed data set, and censored and uncensored observations are equally available for sampling. Let $\mathbf{x}^{\mathrm{T}} = (x_1, \ldots, x_n)$ be a realization of the random sample $\mathbf{X}^{\mathrm{T}} = (X_1, \ldots, X_n)$ with cdf $F(x, \lambda, \tau)$, see (2.1). Moreover, let B be a number of bootstrap replications (resamples). There are two basic types of bootstrap—parametric and non-parametric. In case of the non-parametric bootstrap, the resample $\mathbf{x}^*$ is constructed by sampling with replacement from the data vector $\mathbf{x}$. The non-parametric bootstrap typically makes no assumptions concerning the distribution of the data. However, in our case, the assumption of Weibull distribution is applied, since we deal with censored distribution and need to estimate unknown parameters of the distribution using the ML method.

The algorithm for the non-parametric bootstrap is as follows:

1. Sample n observations randomly with replacement from $\mathbf{x}$ to obtain a bootstrap data set $\mathbf{x}^*$.
2. Calculate ML estimates $\widehat{\lambda}^*$, $\widehat{\tau}^*$ from $\mathbf{x}^*$.
3. Calculate the expected value estimate $\widehat{\mu}^* = \mu\left(\widehat{\lambda}^*, \widehat{\tau}^*\right)$.
4. Repeat steps 1–3 B times to obtain an estimate of the bootstrap distribution.
5. The $(1-\alpha)\%$ confidence interval for estimate $\widehat{\mu}$ is calculated as $\alpha/2$ and $(1-\alpha/2)$ quantile of $\widehat{\mu}_1^*, \ldots, \widehat{\mu}_B^*$.

We denote this confidence interval as $\mathrm{CI}_{\mathrm{boot}}$. The bootstrap estimate of the expected value is calculated as

$$\widehat{\mu} = \frac{1}{B} \sum_{b=1}^{B} \widehat{\mu}_b^*.$$

The parametric bootstrap makes an assumption that a parametric model for the data is known up to the unknown parameters. Therefore, the resample $\mathbf{x}^*$ is constructed by sampling from the distribution with cdf $F(x, \widehat{\lambda}, \widehat{\tau})$ where $\widehat{\lambda}$, $\widehat{\tau}$ are estimated from $\mathbf{x}$ using the ML method.

The algorithm for the parametric bootstrap is very similar to the non-parametric case. However, instead of step 1 in the algorithm, the following 2 steps are used:

1a. Calculate ML estimates $\widehat{\lambda}$, $\widehat{\tau}$ from $\mathbf{x}$.

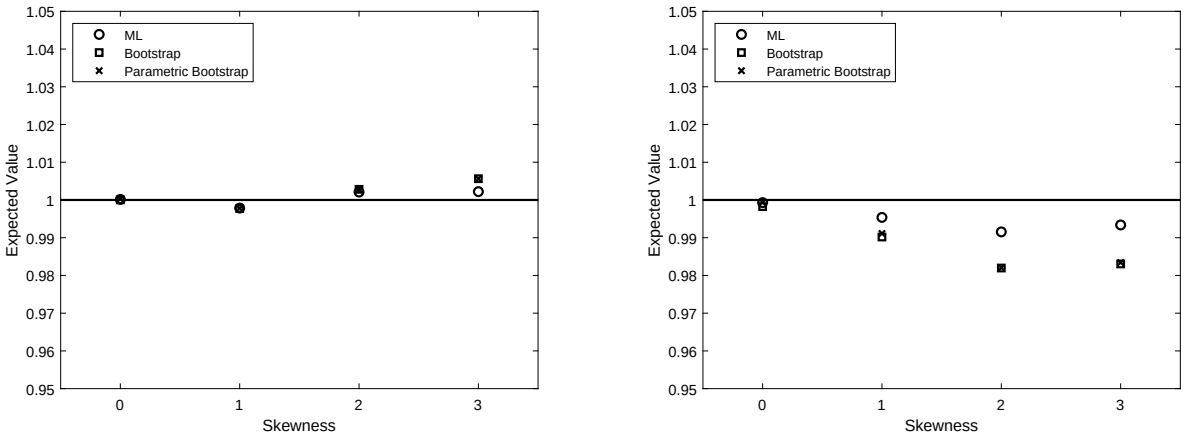
1b. Sample n observations from distribution with cdf $F(x, \widehat{\lambda}, \widehat{\tau})$ to obtain a bootstrap data set $\mathbf{x}^*$.

The obtained confidence interval is denoted as $\mathrm{CI}_{\mathrm{parboot}}$. Davison and Hinkley (1997) discussed the theory behind bootstrap and showed that, under some general conditions, the bootstrap confidence interval is asymptotically valid.

2.2.3 Simulation Study

The performance of the above mentioned methods was assessed using simulations (10,000 repetitions and $B = 500$ bootstrap resamples) for expected values of the Weibull distribution equal to $0.5, 1, 2, 3, 5$, and samples with size $n = 30$ and $n = 100$. Since skewness of the sample distribution can have significant influence on performance of the methods, simulations were carried out for various skewnesses (2.4), specifically $\gamma = 0, 1, 2, 3$. Parameters of the Weibull distribution are uniquely determined by the expected value and the skewness. Detection limits of the censored distribution were selected as quantiles of the Weibull distribution, specifically d_1 equals 5% (45% respectively) and d_2 equals 10% (90% respectively) quantile which corresponds to low (high respectively) censoring level. Since the simulation results are similar for various expected values, attention is paid only to the expected value equal to 1. All the estimates were averaged over 10,000 repetitions, and from now on when speaking about the estimates, we have in mind the estimates averaged over 10,000 repetitions.

It was found out that expected values estimated using the ML and the bootstrap methods are very similar in almost all cases (see Fig. 2.4a). However, in case of a small sample size, a high censoring level and $\gamma > 0$, the ML estimate of the expectation was the best (see Fig. 2.4b).

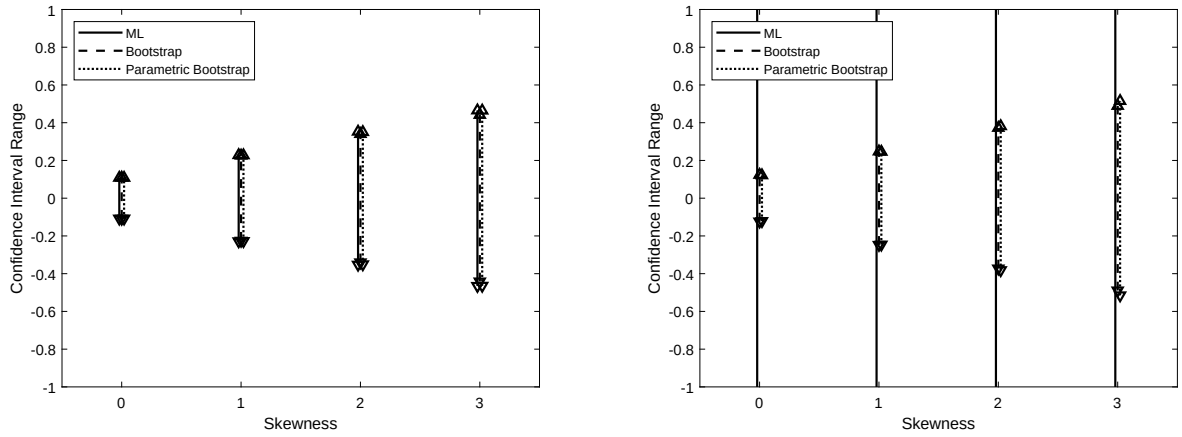


(a) Low censoring

(b) High censoring

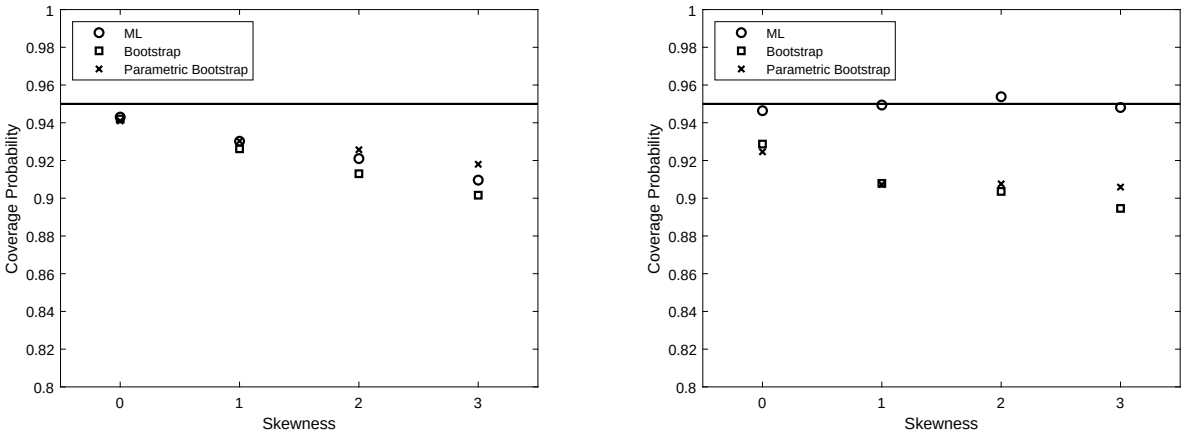
Figure 2.4: Expected value estimates; sample size $n = 30$.

In general, range of confidence intervals gets wider as skewness of the sample goes higher for all sample sizes, censoring levels, and estimation methods. In case of bigger samples ($n = 100$), ranges of all confidence intervals $\mathrm{CI}_{\mathrm{ML}}$, $\mathrm{CI}_{\mathrm{boot}}$ and $\mathrm{CI}_{\mathrm{parboot}}$ are quite similar. Analogous behavior was observed for small sample sizes ($n = 30$) and low censoring level (see Fig. 2.5a). However, in case of a small sample size and a high censoring level, confidence intervals $\mathrm{CI}_{\mathrm{ML}}$ were much wider than $\mathrm{CI}_{\mathrm{boot}}$ and $\mathrm{CI}_{\mathrm{parboot}}$ for all skewnesses (see Fig. 2.5b). It is caused by the fact that when the number of censored values is high, numerical difficulties with estimation of the FIM can result in very wide confidence intervals in some cases.



(a) Low censoring (b) High censoring

Figure 2.5: Range of confidence interval estimates; sample size $n = 30$.



(a) Low censoring (b) High censoring

Figure 2.6: Coverage probabilities of confidence interval estimates; sample size $n = 30$.

In order to assess quality of the confidence interval estimates, it is necessary to cal-

culate coverage probabilities of the confidence intervals. The coverage probability of 95% confidence interval is computed as the proportion of the number of times out of all replications the estimated 95% confidence interval contains the true parameter value. It was found out that $\mathrm{CI}_{\mathrm{ML}}$ has better coverage probability than $\mathrm{CI}_{\mathrm{boot}}$ and $\mathrm{CI}_{\mathrm{parboot}}$ in case of high censoring. The difference is even bigger for a small sample size with $n = 30$ (see Fig. 2.6b). In case of low censoring, coverage probabilities of all confidence intervals $\mathrm{CI}_{\mathrm{ML}}$, $\mathrm{CI}_{\mathrm{boot}}$ and $\mathrm{CI}_{\mathrm{parboot}}$ are quite similar (see Fig. 2.6a).

We add one remark about the number of bootstrap resamples B. When estimating 95% confidence intervals, $B \geq 1000$ is suggested (see e.g. Davison and Hinkley, 1997; Efron and Tibshirani, 1993). Nevertheless, in our case it was found out that for $B \geq 500$ the results were not substantially different.

2.3 Reduction of Weibull Distribution to Exponential

There are situations when the Weibull distribution is too complicated for modelling of given data. In case $\tau = 1$, the model of Weibull distribution can be reduced to the exponential submodel where all the calculations are much easier. To assess suitability of replacement of the censored Weibull distribution with the exponential distribution, asymptotic tests with nuisance parameters can be used (see e.g. Lehmann and Romano, 2005), specifically the Lagrange multiplier (LM) test, the Wald (W) test and the likelihood ratio (LR) test.

The null hypothesis H_0 is expressed as a restriction on the shape parameter τ of the censored Weibull distribution. Specifically, $\mathrm{H}_0 : \tau = 1$ is set against the alternative $\mathrm{H}_1 : \tau \neq 1$, and λ is the nuisance parameter. In case the null hypothesis is not rejected at a specified significance level, the censored exponential distribution can be used instead of the Weibull distribution.

The test statistics are

$$\begin{aligned} LM &= \frac{U_1^2(\widetilde{\lambda}, 1)}{J_{n,22.1}(\widetilde{\lambda}, 1)}, \\ W &= (\widehat{\tau} - 1)^2 J_{n,22.1}(\widehat{\lambda}, \widehat{\tau}), \\ LR &= 2\left[l(\widehat{\lambda}, \widehat{\tau}) - l(\widetilde{\lambda}, 1)\right], \end{aligned} \tag{2.10}$$

where

$$\begin{aligned} U_1(\lambda, \tau) = \frac{\partial l}{\partial \tau} = \sum_{i=1}^{k} N_i \frac{d_i^\tau \ln\left(\frac{d_i}{\lambda}\right) \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right] - d_{i-1}^\tau \ln\left(\frac{d_{i-1}}{\lambda}\right) \exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]}{\lambda^\tau \left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}} \\ + N_0 \frac{(1 - \tau \ln \lambda)}{\tau} + \sum_{i=n-N_0+1}^{n} \ln X_{(i)} + \frac{\ln \lambda}{\lambda^\tau} \sum_{i=n-N_0+1}^{n} X_{(i)}^\tau \end{aligned}$$

$$-\frac{1}{\lambda^\tau}\sum_{i=n-N_0+1}^{n} X_{(i)}^\tau \ln X_{(i)}$$

is the score function and $J_{n,22.1}(\lambda,\tau) = n(J_{22} - J_{21}J^{11}J_{12})$ is a transformation of the expected FIM (2.8). The parameters estimated under the null hypothesis are denoted by tilde, and those estimated under the alternative are denoted by hat. Under the null hypothesis, the test statistics (2.10) have asymptotically χ^2 distribution with one degree of freedom (see e.g. Lehmann and Romano, 2005). The null hypothesis is rejected at a prescribed significance level when the test statistics exceed the critical value of the χ^2 distribution.

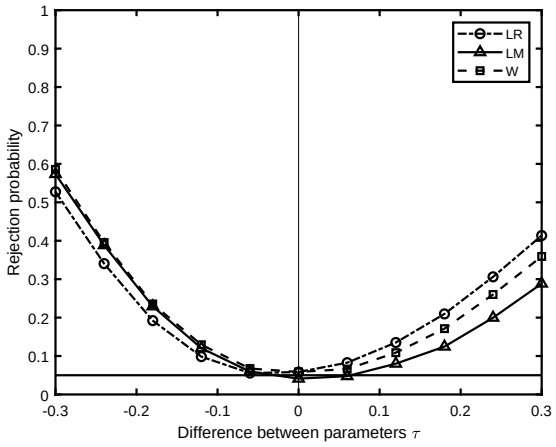
2.3.1 Power of the Tests

Performance of the tests using statistics (2.10) was assessed by means of simulated power functions (10,000 repetitions). Since the majority of researchers deal with censored data with one or two detection limits, two levels of censoring were considered. Specifically, single censoring with one detection limit, and double censoring with two detection limits. The detection limits d_1, d_2, were selected as quantiles of Weibull distribution using equations $q_i = F(d_i,\lambda,\tau)$, where q_i are given in Table 2.9. For example, the q_1 given in column "Double" in Table 2.9 denotes the proportion of doubly censored values, and describes the given censoring scheme. The censoring scheme "Low" represents the smallest proportion (10%) of censored data, and the censoring scheme "High" represents the largest proportion (90%) of censored data in case of singly and doubly censored samples. Since λ is the scale parameter, and ML estimators are scale invariant, we take $\lambda = 1$ without the loss of generality. This fact was also verified using simulations. The power functions were calculated for singly and doubly left-censored samples with size $n = 10, 20, 30, 50, 100$.

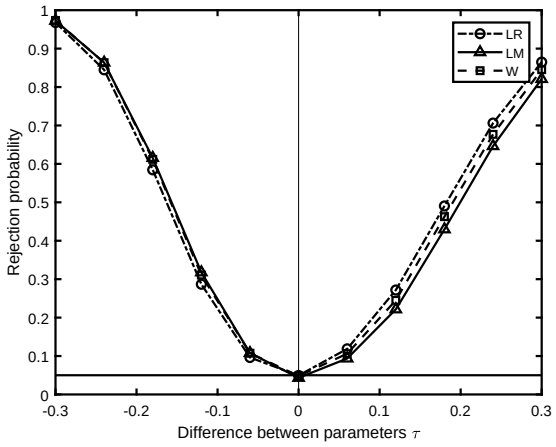
Table 2.9: Quantiles for determination of detection limit values considering single and double censoring and various censoring schemes.

	Single	Double	
Censoring	q_1	q_1	q_2
Low	0.10	0.05	0.10
Medium	0.50	0.25	0.50
High	0.90	0.45	0.90

In case of double censoring, all the test statistics perform poorly for small sample sizes



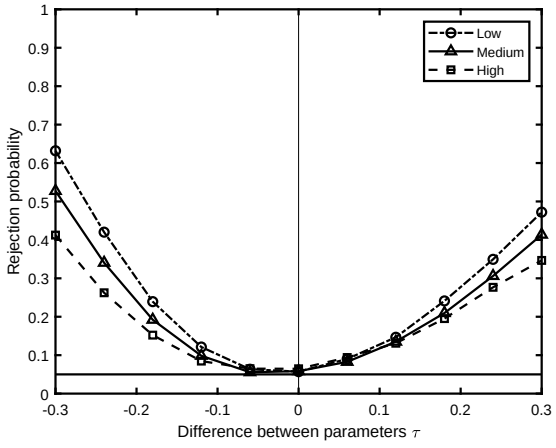
(a) $n = 30$



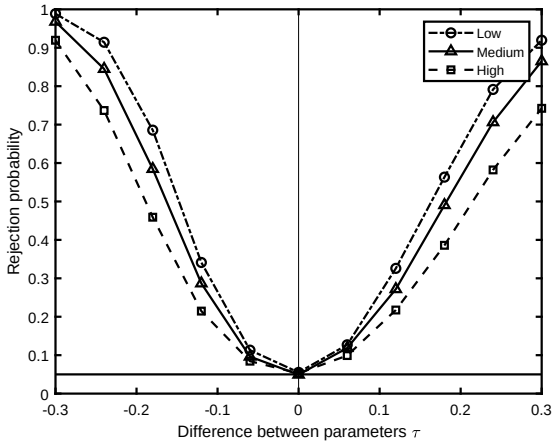
(b) $n = 100$

Figure 2.7: Power functions for test statistics (2.10), double censoring and medium number of censored values.

($n < 30$; not shown in figures). Furthermore, all the test statistics perform very similarly (see Fig. 2.7) for sample size $n = 100$. Overall, LR test statistic has the highest and LM test statistic the lowest power. When comparing the power functions considering various censoring schemes, Fig. 2.8 shows what difference between power functions can be expected in case of LR test statistic. Similar behavior was observed for test statistics LM and W (not shown in figures).



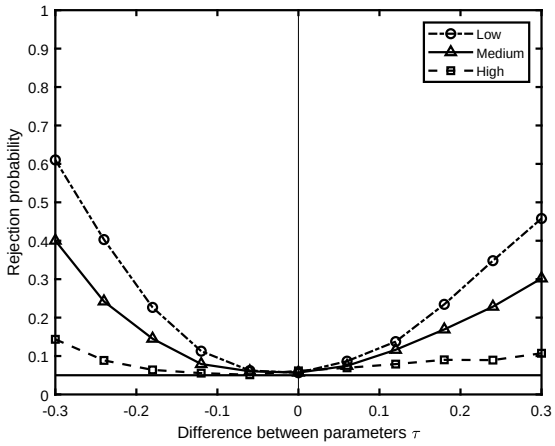
(a) $n = 30$



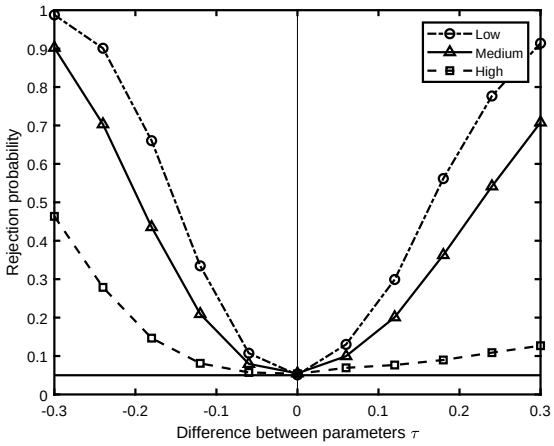
(b) $n = 100$

Figure 2.8: Power functions for test statistic LR, double censoring and a various number of censored values.

In case of single censoring, all the test statistics perform poorly for small sample sizes ($n < 30$; not shown in figures). Moreover, when the number of censored values is high, all the tests are practically unusable even for sample size $n = 100$ (see Fig. 2.9). All the test

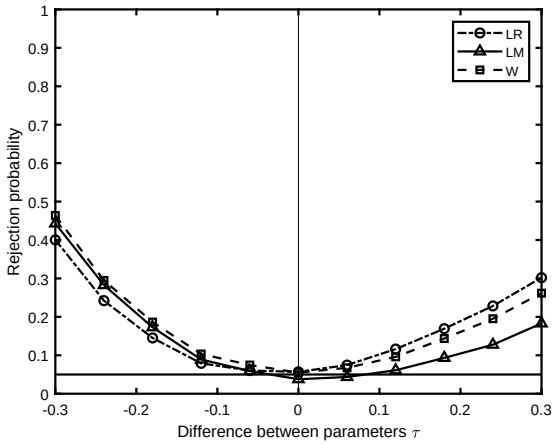


(a) $n = 30$

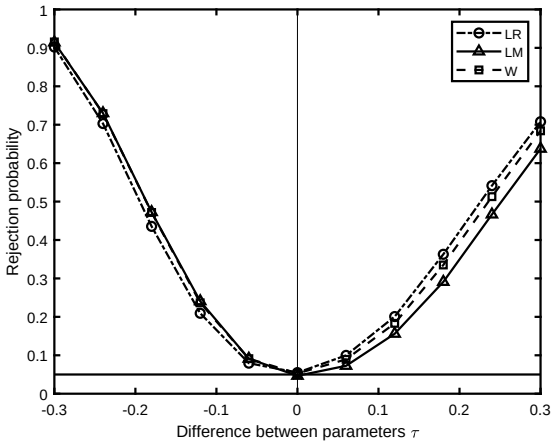


(b) $n = 100$

Figure 2.9: Power functions for test statistic LR, single censoring and a various number of censored values.



(a) $n = 30$



(b) $n = 100$

Figure 2.10: Power functions for test statistics (2.10), single censoring and medium number of censored values.

statistics perform very similarly (see Fig. 2.10) for sample size $n = 100$ and low/medium number of censored values. Furthermore, LR test statistic has the highest and LM test statistic the lowest power.

Chapter 3

Comparison of Two Left-Censored Weibull Samples

In order to compare two independent Type I multiply left-censored samples from the Weibull distribution, we extend the one-sample model described in Chapter 2 to the two-sample model. Let $X_{j,1}, \ldots, X_{j,n_j}$, $j = 1, 2$, be two independent Type I multiply left-censored samples from the Weibull distribution with cdf (2.1), pdf (2.2) and parameters $\lambda_1 = \lambda$, $\tau_1 = \tau$ in case of the first sample ($j = 1$), and $\lambda_2 = \lambda + \alpha$, $\tau_2 = \tau + \beta$ in case of the second sample ($j = 2$). The ordered sample of $X_{j,1}, \ldots, X_{j,n_j}$, $j = 1, 2$, is denoted as $X_{j,(1)} \leq \cdots \leq X_{j,(n_j)}$, and $N_{j,i}$ are frequencies corresponding to frequencies N_i, $i = 0, 1, \ldots, k$, from Chapter 2, where j denotes the sample number.

The log-likelihood function of the two joint censored samples is

$$\begin{aligned} l_{\mathrm{R}}(\alpha, \beta, \lambda, \tau) = {} & l(\lambda, \tau, N_{1,0}, \ldots, N_{1,k}, X_{1,(n_1 - N_{1,0}+1)}, \ldots, X_{1,(n_1)}) \\ & + l(\lambda + \alpha, \tau + \beta, N_{2,0}, \ldots, N_{2,k}, X_{2,(n_2 - N_{2,0}+1)}, \ldots, X_{2,(n_2)}), \end{aligned}$$

where l is the log-likelihood function (2.6) in the one-sample model, specifically

$$\begin{aligned} l_{\mathrm{R}}(\alpha, \beta, \lambda, \tau) = {} & \log\left(\frac{n_1!}{N_{1,1}! \cdots N_{1,k}!}\right) + \sum_{i=1}^{k} N_{1,i} \log\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\} \\ & + N_{1,0} \log\left(\frac{\tau}{\lambda^{\tau}}\right) + (\tau - 1) \sum_{i=n_1 - N_{1,0}+1}^{n_1} \log\left(X_{1,(i)}\right) - \frac{1}{\lambda^{\tau}} \sum_{i=n_1 - N_{1,0}+1}^{n_1} X_{1,(i)}^{\tau} \\ & + \log\left(\frac{n_2!}{N_{2,1}! \cdots N_{2,k}!}\right) + \sum_{i=1}^{k} N_{2,i} \log\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda + \alpha}\right)^{\tau+\beta}\right] - \exp\left[-\left(\frac{d_i}{\lambda + \alpha}\right)^{\tau+\beta}\right]\right\} \\ & + N_{2,0} \log\left[\frac{\tau + \beta}{(\lambda + \alpha)^{\tau+\beta}}\right] + (\tau + \beta - 1) \sum_{i=n_2 - N_{2,0}+1}^{n_2} \log\left(X_{2,(i)}\right) - \frac{1}{(\lambda + \alpha)^{\tau+\beta}} \sum_{i=n_2 - N_{2,0}+1}^{n_2} X_{2,(i)}^{\tau+\beta}. \end{aligned} \tag{3.1}$$

As in the one-sample model, the ML estimates $\widehat{\alpha}$, $\widehat{\beta}$, $\widehat{\lambda}$, $\widehat{\tau}$ of parameters α, β, λ, τ can be obtained by maximization of the log-likelihood function (3.1).

The variability of ML estimates $\widehat{\alpha}$, $\widehat{\beta}$, $\widehat{\lambda}$, $\widehat{\tau}$ can be calculated from the sample or the expected FIM. The expected FIM is

$$\boldsymbol{J}_n^{\mathrm{R}}(\alpha,\beta,\lambda,\tau) = \begin{bmatrix} J_{11}^{\mathrm{R}} & J_{12}^{\mathrm{R}} & J_{13}^{\mathrm{R}} & J_{14}^{\mathrm{R}} \\ J_{21}^{\mathrm{R}} & J_{22}^{\mathrm{R}} & J_{23}^{\mathrm{R}} & J_{24}^{\mathrm{R}} \\ J_{31}^{\mathrm{R}} & J_{32}^{\mathrm{R}} & J_{33}^{\mathrm{R}} & J_{34}^{\mathrm{R}} \\ J_{41}^{\mathrm{R}} & J_{42}^{\mathrm{R}} & J_{43}^{\mathrm{R}} & J_{44}^{\mathrm{R}} \end{bmatrix} = \begin{bmatrix} -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\alpha^2} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\alpha\partial\beta} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\alpha\partial\lambda} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\alpha\partial\tau} \\ -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\beta\partial\alpha} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\beta^2} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\beta\partial\lambda} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\beta\partial\tau} \\ -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\lambda\partial\alpha} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\lambda\partial\beta} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\lambda^2} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\lambda\partial\tau} \\ -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\tau\partial\alpha} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\tau\partial\beta} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\tau\partial\lambda} & -\mathrm{E}\frac{\partial^2 l_{\mathrm{R}}}{\partial\tau^2} \end{bmatrix}, \quad (3.2)$$

where

$$\begin{aligned}
J_{11}^{\mathrm{R}} &= J_{13}^{\mathrm{R}} = J_{31}^{\mathrm{R}} = n_2 J_{11}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),\\
J_{12}^{\mathrm{R}} &= J_{21}^{\mathrm{R}} = J_{14}^{\mathrm{R}} = J_{41}^{\mathrm{R}} = J_{23}^{\mathrm{R}} = J_{32}^{\mathrm{R}}\\
&= n_2 J_{12}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),\\
J_{22}^{\mathrm{R}} &= J_{24}^{\mathrm{R}} = J_{42}^{\mathrm{R}} = n_2 J_{22}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),\\
J_{33}^{\mathrm{R}} &= n_1 J_{11}(\lambda,\tau,N_{1,0},\ldots,N_{1,k},X_{1,(n_1-N_{1,0}+1)},\ldots,X_{1,(n_1)})\\
&\quad + n_2 J_{11}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),\\
J_{44}^{\mathrm{R}} &= n_1 J_{22}(\lambda,\tau,N_{1,0},\ldots,N_{1,k},X_{1,(n_1-N_{1,0}+1)},\ldots,X_{1,(n_1)})\\
&\quad + n_2 J_{22}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),\\
J_{34}^{\mathrm{R}} &= J_{43}^{\mathrm{R}} = n_1 J_{12}(\lambda,\tau,N_{1,0},\ldots,N_{1,k},X_{1,(n_1-N_{1,0}+1)},\ldots,X_{1,(n_1)})\\
&\quad + n_2 J_{12}(\lambda+\alpha,\tau+\beta,N_{2,0},\ldots,N_{2,k},X_{2,(n_2-N_{2,0}+1)},\ldots,X_{2,(n_2)}),
\end{aligned} \quad (3.3)$$

and J_{11}, J_{12}, J_{22} are elements of the expected FIM (2.8) in the one-sample model. The sample FIM $\widetilde{\boldsymbol{J}}_n^{\mathrm{R}}(\alpha,\beta,\lambda,\tau)$ can be obtained in a similar way by replacing of $n_j J_{11}$, $n_j J_{12}$, $n_j J_{22}$, $j = 1,2$, in (3.3) by corresponding elements of the sample FIM (2.7) for each individual sample j.

3.1 Comparison of Distributions

For comparison of two independent censored samples from Weibull distribution, asymptotic tests with nuisance parameters can be used (see e.g. Lehmann and Casella, 1998), specifically the Lagrange multiplier (LM) test, the Wald (W) test and the likelihood ratio (LR) test. The null hypothesis H_0 is that distributions of both samples are equal. As it was stated at the beginning of this chapter, parameters α and β describe the difference between distributions of the first and the second sample. In case $\alpha = 0$ and $\beta = 0$, distributions of the two samples are identical. The null hypothesis $\mathrm{H}_0 : (\alpha,\beta)^{\mathrm{T}} = (0,0)^{\mathrm{T}}$ is set against the alternative $\mathrm{H}_1 : (\alpha,\beta)^{\mathrm{T}} \neq (0,0)^{\mathrm{T}}$, where λ and τ are nuisance parameters.

The test statistics are

$$\begin{aligned} LM &= \boldsymbol{U}_1(0,0,\widetilde{\lambda},\widetilde{\tau})\left[\boldsymbol{J}^{\mathrm{R}}_{n,11.2}(0,0,\widetilde{\lambda},\widetilde{\tau})\right]^{-1}\boldsymbol{U}_1^{\mathrm{T}}(0,0,\widetilde{\lambda},\widetilde{\tau}),\\ W &= (\widehat{\alpha},\widehat{\beta})\left[\boldsymbol{J}^{\mathrm{R}}_{n,11.2}(\widehat{\alpha},\widehat{\beta},\widehat{\lambda},\widehat{\tau})\right](\widehat{\alpha},\widehat{\beta})^{\mathrm{T}},\\ LR &= 2\left[l_{\mathrm{R}}(\widehat{\alpha},\widehat{\beta},\widehat{\lambda},\widehat{\tau}) - l_{\mathrm{R}}(0,0,\widetilde{\lambda},\widetilde{\tau})\right], \end{aligned} \tag{3.4}$$

where

$$\boldsymbol{U}_1(\alpha,\beta,\lambda,\tau) = \left(\frac{\partial l_{\mathrm{R}}}{\partial\alpha},\frac{\partial l_{\mathrm{R}}}{\partial\beta}\right) = (u_1,u_2),$$

$$\begin{aligned} u_1 = {} & \sum_{i=1}^{k} N_i \frac{(\tau+\beta)\left\{d_{i-1}^{\tau+\beta}\exp\left[-\left(\frac{d_{i-1}}{\lambda+\alpha}\right)^{\tau+\beta}\right] - d_i^{\tau+\beta}\exp\left[-\left(\frac{d_i}{\lambda+\alpha}\right)^{\tau+\beta}\right]\right\}}{(\lambda+\alpha)^{\tau+\beta+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda+\alpha}\right)^{\tau+\beta}\right] - \exp\left[-\left(\frac{d_i}{\lambda+\alpha}\right)^{\tau+\beta}\right]\right\}} - N_0\frac{\tau+\beta}{\lambda+\alpha}\\ & + \frac{\tau+\beta}{(\lambda+\alpha)^{\tau+\beta+1}}\sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau+\beta}, \end{aligned}$$

$$\begin{aligned} u_2 = {} & \sum_{i=1}^{k} N_i \frac{d_i^{\tau+\beta}\log\left(\frac{d_i}{\lambda+\alpha}\right)\exp\left[-\left(\frac{d_i}{\lambda+\alpha}\right)^{\tau+\beta}\right] - d_{i-1}^{\tau+\beta}\log\left(\frac{d_{i-1}}{\lambda+\alpha}\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda+\alpha}\right)^{\tau+\beta}\right]}{(\lambda+\alpha)^{\tau+\beta}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda+\alpha}\right)^{\tau+\beta}\right] - \exp\left[-\left(\frac{d_i}{\lambda+\alpha}\right)^{\tau+\beta}\right]\right\}}\\ & + N_0\frac{[1-(\tau+\beta)\log(\lambda+\alpha)]}{\tau+\beta} + \sum_{i=n-N_0+1}^{n}\log X_{(i)} + \frac{\log(\lambda+\alpha)}{(\lambda+\alpha)^{\tau+\beta}}\sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau+\beta}\\ & - \frac{1}{(\lambda+\alpha)^{\tau+\beta}}\sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau+\beta}\log X_{(i)}, \end{aligned}$$

is the score function and

$$\boldsymbol{J}^{\mathrm{R}}_{n,11.2}(\alpha,\beta,\lambda,\tau) = \begin{bmatrix} J^{\mathrm{R}}_{11} & J^{\mathrm{R}}_{12}\\ J^{\mathrm{R}}_{21} & J^{\mathrm{R}}_{22}\end{bmatrix} - \begin{bmatrix} J^{\mathrm{R}}_{13} & J^{\mathrm{R}}_{14}\\ J^{\mathrm{R}}_{23} & J^{\mathrm{R}}_{24}\end{bmatrix}\begin{bmatrix} J^{\mathrm{R}}_{33} & J^{\mathrm{R}}_{34}\\ J^{\mathrm{R}}_{43} & J^{\mathrm{R}}_{44}\end{bmatrix}^{-1}\begin{bmatrix} J^{\mathrm{R}}_{31} & J^{\mathrm{R}}_{32}\\ J^{\mathrm{R}}_{41} & J^{\mathrm{R}}_{42}\end{bmatrix}$$

is a transformation of the expected FIM (3.2). The parameters estimated under the null hypothesis are denoted by tilde and those estimated under the alternative are denoted by hat. Under the null hypothesis, the test statistics (3.4) have asymptotically χ^2 distribution with two degrees of freedom (see e.g. Lehmann and Romano, 2005). The null hypothesis is rejected at a prescribed significance level when the test statistics exceed the critical value of the χ^2 distribution.

3.1.1 Power of the Tests

Performance of the tests using statistics (3.4) was studied using simulated power functions (10,000 repetitions) and the significance level was 0.05. The power functions were calculated in case of comparing doubly left-censored samples ($n = 30$ and $n = 100$) from the Weibull distribution with various values of parameters λ, τ considering detection limit d_1 equals 5% (45% respectively) and d_2 equals 10% (90% respectively) quantile of Weibull distribution, i.e. low (high respectively) censoring level. Since the power functions of all the test statistics practically coincide for $n \geq 100$, results are visualized only for $n = 30$ and high censoring level, which was observed when dealing with real data (Fusek and Michálek, 2013).

In case there is a difference in scale parameter of the distributions and $\beta = 0$, all test statistics perform rather well (see Figs. 3.1a, c, e). However, when a value of τ is low ($\tau = 0.5$), the test statistics perform poorly for small sample size ($n = 30$; not shown in figures). This can be caused by high skewness of the Weibull distribution in case $\tau < 1$. The LR test statistic outperforms the LM and W statistics in all cases. Moreover, the LM statistic performs the worst. If there is a difference in shape of the distributions and $\alpha = 0$, performance of test statistics (3.4) for small sample size ($n = 30$) and $\beta > 0$ is not particularly good (see Figs. 3.1b, d, f). This can be caused by a small difference between expected values of the two Weibull samples for $\beta > 0$ in comparison to $\beta < 0$ (see the differences between expected values on the top x-axis in Figs. 3.1b, d, f). The LR test statistic outperforms the LM and W statistics in all cases. Both LM and W statistics perform rather similar. However, the disadvantage of the LR test statistic is that it works at a higher significance level than the declared 0.05.

3.2 Comparison of Expected Values

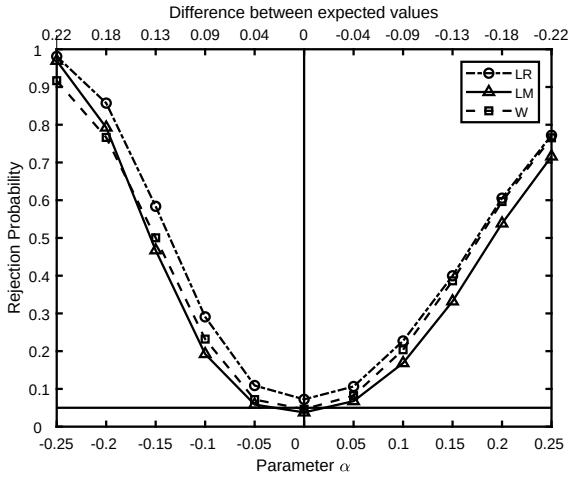
For comparison of means μ_1, μ_2 of two independent censored samples from Weibull distribution, the test based on Wald's test statistic (see e.g. Lehmann and Romano, 2005) can be used. The null hypothesis $\mathrm{H}_0 : \mu_1 - \mu_2 = 0$ is set against the alternative $\mathrm{H}_1 : \mu_1 - \mu_2 \neq 0$.

The test statistic is

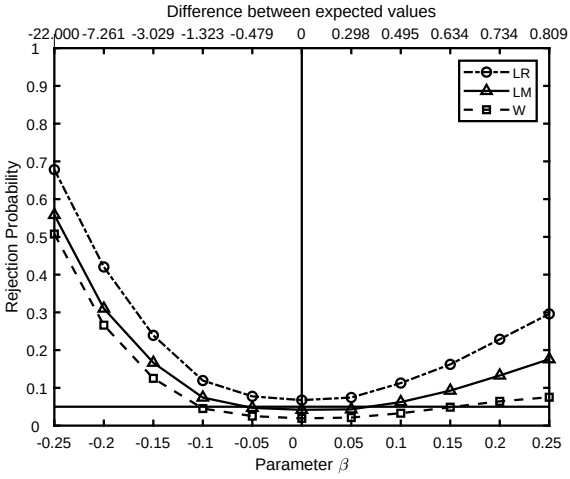
$$W = \frac{\widehat{\mu}_1 - \widehat{\mu}_2}{\sqrt{\widehat{\mathrm{Var}}\,(\widehat{\mu}_1) + \widehat{\mathrm{Var}}\,(\widehat{\mu}_2)}}, \tag{3.5}$$

where $\widehat{\mu}_i = \mu(\widehat{\lambda}_i, \widehat{\tau}_i)$ can be calculated from (2.3) and $\widehat{\mathrm{Var}}\,(\widehat{\mu}_i) = \mathrm{Var}\left(\mu(\widehat{\lambda}_i, \widehat{\tau}_i)\right)$ can be calculated from (2.9) for $i = 1, 2$. Under the null hypothesis, the test statistic (3.5) is considered to be asymptotically normal $\mathrm{N}(0, 1)$.

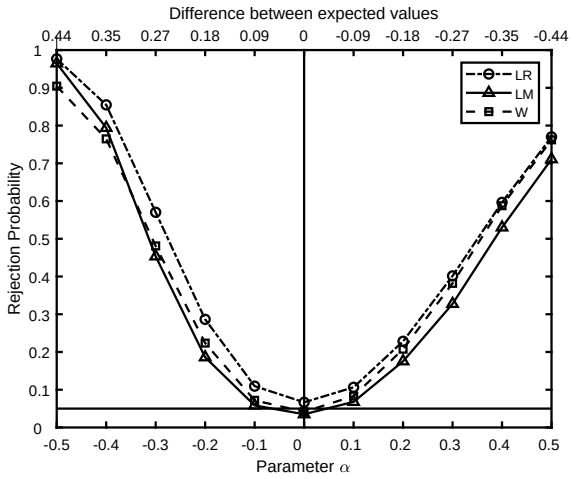
In order to compare means of two independent censored samples, there is another option. We can use the asymptotic t-test. Nevertheless, since we deal with censored



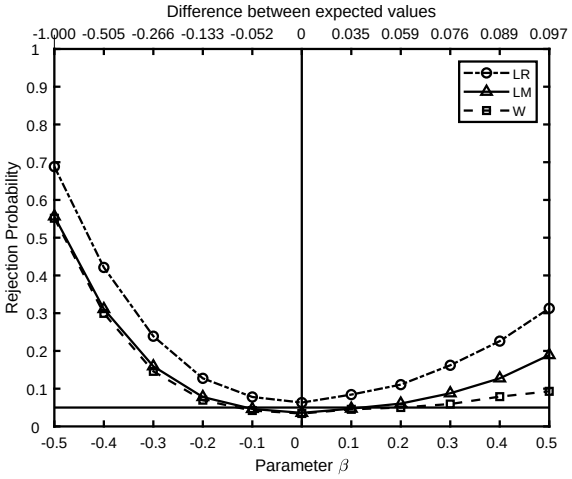
(a) Parameter α; $\beta = 0$, $\lambda = 0.5$, $\tau = 2$



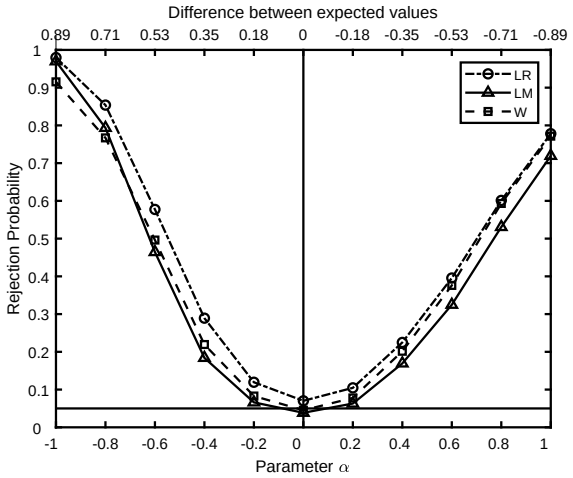
(b) Parameter β; $\alpha = 0$, $\lambda = 1$, $\tau = 0.5$



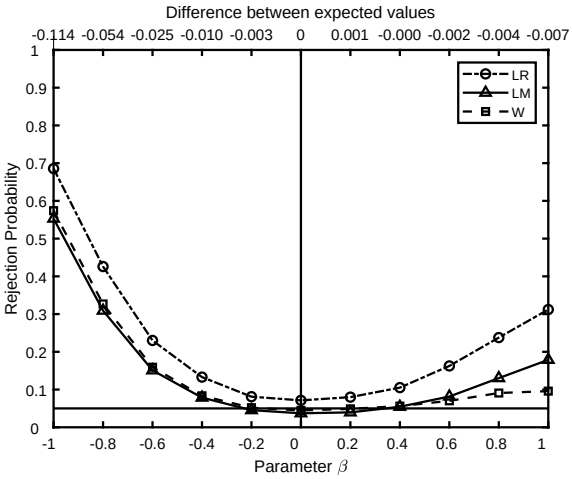
(c) Parameter α; $\beta = 0$, $\lambda = 1$, $\tau = 2$



(d) Parameter β; $\alpha = 0$, $\lambda = 1$, $\tau = 1$



(e) Parameter α; $\beta = 0$, $\lambda = 2$, $\tau = 2$



(f) Parameter β; $\alpha = 0$, $\lambda = 1$, $\tau = 2$

Figure 3.1: Power functions for test statistics (3.4), high censoring level and sample size $n = 30$; differences between expected values on the top x-axis.

observations, certain adjustments have to be done. The usual approach in such a situation is based on replacing values between detection limits d_{i-1} and d_i, $i = 1, \ldots, k$, by constants lying between the individual detection limits, often by the midpoint of such an interval (see e.g. El-Shaarawi and Esterby, 1992). The null and the alternative hypotheses remain the same as above and the test statistic is

$$T = \frac{\overline{X}_1 - \overline{X}_2}{\sqrt{\frac{S_1^2}{n} + \frac{S_2^2}{n}}}, \tag{3.6}$$

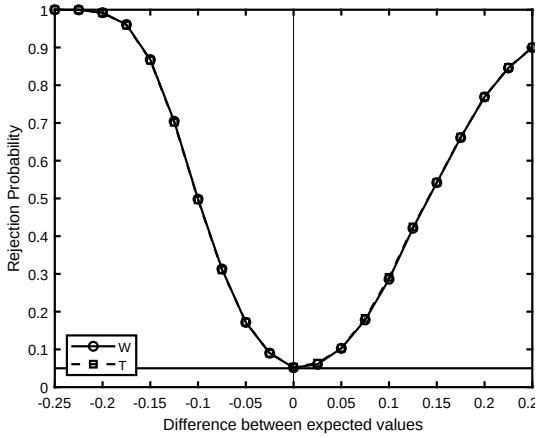
where $\overline{X}_1$ ($\overline{X}_2$ respectively) is the sample mean and S_1^2 (S_2^2 respectively) is the sample variance of the first (second respectively) sample. Under the null hypothesis of equal means, the statistic (3.6) is considered to be asymptotically normal $\mathrm{N}(0, 1)$.

Clearly, an advantage of the T statistic is that it can be used for samples with various distributions as long as assumptions of the central limit theorem are fulfilled. However, performance of methods based on replacement of censored values by constants has previously been examined (El-Shaarawi and Esterby, 1992; Helsel and Cohn, 1988; Lubin et al., 2004; Singh and Nocerino, 2002), and it was shown that it is not particularly good. More information about how substituting values for censored observations can ruin results can be found in Helsel (1990, 2006) and Hornung and Reed (1990).

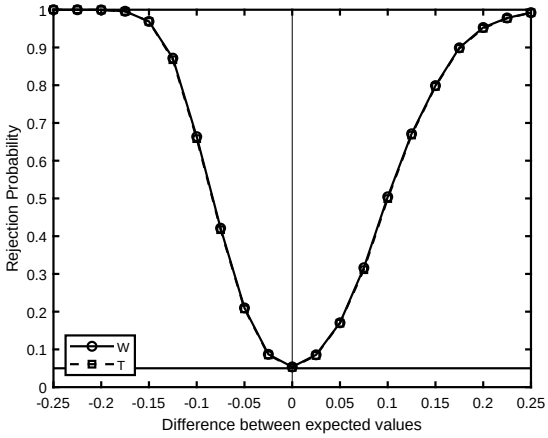
3.2.1 Power of the Tests

Performance of tests based on statistics (3.5), (3.6) was verified by means of simulated power functions (10,000 repetitions) for expected values of Weibull distribution equal to $0.5, 1, 2, 3, 5$. Simulations were focused on doubly left-censored samples ($n = 30$ and $n = 100$) because they are often present when analyzing real data. Since the skewness of the sample distribution can have significant influence on performance of both tests, simulations were carried out for various skewnesses γ_i of samples $i = 1, 2$, specifically $\gamma_i = -1, 0, 1, 2, 3$. Parameters of the Weibull distribution are uniquely determined by the expected value and the skewness. Detection limits of the censored distribution were selected as quantiles of the Weibull distribution, specifically d_1 equals 5% (45% respectively) and d_2 equals 10% (90% respectively) quantile which corresponds to low (high respectively) censoring level. In case of statistic (3.6), all censored values are replaced by midpoints of intervals $(d_0, d_1]$ and $(d_1, d_2]$. Since the power functions of all the test statistics have similar behavior for various expected values and sample sizes, they are illustrated in Fig. 3.2 only for expected value equal to 0.5 and sample size $n = 100$.

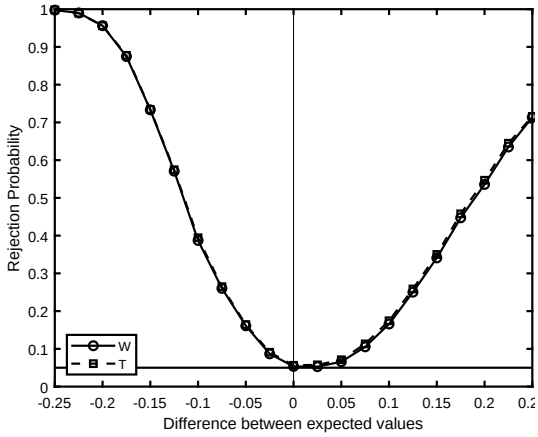
In case of low censoring, performances of both tests are rather similar (see Fig. 3.2a), especially when skewnesses of both samples are similar (see Fig. 3.2b). However, if there is a big difference between skewnesses of the samples, power functions of both test statistics are slightly biased (see Fig. 3.2c). In case of high censoring, test statistic (3.5) performs



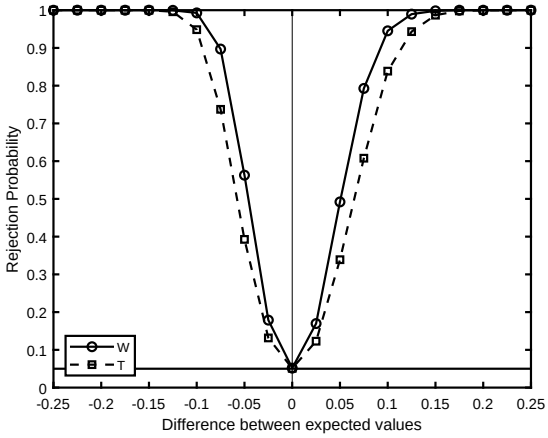
(a) Low censoring; $\gamma_1 = 1$, $\gamma_2 = 2$



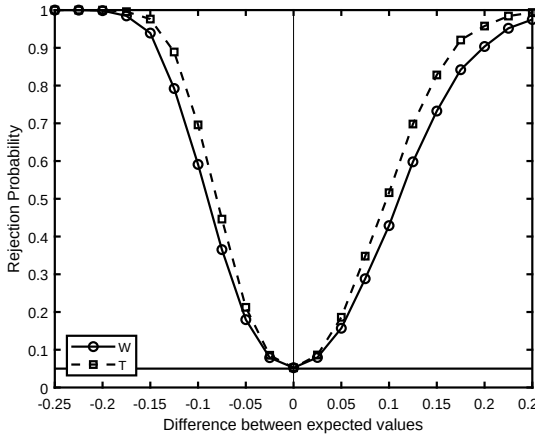
(b) Low censoring; $\gamma_1 = 1$, $\gamma_2 = 1$



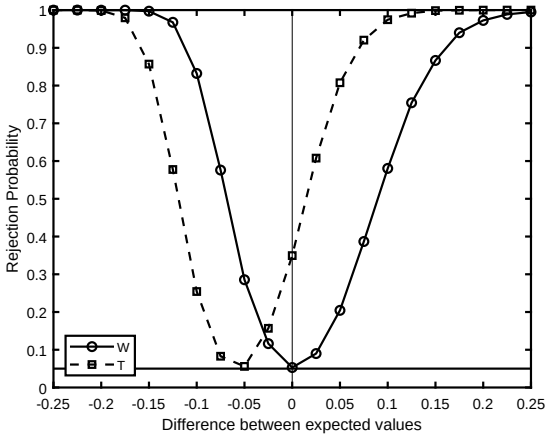
(c) Low censoring; $\gamma_1 = 1$, $\gamma_2 = 3$



(d) High censoring; $\gamma_1 = 0$, $\gamma_2 = 0$



(e) High censoring; $\gamma_1 = 1$, $\gamma_2 = 1$



(f) High censoring; $\gamma_1 = 0$, $\gamma_2 = 1$

Figure 3.2: Power functions for test statistics (3.5), (3.6); sample size $n = 100$.

better in almost all cases (see Fig. 3.2d). The exception is situation when skewnesses of both samples are equal and ≥ 1 (see Fig. 3.2e). Otherwise, test statistic (3.6) performs poorly since its power function is biased. Specifically, Fig. 3.2f shows that in case both samples have the same expected values, the rejection probability of the null hypothesis is higher (close to 0.4) than the prescribed significance level 0.05. Moreover, the lowest rejection probability is encountered if the difference between expected values of both samples is about 0.05. Similar to low censoring, the power function of test statistic (3.5) is slightly biased if skewnesses of the samples vary significantly.

Chapter 4

Goodness-of-Fit Tests

When analyzing real data using the parametric approach, it is assumed that data has a specific distribution with cdf $F(x, \boldsymbol{\theta})$, where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k) \in \boldsymbol{\Theta} \subset \mathbb{R}^k$ is a vector of parameters. In environmental studies, data are typically skewed and various distributions such as the lognormal (Baccarelli et al., 2005; El-Shaarawi, 1989), the gamma (Hrdličková et al., 2008; Singh et al., 2002) and the Weibull (Fusek et al., 2015, 2020; Mbengue et al., 2018) distributions are often used. Since selecting an unsuitable probability distribution can lead to biased estimates and potentially misleading inferences, goodness-of-fit tests are of a great importance. There are several goodness-of-fit tests available in the literature based on a complete sample and an excellent overview on this topic can be found in d'Agostino and Stephens (1986). Nevertheless, there has been relatively little work done on the problem of goodness-of-fit for Type I censored data and attention was usually paid only to right-censoring (Bispo et al., 2011; Pakyari and Balakrishnan, 2013; Pakyari and Nia, 2017). In this chapter, three tests (Kolmogorov-Smirnov, Cramér-von Mises, Anderson-Darling) based on the empirical distribution function (EDF) are considered, and their power is investigated by varying the null and the alternative distributions, the sample size and the degree of censoring. It can bring readers valuable information about the type II error that can be expected when having a dataset with a specific size and a number of censored values.

Following probability distributions are used:

1) The Weibull distribution with parameter $\boldsymbol{\theta} = (\lambda, \tau) \in (0, \infty) \times (0, \infty)$, and cdf

$$F(x, \boldsymbol{\theta}) = \begin{cases} 1 - \exp\left[-\left(\frac{x}{\lambda}\right)^{\tau}\right] & \text{for } x \geq 0, \\ 0 & \text{for } x < 0, \end{cases} \tag{4.1}$$

where λ is the scale parameter and τ is the shape parameter.

2) The lognormal distribution with parameter $\boldsymbol{\theta} = (\mu, \sigma) \in (-\infty, \infty) \times (0, \infty)$, and cdf

$$F(x, \boldsymbol{\theta}) = \begin{cases} \frac{1}{\sigma\sqrt{2\pi}} \int_0^x \frac{1}{t} \exp\left[-\frac{(\log(t)-\mu)^2}{2\sigma^2}\right] \mathrm{d}t & \text{for } x > 0, \\ 0 & \text{for } x \leq 0, \end{cases} \tag{4.2}$$

where μ is the location parameter and σ is the scale parameter of the variable's natural logarithm.

3) The gamma distribution with parameter $\boldsymbol{\theta} = (\lambda, \kappa) \in (0, \infty) \times (0, \infty)$, and cdf

$$F(x, \boldsymbol{\theta}) = \begin{cases} \frac{1}{\lambda^\kappa \Gamma(\kappa)} \int_0^x t^{\kappa-1} \exp\left(-\frac{t}{\lambda}\right) \mathrm{d}t & \text{for } x > 0, \\ 0 & \text{for } x \leq 0, \end{cases} \tag{4.3}$$

where λ is the scale parameter and κ is the shape parameter.

4) The Gumbel distribution with parameter $\boldsymbol{\theta} = (\mu, \sigma) \in (-\infty, \infty) \times (0, \infty)$, and cdf

$$F(x, \boldsymbol{\theta}) = 1 - \exp\left[-\exp\left(\frac{x-\mu}{\sigma}\right)\right] \text{ for } x \in \mathbb{R}, \tag{4.4}$$

where μ is the location parameter and σ is the scale parameter.

5) The normal distribution with parameter $\boldsymbol{\theta} = (\mu, \sigma) \in (-\infty, \infty) \times (0, \infty)$, and cdf

$$F(x, \boldsymbol{\theta}) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^x \exp\left[-\frac{(t-\mu)^2}{2\sigma^2}\right] \mathrm{d}t \text{ for } x \in \mathbb{R}, \tag{4.5}$$

where μ is the location parameter and σ is the scale parameter.

4.1 Goodness-of-Fit Test Statistics

Let $X_1, \ldots, X_n$ be a random sample from a distribution with cdf $F(x)$. We consider a problem of testing a composite hypothesis

$$\mathrm{H}_0 : F(x) \in \left\{F_0(x, \boldsymbol{\theta}), \boldsymbol{\theta} \in \boldsymbol{\Theta} \subset \mathbb{R}^k\right\},$$

where F_0 is a cdf of a known parametric family. In case $\boldsymbol{\theta}$ is fully specified, then H_0 is a simple hypothesis and the distribution theory of EDF statistics is well developed. When $\boldsymbol{\theta}$ is unknown, it can be replaced by its estimate $\widehat{\boldsymbol{\theta}}$, and distributions of EDF statistics depend on the tested distribution, the estimated parameters and the sample size. It is well known fact (d'Agostino and Stephens, 1986) that in case the unknown components in $\boldsymbol{\theta}$ are location or scale parameters, distributions of EDF statistics do not depend on the true values of the unknown parameters, and depend only on the tested distribution and on the

sample size. When the unknown component in $\boldsymbol{\theta}$ is the shape parameter, distributions of EDF statistics depend on the true value of this parameter. In our case, it was possible to transform the distributions depending on the shape parameter to another distributions depending on the location and scale parameters only. Specifically, if a random variable X has the Weibull distribution, then $\log(X)$ has the Gumbel distribution. Therefore, testing the null hypothesis that the data follow the Weibull distribution (4.1) is equivalent to testing that the log-transformed data follow the Gumbel distribution with location parameter $\mu = \log(\lambda)$, scale parameter $\sigma = 1/\tau$, and cdf (4.4). Moreover, a random variable X has the lognormal distribution if $\log(X)$ has the normal distribution. For that reason, testing the null hypothesis that the data follow the lognormal distribution (4.2) is equivalent to testing that the log-transformed data follow the normal distribution with mean μ, standard deviation σ, and cdf (4.5).

Critical values of the EDF statistics can be obtained by means of Monte Carlo simulations using the following steps:

1) Generate a Type I doubly left-censored sample $X_1, \ldots, X_n$ with a pre-chosen sample size n and detection limits from the distribution being tested. Detection limits are selected as quantiles of the tested distribution depending on the degree of censoring.

2) Calculate the ML estimates of the unknown parameters of the selected distribution.

3) Calculate the EDF statistic.

4) Repeat steps 1–3 a large number of times and determine the $(1-\alpha)$th quantile of the test statistic as the required critical value of that goodness-of-fit statistic.

Three test statistics based on the EDF $F_n(x)$ are applied (see d'Agostino and Stephens, 1986, for more details).

4.1.1 Kolmogorov-Smirnov Statistic

The Kolmogorov-Smirnov (KS) statistic is defined by

$$D = \sup_{d_2 \le x < \infty} |F_n(x) - F_0(x)|$$

with the useful alternative form for computational purposes

$$D = \max_{n-N_0+1 \le i \le n} \left\{ \left| \frac{i}{n} - F_0\left(x_{(i)}, \widehat{\boldsymbol{\theta}}\right) \right|, \left| F_0\left(x_{(i)}, \widehat{\boldsymbol{\theta}}\right) - \frac{i-1}{n} \right|, \left| F_0\left(d_2, \widehat{\boldsymbol{\theta}}\right) - \frac{n-N_0}{n} \right| \right\}.$$

4.1.2 Cramér-von Mises Statistic

The Cramér-von Mises (CM) statistic is defined by

$$W^2 = n \int_{d_2}^{\infty} [F_n(x) - F_0(x)]^2 \, \mathrm{d}F_0(x)$$

with an alternative form for computational purposes

$$W^2 = \sum_{i=1}^{N_0+1} \left(Z_{(i)} - \frac{2i-1}{2n} \right)^2 + \frac{N_0+1}{12n^2} + \frac{n}{3} \left(Z_{(N_0+1)} - \frac{N_0+1}{n} \right)^3,$$

where $Z_{(i)} = 1 - F_0(x_{(n-i+1)}, \widehat{\boldsymbol{\theta}})$, $i = 1, \ldots, N_0$, and $Z_{(N_0+1)} = 1 - F_0(d_2, \widehat{\boldsymbol{\theta}})$.

4.1.3 Anderson-Darling Statistic

The Anderson-Darling (AD) statistic is a modification of the CM statistic placing more weight in the tails of the underlying distribution. It is defined by

$$A^2 = n \int_{d_2}^{\infty} \frac{[F_n(x) - F_0(x)]^2}{F_0(x)[1 - F_0(x)]} \, \mathrm{d}F_0(x)$$

with an alternative form for computational purposes

$$\begin{aligned} A^2 = & -\frac{1}{n} \sum_{i=1}^{N_0+1} (2i-1) \left[\log(Z_{(i)}) - \log(1 - Z_{(i)}) \right] - 2 \sum_{i=1}^{N_0+1} \log(1 - Z_{(i)}) \\ & - \frac{1}{n} \left[(N_0 + 1 - n)^2 \log(1 - Z_{(N_0+1)}) - (N_0+1)^2 \log(Z_{(N_0+1)}) + n^2 Z_{(N_0+1)} \right], \end{aligned}$$

where again $Z_{(i)} = 1 - F_0(x_{(n-i+1)}, \widehat{\boldsymbol{\theta}})$, $i = 1, \ldots, N_0$, and $Z_{(N_0+1)} = 1 - F_0(d_2, \widehat{\boldsymbol{\theta}})$.

4.2 Simulation Study

The empirical significance level as well as the power of the above mentioned tests was studied by means of Monte Carlo simulations. Tested models included the Weibull (denoted by $\mathrm{Wbl}(\lambda, \tau)$), lognormal (denoted by $\mathrm{LN}(\mu, \sigma)$) and gamma (denoted by $\mathrm{Gam}(\lambda, \kappa)$) distributions as these are among the most frequently used distributions when modelling censored environmental data. In case of the Weibull (lognormal respectively) distribution, the previously described transformation to the Gumbel (normal respectively) distribution was applied. The power of the goodness-of-fit tests was estimated by the proportion of the correct rejections of the null hypothesis at the significance level of $\alpha = 0.05$. The power of each statistic was simulated from 100,000 replications considering sample sizes

Table 4.1: Estimated power for various alternatives and censoring schemes when testing for the Weibull distribution; $n = 30, 100$.

		$n = 30$				$n = 100$			
Alt. model	Stat.	c_1	c_2	c_3	c_4	c_1	c_2	c_3	c_4
Wbl(1,0.5)	KS	0.0504	0.0493	0.0485	0.0499	0.0506	0.0505	0.0501	0.0500
	CM	0.0508	0.0494	0.0500	0.0488	0.0502	0.0503	0.0506	0.0515
	AD	0.0505	0.0493	0.0501	0.0490	0.0500	0.0496	0.0505	0.0506
Wbl(1,2)	KS	0.0493	0.0497	0.0496	0.0506	0.0501	0.0506	0.0511	0.0505
	CM	0.0498	0.0498	0.0500	0.0496	0.0509	0.0499	0.0510	0.0503
	AD	0.0496	0.0494	0.0498	0.0496	0.0507	0.0503	0.0514	0.0498
LN(0,0.5)	KS	0.2083	0.1679	0.1487	0.1324	0.5902	0.4462	0.3812	0.3503
	CM	0.2396	0.1891	0.1751	0.1612	0.6835	0.5303	0.4731	0.4238
	AD	0.2396	0.2044	0.1866	0.1631	0.6906	0.5607	0.4919	0.4130
LN(0,2)	KS	0.2073	0.1701	0.1481	0.1318	0.5854	0.4464	0.3858	0.3514
	CM	0.2399	0.1901	0.1759	0.1605	0.6819	0.5328	0.4793	0.4249
	AD	0.2388	0.2063	0.1860	0.1624	0.6892	0.5623	0.4970	0.4131
Gam(0.5,0.5)	KS	0.0696	0.0643	0.0628	0.0619	0.1278	0.1074	0.0992	0.0911
	CM	0.0720	0.0639	0.0617	0.0545	0.1469	0.1181	0.1069	0.0842
	AD	0.0726	0.0615	0.0597	0.0529	0.1546	0.1176	0.1053	0.0819
Gam(0.5,2)	KS	0.0627	0.0605	0.0588	0.0559	0.0952	0.0848	0.0768	0.0746
	CM	0.0676	0.0637	0.0628	0.0611	0.1093	0.0921	0.0869	0.0841
	AD	0.0683	0.0664	0.0653	0.0621	0.1141	0.0968	0.0913	0.0847

$n = 10, 20, 30, 50, 100, 200$ and censoring schemes $c_1, \ldots, c_4$, which represent proportions of censored observations between 10% and 70% (with a step of 20%). For example, c_3 represents 50% of censored values. Detection limits d_1, d_2 were selected as quantiles of the particular distribution using equations $q_i = F(d_i, \boldsymbol{\theta})$, $i = 1, 2$, where $q_2 = 0.1, 0.3, 0.5, 0.7$ and $q_1 = q_2/2$. Critical values of the test statistics were obtained by means of Monte Carlo simulations using 2,000,000 repetitions. When the alternative model is the model from which the data are simulated, the rejection probabilities give the power of the tests. In case the null hypothesis is true, it is expected that the statistics maintain the type I error rate. Overall, differences between the nominal level of 0.05 and the actual levels were very small for various censoring schemes and sample sizes, which shows a reliable performance of the goodness-of-fit statistics for left-censored data (see Tables 4.1–4.3).

Table 4.1 shows that power of all the test statistics is very low when data generated from the gamma distribution are tested for the Weibull distribution. Similar behavior is observed when data generated from Gam(0.5,2) are tested for the lognormal distribution (Table 4.2), and data generated from LN(0,0.5) and Wbl(1,2) are tested for the gamma distribution (Table 4.3). It is caused by the fact that it is very difficult to distinguish

Table 4.2: Estimated power for various alternatives and censoring schemes when testing for the lognormal distribution; $n = 30, 100$.

		$n = 30$				$n = 100$			
Alt. model	Stat.	c_1	c_2	c_3	c_4	c_1	c_2	c_3	c_4
LN(0,0.5)	KS	0.0491	0.0492	0.0507	0.0497	0.0507	0.0500	0.0497	0.0499
	CM	0.0487	0.0500	0.0502	0.0484	0.0505	0.0495	0.0494	0.0494
	AD	0.0485	0.0503	0.0508	0.0493	0.0509	0.0497	0.0497	0.0484
LN(0,2)	KS	0.0488	0.0496	0.0500	0.0508	0.0506	0.0496	0.0500	0.0492
	CM	0.0490	0.0495	0.0501	0.0491	0.0515	0.0498	0.0498	0.0497
	AD	0.0490	0.0495	0.0494	0.0493	0.0512	0.0500	0.0500	0.0499
Wbl(1,0.5)	KS	0.2188	0.1530	0.1219	0.0921	0.6180	0.4565	0.3461	0.2335
	CM	0.2636	0.1757	0.1195	0.0731	0.7501	0.5660	0.3809	0.1962
	AD	0.2673	0.1796	0.1227	0.0781	0.7870	0.6016	0.4099	0.2253
Wbl(1,2)	KS	0.2175	0.1543	0.1228	0.0919	0.6177	0.4552	0.3459	0.2320
	CM	0.2635	0.1758	0.1198	0.0735	0.7493	0.5653	0.3820	0.1954
	AD	0.2685	0.1792	0.1237	0.0786	0.7858	0.6003	0.4102	0.2235
Gam(0.5,0.5)	KS	0.3763	0.2675	0.2014	0.1336	0.8906	0.7563	0.6158	0.4062
	CM	0.4778	0.3221	0.1965	0.1012	0.9664	0.8753	0.6633	0.3301
	AD	0.5026	0.3394	0.2137	0.1169	0.9803	0.9077	0.7223	0.4100
Gam(0.5,2)	KS	0.1250	0.0970	0.0831	0.0696	0.3406	0.2421	0.1916	0.1414
	CM	0.1432	0.1065	0.0814	0.0589	0.4249	0.2961	0.2079	0.1227
	AD	0.1410	0.1052	0.0815	0.0600	0.4476	0.3110	0.2159	0.1314

between the gamma, lognormal and Weibull distributions in some cases (see Fig. 4.1).

As expected, the statistical power of the studied tests increases with increase in the sample size, and decreases with the increasing proportion of censored values. The relation between the power of the test and the sample size is visualized for several cases in Fig. 4.2. Note that the AD test seems to have the best performance for most cases in comparison to the CM and KS tests. In general, there is not much difference between the powers of the AD and CM tests and the KS test usually performs the worst. Let us look more closely at the tests' performance with regards to the proportion of censored values in a sample. If there is at most 50% of censored values (schemes c_1-c_3) in a sample, the AD test can be used without much hesitation. Nevertheless, when the proportion of censored values is high (70%; scheme c_4), the KS and CM tests sometimes outperform the AD test. In case of testing data with sample size $n < 100$ for the lognormal distribution, the KS test has the highest power (i.e. the lowest type II error), see Fig. 4.3. When testing lognormally distributed data with sample size $n > 50$ for the Weibull distribution and/or data generated from LN(0,2) for the gamma distribution, the CM test has the highest power. There are few other cases in which the KS test performs the best, specifically when

Table 4.3: Estimated power for various alternatives and censoring schemes when testing for the gamma distribution; $n = 30, 100$.

		$n = 30$				$n = 100$			
Alt. model	Stat.	c_1	c_2	c_3	c_4	c_1	c_2	c_3	c_4
Gam(0.5,0.5)	KS	0.0501	0.0507	0.0496	0.0505	0.0493	0.0506	0.0501	0.0505
	CM	0.0497	0.0516	0.0515	0.0512	0.0499	0.0498	0.0510	0.0509
	AD	0.0501	0.0514	0.0504	0.0509	0.0501	0.0494	0.0506	0.0507
Gam(0.5,2)	KS	0.0501	0.0505	0.0507	0.0501	0.0499	0.0497	0.0497	0.0512
	CM	0.0502	0.0504	0.0499	0.0502	0.0507	0.0498	0.0501	0.0504
	AD	0.0501	0.0502	0.0502	0.0498	0.0511	0.0503	0.0502	0.0509
LN(0,0.5)	KS	0.0963	0.0883	0.0829	0.0768	0.2097	0.1706	0.1521	0.1419
	CM	0.1061	0.0967	0.0933	0.0904	0.2486	0.2033	0.1848	0.1709
	AD	0.1152	0.1068	0.1019	0.0961	0.2640	0.2213	0.1956	0.1712
LN(0,2)	KS	0.5613	0.4790	0.4177	0.3751	0.9746	0.9395	0.8968	0.8565
	CM	0.6307	0.5401	0.4826	0.4389	0.9893	0.9678	0.9395	0.9002
	AD	0.6286	0.5504	0.4891	0.4293	0.9893	0.9701	0.9409	0.8901
Wbl(1,0.5)	KS	0.1385	0.1229	0.1133	0.1064	0.3723	0.3148	0.2817	0.2664
	CM	0.1610	0.1424	0.1348	0.1324	0.4465	0.3814	0.3469	0.3266
	AD	0.1648	0.1501	0.1396	0.1311	0.4568	0.4006	0.3612	0.3209
Wbl(1,2)	KS	0.0833	0.0722	0.0686	0.0645	0.1741	0.1391	0.1224	0.1011
	CM	0.0887	0.0743	0.0674	0.0546	0.2068	0.1610	0.1300	0.0896
	AD	0.0830	0.0693	0.0640	0.0516	0.2078	0.1611	0.1287	0.0892

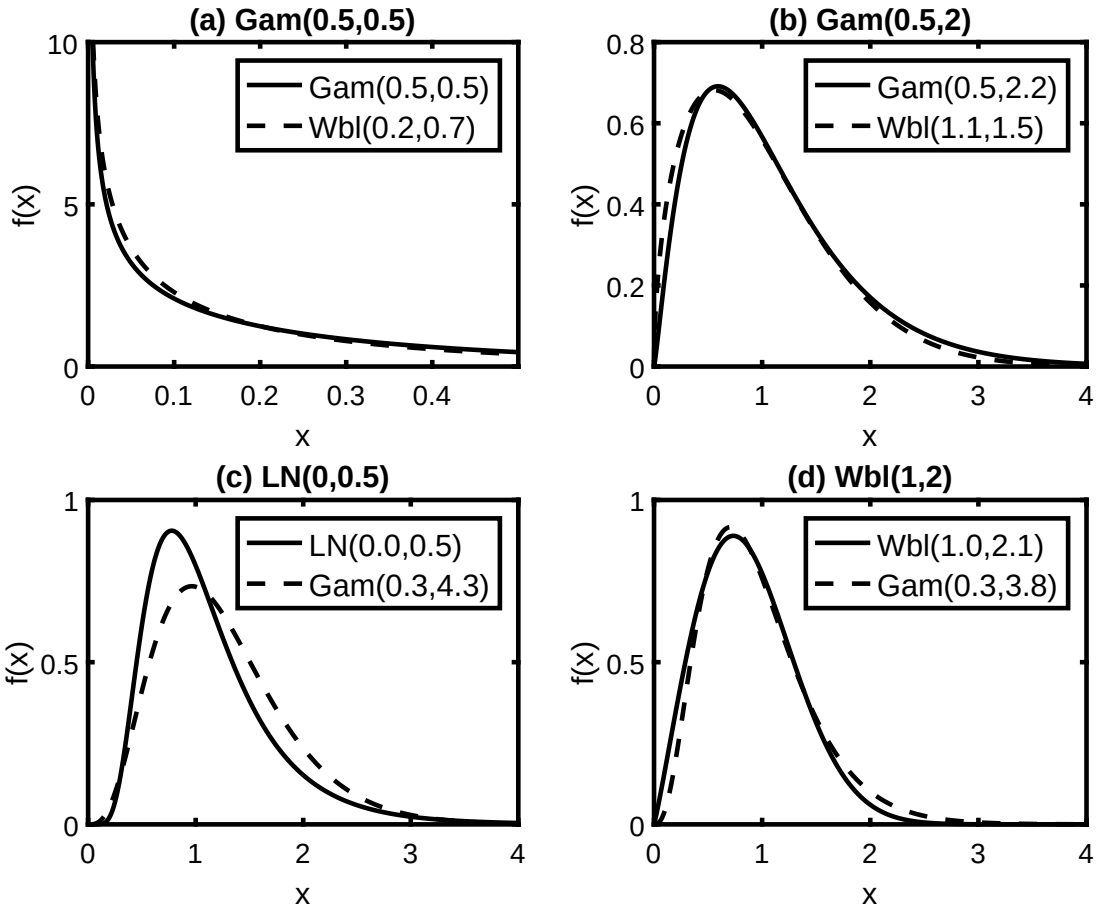


Figure 4.1: Densities of some alternative distributions (solid lines) compared with densities of the fitted distributions (dashed lines) for $n = 30$ and 30% of censored values.

data generated from Gam(0.5,0.5) are tested for the Weibull distribution and/or when data generated from Wbl(1,2) are tested for the gamma distribution. Similarly, when data generated from Wbl(1,0.5) are tested for the gamma distribution, the CM test performs the best. Nevertheless, in these three cases, the differences in tests' powers are very small and they can be considered negligible from the practical point of view.

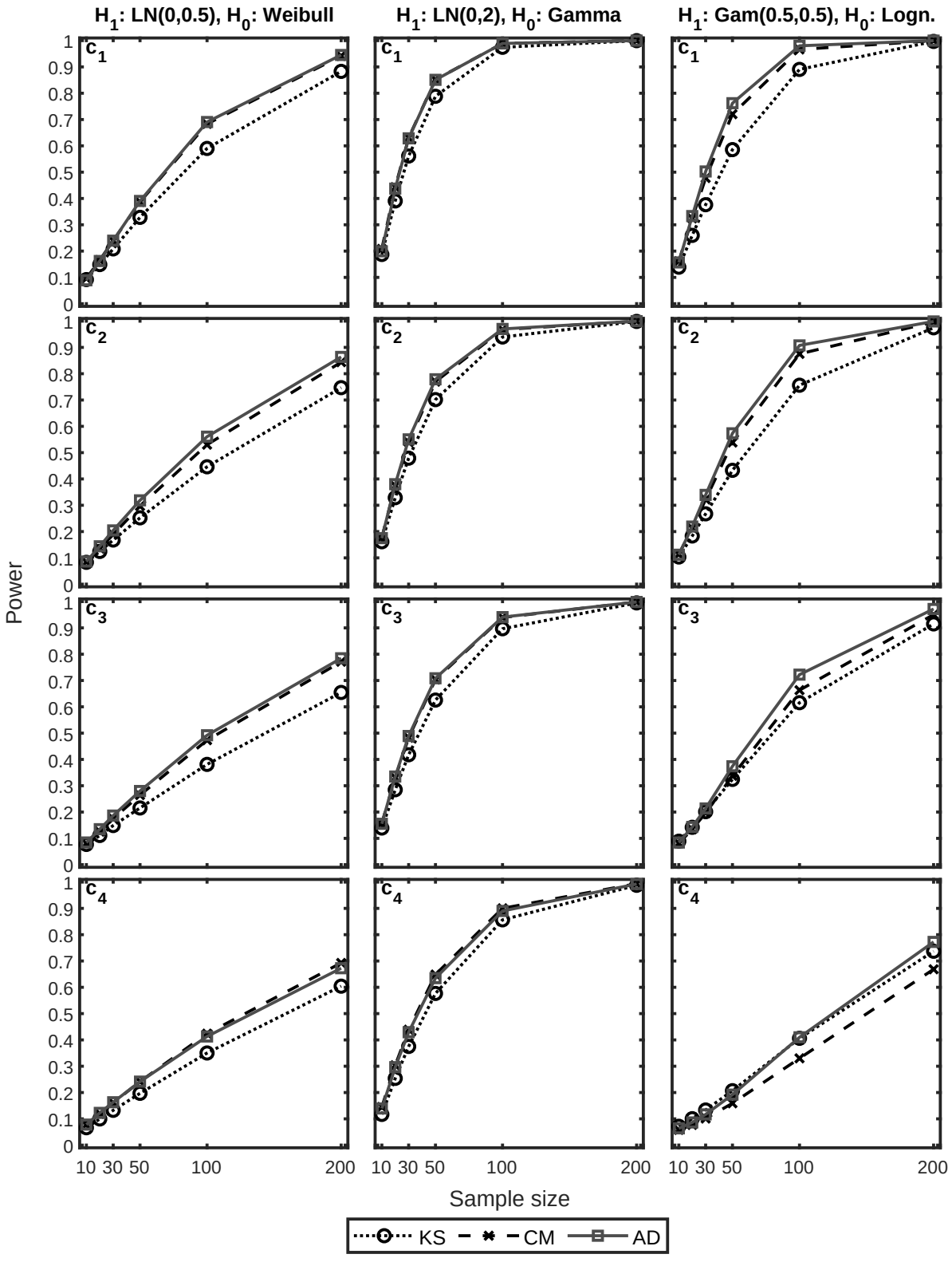


Figure 4.2: Estimated power for various alternatives as a function of the sample size and the proportion of censored values c_1 (10%), c_2 (30%), c_3 (50%), c_4 (70%) when testing for the Weibull (left), gamma (middle) and lognormal (right) distributions.

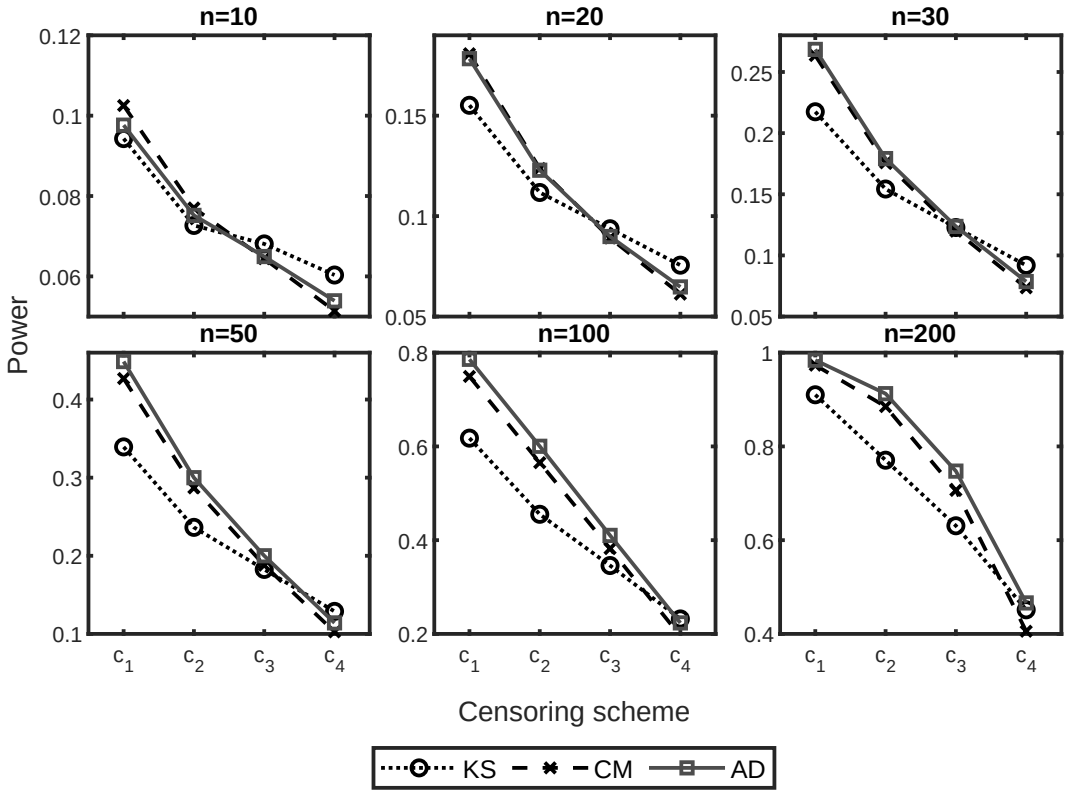


Figure 4.3: Estimated power for Wbl(1,2) alternative as a function of the sample size n and the proportion of censored values c_1 (10%), c_2 (30%), c_3 (50%), c_4 (70%) when testing for lognormal distribution.

Chapter 5

Applications

When dealing with environmental or microbiological data, measured values are often found below the detection limits of a measurement method, and only the number of values below the detection limits can be determined. There are usually two detection limits. One of them is called the limit of detection (LOD), which is the lowest quantity of a substance that can be distinguished from the absence of that substance (a blank value) within a stated confidence limit. The other one is called the limit of quantification (LOQ), which is the lowest analyte concentration that can be quantitatively detected with a stated accuracy and precision. In such case, we are dealing with Type I doubly left-censored data (Busschaert et al., 2010; Fusek et al., 2015; Pouillot et al., 2013; Shorten et al., 2006; Valero et al., 2017). In this chapter, statistical methods described in previous chapters are used for analyses of environmental data. Two approaches are used. The first one is based on the censored exponential and Weibull distributions. The second one is based on the so-called "replacement method," where all values under the detection limits are replaced by midpoints of intervals $(0, \mathrm{LOD}]$ and $(\mathrm{LOD}, \mathrm{LOQ}]$.

5.1 Musk Compounds

Synthetic aromatic substances or musk compounds are lipophilic contaminants able to accumulate in various components of the environment. They represent a group of persistent pollutants, and may occur in environmental matrices and human tissues. Synthetic aromatic substances were launched on the market in the early 20th century and the volume of their production has significantly increased in recent years (Luckenbach and Epel, 2005). Since they have potential carcinogenic properties, efforts are currently being made to limit or prohibit their use in many regions worldwide.

In general, musk compounds can be divided into four groups: linear, macrocyclic, polycyclic and nitro musk compounds. The last two groups are used most frequently as substitutes for natural musks in fragrances and personal hygiene products (OSPAR, 2004). Galaxolide (HHCB) and tonalide (AHTN) are examples of the most important polycyclic

musk compounds. Musk xylene, musk ketone and musk ambrette are well-known nitro musk compounds (i.e. compounds containing one or more nitro groups in a molecule). The production of nitro musk compounds, that are generally included in a group of substances posing a risk to the environment, has decreased over the last years (Bester, 2009; Rimkus, 1999). By contrast, production of polycyclic synthetic aromatic substances, which are less toxic, has increased because of their frequent use as additives in many personal care products, e.g. soaps, shampoos, deodorants, body lotions, perfumes, cleaning and disinfecting agents, air fresheners and industrial cleaning agents (see e.g. Sumner et al., 2010). Synthetic aromatic substances were also detected in samples of air and dust collected in indoor environments (Regueiro et al., 2009). They often penetrate into the environment through wastewater because of their ineffective removal in the wastewater treatment plant (WWTP), see e.g. Gómez et al. (2006) and references inside. Accumulation of these substances in the environment (surface water, sediment) results in their occurrence in food chain, especially in aquatic ecosystems. A number of studies revealed the presence of musk compounds in tissues of aquatic animals. These compounds can also be found in human body, for example in fat tissue, human milk and blood plasma (see e.g. Lignell et al., 2008; Zlámalová Gargošová et al., 2013), as a consequence of fish consumption.

The goal is:

a) to model musk compound concentrations using methods for censored samples;

b) to evaluate the amount of musk compounds in fish caught upstream and downstream the WWTP;

c) to compare mean concentrations and distributions of concentrations of musk compounds in fish caught upstream and downstream the WWTP.

5.1.1 Data

The sample of aquatic biota consists of 60 fish from the carp family, specifically of the European chub (Leuciscus cephalus), which were caught in the Svratka River, Czech Republic, near the WWTP Brno-Modřice by Morava River Basin Administration employees. Fish were caught on 10th November 2009; half of them came from a watercourse upstream (Group 1), and half of them from a watercourse downstream (Group 2) from the WWTP. The fish were transported to the laboratory of the Institute of Veterinary Hygiene and Ecology of Veterinary and Pharmaceutical University in Brno, and examined by a veterinarian. Relevant characteristics were noted and then muscle, skin and guts were separated. Muscle tissue was selected for the musk compound analysis because it is considered to be representative of all of the body. The muscle tissue was homogenized (using a blender), subsequently frozen at -20 °C and kept frozen until the analysis. Fish of approximately the same age were chosen for the analysis. As a result, four nitro (musk ambrette - AMB,

Table 5.1: Musk compounds distribution in fish samples upstream and downstream the WWTP.

	Upstream			Downstream			LOD [μg/kg]	LOQ [μg/kg]
	N_1^a	N_2^b	N_0^c	N_1	N_2	N_0		
PH	18	12	0	23	6	1	0.55	1.82
AMB	28	2	0	28	2	0	1.46	4.88
TR	24	6	0	22	8	0	1.11	3.68
HHCB	3	23	4	0	22	8	8.95	29.83
AHTN	6	17	7	8	4	18	1.98	6.62
MX	22	4	4	23	6	1	0.75	2.50
TIB	27	1	2	28	2	0	0.15	0.51
MK	0	17	13	0	19	11	0.57	1.90

[a] N_1 - the number of values below the LOD
[b] N_2 - number of values in the interval (LOD,LOQ]
[c] N_0 - number of uncensored values

musk xylene - MX, musk tibetene - TIB, musk ketone - MK), and four polycyclic musk compounds (phantolide - PH, traseolide - TR, galaxolide - HHCB, tonalide - AHTN) were detected. Details of the chemical analyses can be found in Fusek et al. (2015). The LOD and the LOQ were calculated using calibration curves of particular analytes, see Kellner (1998) for more information. Frequencies of censored and uncensored musk compound concentrations are presented in Table 5.1 together with the specified detection limits.

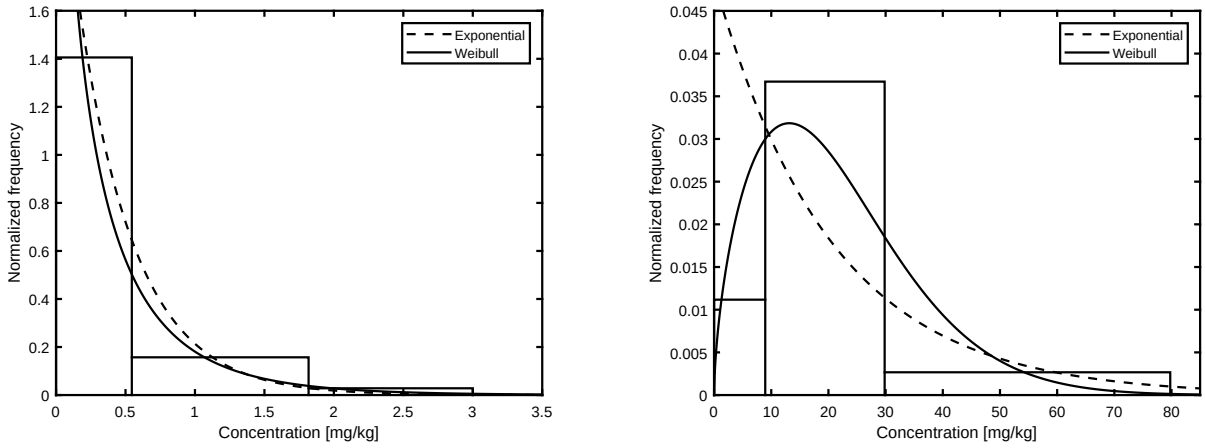


Figure 5.1: Histogram (normalized to the pdf) of a) PH concentrations downstream, b) HHCB concentrations upstream the WWTP with exponential and Weibull densities.

5.1.2 Results

The suitability of the exponential and the Weibull distributions for modelling of BA concentrations was tested using Pearson's χ^2 goodness-of-fit test and Cramér-von Mises test for censored data that was implemented in Matlab (version R2022b). Moreover, graphical analysis of the data was used in order to choose the model distribution. Specifically, Q-Q plots and correspondence between the histogram (normalized to the pdf) and the exponential (Weibull respectively) density was assessed. It was found out that it is possible to use the exponential distribution for modelling of PH, AMB, TR, TIB and MK (see Fig. 5.1a for an example). In case of HHCB and MX, it was necessary to use the Weibull distribution (see Fig. 5.1b for an example). In case of AHTN in fish caught downstream the WWTP, neither the exponential nor the Weibull distribution was suitable and we applied the more flexible Weibull distribution just for illustration purposes.

Mean musk compound concentrations were estimated together with their 95% confidence limits using methods for censored exponential and Weibull distributions (see Table 5.2), and using the replacement method, where all censored values were replaced by midpoints of intervals $(0, \mathrm{LOD}]$ and $(\mathrm{LOD}, \mathrm{LOQ}]$ (see Table 5.3). It can be seen that both estimates are quite similar. Mean musk compound concentration estimates based on censored distributions are of lower values than those estimated using the replacement method in most cases. In order to assess the estimation quality, a simulation study was carried out in Fusek et al. (2015). The authors showed that behavior of mean and variance estimates based on the censored distribution and the replacement method (using the sample mean and the sample variance) are rather similar in case of low censoring. On the other hand, when the number of censored values is high, performance of the estimates based on the replacement method is not particularly good.

Results of the comparison of mean musk compound concentrations in fish caught upstream and downstream the WWTP are presented in Table 5.4. There is no significant difference between the two groups in most cases. In case of methods for censored distributions, there is a significant difference in mean concentrations of TIB between fish caught upstream and downstream the WWTP at the significance level of 0.05. On the other hand, the replacement method was not able to reveal the difference between mean concentrations of TIB in fish caught upstream and downstream the WWTP. Another part of the analysis was to compare distributions of musk compound concentrations in fish caught upstream and downstream the WWTP. It was found out that all tests (the likelihood ratio test, the Lagrange multiplier test, and the Wald test) give similar results. There is no significant difference between the two groups at the significance level of 0.05 with the exception of TIB.

To summarize the results, it was found out that the WWTP has no significant influence on concentrations of musk compounds in fish tissue at the significance level of 0.05 with the exception of musk tibetene.

Table 5.2: Mean musk compound concentrations (in μg/kg) with their standard deviations (SD) and 95% lower (LCL) and upper (UCL) confidence limits estimated using the censored exponential (PH, AMB, TR, TIB) and Weibull (HHCB, AHTN, MX, MK) distributions.

	Upstream				Downstream			
	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL
PH	0.512	0.107	0.303	0.721	0.411	0.088	0.239	0.583
AMB	0.540	0.136	0.274	0.806	0.540	0.136	0.274	0.806
TR	0.669	0.147	0.381	0.957	0.792	0.170	0.459	1.126
HHCB	21.482	2.676	16.238	26.726	26.008	2.593	20.926	31.091
AHTN	4.664	0.610	3.468	5.860	6.140	0.802	4.568	7.712
MX	0.934	0.405	0.141	1.727	0.544	0.151	0.249	0.839
TIB	0.201	0.040	0.122	0.280	0.057	0.014	0.029	0.085
MK	2.194	0.411	1.389	3.000	1.918	0.361	1.210	2.625

Table 5.3: Mean musk compound concentrations (in μg/kg) with their standard deviations (SD) and 95% lower (LCL) and upper (UCL) confidence limits estimated using the replacement method.

	Upstream				Downstream			
	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL
PH	0.636	0.083	0.474	0.798	0.513	0.085	0.346	0.680
AMB	0.895	0.113	0.673	1.116	0.895	0.113	0.673	1.116
TR	0.921	0.137	0.653	1.189	1.044	0.151	0.747	1.340
HHCB	21.923	2.516	16.991	26.855	25.606	2.347	21.006	30.205
AHTN	4.757	0.559	3.662	5.852	6.170	0.717	4.765	7.575
MX	1.064	0.253	0.568	1.559	0.716	0.124	0.472	0.959
TIB	0.211	0.094	0.027	0.395	0.094	0.012	0.071	0.118
MK	2.232	0.381	1.485	2.980	1.966	0.241	1.493	2.439

Table 5.4: Comparison of mean musk compound concentrations between fish caught upstream and downstream the WWTP using methods for censored distributions with statistic (3.5) (p-value p_{cen}), and the replacement method with statistic (3.6) (p-value p_{rep}). Comparison of distributions of musk compound concentrations using the likelihood ratio test (p-value p_{LR}), the Lagrange multiplier test (p-value p_{LM}), the Wald test (p-value p_{W}) and statistics (3.4).

	Comparison of means		Comparison of distributions		
	p_{cen}	p_{rep}	p_{LR}	p_{LM}	p_{W}
PH	0.47	0.30	0.45	0.44	0.47
AMB	1.00	1.00	1.00	1.00	1.00
TR	0.58	0.55	0.58	0.57	0.58
HHCB	0.22	0.28	0.36	0.33	0.38
AHTN	0.14	0.12	0.28	0.28	0.31
MX	0.37	0.22	0.37	0.42	0.47
TIB	$< 0.01^*$	0.22	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$
MK	0.61	0.56	0.61	0.60	0.61

* - rejection of the hypothesis at the significance level of 0.05

5.2 Biogenic Amines

Biogenic amines (BAs; e.g. histamine, tyramine, fenyletylamine, tryptamine, putrescine, kadaverine, spermine and spermidine) are biologically active organic bases with a low molecular weight which are synthesized by living organisms for their own needs. They pass into food and beverages through ingredients (usually a small amount) and are also generated by microbial decarboxylation of amino acids. The intake of BAs into the body is regulated by a detoxification system composed of monoamine oxidases, diamino oxidases and histidine methyl-transferases. High intake of BAs (in general over 100 mg/kg of food) or the presence of factors that reduce the effectiveness of the detoxification system can lead to intoxication which may endanger health and, in some cases, life (Halász et al., 1994; Shalaby, 1996; Silla Santos, 1996; Ten Brink et al., 1990). For example, in case of histamine, there is a legislatively based concentration limit of 100 mg/kg (200 mg/kg, respectively) in fish and fishery products (Commission Regulation EC 2073/2005). Moreover, lower limits for specific BAs have been proposed in literature, e.g. 10 mg/kg of histamine, 80 mg/kg of tyramine, and 3 mg/kg of phenylethylamine (Halász et al., 1994; Ten Brink et al., 1990).

Freshwater and saltwater fish are an important part of our diet owing to a high content of polyunsaturated fatty acids, minerals and other biologically active substances. Nevertheless, fish meat represents a system with very short shelf-life due to very fast post-mortem changes which are related to frequent occurrence of BAs. Frequent contaminants

of fish include bacteria from the *Enterobacteriaceae* family and the genera Pseudomonas. In addition, the lactic acid bacteria, e.g. representatives of the genera Lactobacillus and Enterococcus, can also contribute to production of BAs (Apetrei and Apetrei, 2015; Arnold and Brown, 1978; Jaw et al., 2012; Kaale et al., 2011; Prester, 2011; Rawles et al., 1996; Zhang et al., 2010). The content of BAs in fish meat was previously studied in Buňka et al. (2013). They found out that the BA content was higher than 100 mg/kg in approximately 15% of samples. Moreover, in 6 samples the concentrations were so high that they failed to comply with legislative requirements established in Commission Regulation EC 2073/2005. Such high concentrations have a significant impact on food safety, and may endanger health or even life of sensitive individuals, which emphasizes the importance of monitoring BAs in these commodities.

Since in the previous study by Buňka et al. (2013) the concentrations below detection limits were not taken into account, the goal is:

a) to model concentration of BAs using methods for censored samples;

b) to evaluate the amount of BAs in various fish species (Atlantic salmon, Atlantic cod, striped catfish);

c) to compare mean BA concentrations and distributions of concentrations among the species;

d) to determine the risk of exceeding certain BA limits for various fish species.

5.2.1 Data

In total 54 samples of fish commonly consumed in Central Europe were analyzed. There were 18 samples of Atlantic salmon (Salmo salar), 17 samples of Atlantic cod (Gadus morhua), and 19 samples of striped catfish (Pangasius hypophthalmus). The fish were bought in retail stores, stored on ice, and the samples were extracted from commonly consumed parts of the fish. The same parts of the fish muscle tissue were used. The period between buying the fish and start of lyophilization of the samples in the laboratory did not exceed 6 hours, and the samples were stored in a fridge at 2 ± 1 °C. The samples were extracted immediately after the lyophilization.

The extraction and determination of BAs (histamine - HIM, tyramine - TYM, phenylethylamine - PHE, tryptamine - TRM, putrescine - PUT, cadaverine - CAD, spermidine - SPD, spermine - SPN) were carried out according to Buňka et al. (2013). The BA content in samples was determined using high performance liquid chromatography (LabAlliance, State College, USA; Agilent Technologies, Agilent, Palo Alto, USA) after preceding derivatization with dansyl chloride. Every sample was analyzed eight times (2 extracts of each sample, times 2 derivatizations of each extract, times 2 analyses of each derivatized extract). Results (in mg/kg) are expressed for the fresh matter before lyophilization. The

Table 5.5: Biogenic amines distribution in fish samples.

	Atlantic salmon			Atlantic cod			Striped catfish			LOD [mg/kg]	LOQ [mg/kg]
	N_1^a	N_2^b	N_0^c	N_1	N_2	N_0	N_1	N_2	N_0		
TRM	17	1	0	15	2	0	15	4	0	0.13	0.35
PHE	12	2	4	9	1	7	16	1	2	0.06	0.21
PUT	0	0	18	0	0	17	2	1	16	0.16	0.82
CAD	7	1	10	4	1	12	10	1	8	0.09	0.26
HIM	10	2	6	4	1	12	16	3	0	0.11	0.38
TYM	10	0	8	4	0	13	13	2	4	0.01	0.08
SPD	0	0	18	1	1	15	0	0	19	0.13	0.29
SPN	0	0	18	0	0	17	1	0	18	0.02	0.13

[a] N_1 - the number of values below the LOD

[b] N_2 - number of values in the interval (LOD,LOQ]

[c] N_0 - number of uncensored values

LOD and the LOQ were determined according to standard chromatography procedures (Lister, 2005; Wenzl et al., 2016) and in accordance with ISO 17025 (ISO, 2017). Frequencies of censored and uncensored BA concentrations for various fish species are presented in Table 5.5 together with the specified detection limits.

5.2.2 Results

The suitability of the exponential and the Weibull distributions for modelling of BA concentrations was tested using Pearson's χ^2 goodness-of-fit test and Cramér-von Mises test for censored data that was implemented in Matlab (version R2022b). Moreover, graphical analysis of the data was used in order to choose the model distribution. Specifically, Q-Q plots and correspondence between the histogram (normalized to the pdf) and the exponential (Weibull respectively) density was assessed. It was found out that the Weibull distribution is suitable (despite some anomalies caused by extreme values or missing values in the interval (LOD,LOQ]) for modelling of all the BAs. In addition, it was possible to use the exponential distribution for modelling of TRM, CAD, HIM and TYM (see Fig. 5.2a for an example). In case of PHE, PUT, SPD and SPN, it was necessary to use the Weibull distribution (see Fig. 5.2b for an example).

Estimation of BA Concentrations

Mean BA concentrations were estimated together with their 95% confidence limits using methods for censored exponential and Weibull distributions and the results are in Table 5.6. It can be seen that concentrations of TRM, PHE, TYM, SPD and SPN are relatively low and do not pose a high risk to consumers' health. Nevertheless, the amount of PUT was

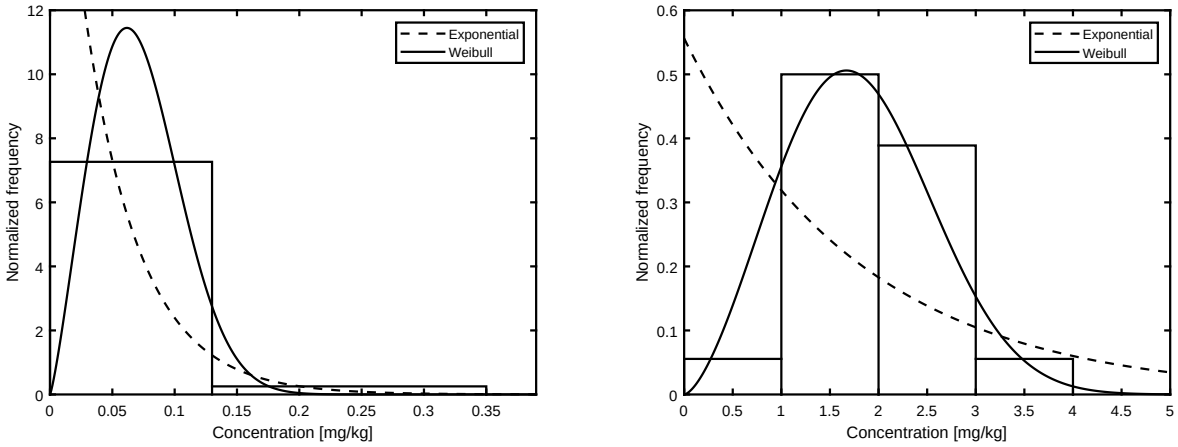


Figure 5.2: Histogram (normalized to the pdf) of a) TRM, b) SPN concentrations in Atlantic salmon with exponential and Weibull densities.

relatively high and can have a negative impact on food safety, and ultimately on consumers' health, especially in combination with alcohol consumption, which inhibits the detoxification system in the human body (Shalaby, 1996; Silla Santos, 1996; Ten Brink et al., 1990). Similar conclusions can be made in case of CAD in Atlantic cod and Atlantic salmon and HIM in Atlantic salmon, where the concentrations of BAs are also high.

In Table 5.7, there are mean BA concentrations together with their 95% confidence limits that were estimated using the replacement method, where all censored values were replaced by midpoints of intervals $(0, \text{LOD}]$ and $(\text{LOD}, \text{LOQ}]$. In a situation where there are no uncensored values, the ability of estimating mean concentrations is very limited. In case of TRM (and HIM for striped catfish), the replacement method overestimates the mean concentration and underestimates its variability in comparison to the use of censored distribution. When both censored and uncensored values are present, the estimates of mean concentrations are quite similar with the exception of PHE, where the replacement method underestimates the mean concentration.

Comparison of BA Concentrations

Results of the comparison of mean BA concentrations are presented in Table 5.8. First of all, let us focus on the methods for censored distributions. There is a significant difference in mean concentrations of HIM, TYM and SPD among all three species at the significance level of 0.05. Moreover, in case of CAD, only Atlantic salmon and Atlantic cod have similar mean concentrations. In case of SPN, only Atlantic cod and striped catfish have similar mean concentrations. Furthermore, let us focus on the replacement method, where the equality of mean concentrations was tested using the asymptotic t-test. Contradictory results were obtained in case of comparison of a) Atlantic salmon and Atlantic cod for HIM and SPD, and b) Atlantic salmon and striped catfish for SPD, where the replacement

Table 5.6: Mean BA concentrations (in mg/kg) with their standard deviations (SD) and 95% lower (LCL) and upper (UCL) confidence limits estimated using the censored exponential (TRM, CAD, HIM, TYM) and Weibull (PHE, PUT, SPD, SPN) distributions.

	Atlantic salmon				Atlantic cod				Striped catfish			
	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL
TRM	0.045	0.015	0.015	0.074	0.060	0.018	0.024	0.095	0.079	0.021	0.037	0.121
PHE	0.492	0.565	0.000	1.601	0.670	0.512	0.000	1.674	0.860	2.886	0.000	6.517
PUT	38.867	13.787	11.845	65.890	36.367	2.738	31.001	41.732	25.210	6.844	11.795	38.624
CAD	8.335	1.968	4.478	12.192	10.447	2.538	5.474	15.421	0.396	0.094	0.213	0.580
HIM	12.470	2.944	6.700	18.240	3.807	0.928	1.987	5.627	0.059	0.017	0.026	0.092
TYM	5.165	1.218	2.777	7.552	0.504	0.123	0.262	0.745	0.093	0.022	0.049	0.137
SPD	5.136	1.556	2.087	8.186	0.747	0.115	0.522	0.971	1.817	0.307	1.215	2.420
SPN	1.801	0.178	1.452	2.150	0.741	0.088	0.568	0.913	0.690	0.123	0.449	0.930

Table 5.7: Mean BA concentrations (in mg/kg) with their standard deviations (SD) and 95% lower (LCL) and upper (UCL) confidence limits estimated using the replacement method.

	Atlantic salmon				Atlantic cod				Striped catfish			
	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL	Mean	SD	LCL	UCL
TRM	0.075	0.010	0.056	0.094	0.086	0.014	0.058	0.113	0.102	0.017	0.069	0.135
PHE	0.334	0.147	0.046	0.621	0.491	0.152	0.193	0.790	0.298	0.227	0.000	0.743
PUT	38.988	13.065	13.380	64.596	36.479	2.676	31.234	41.724	24.481	4.607	15.451	33.511
CAD	8.335	3.223	2.018	14.652	10.447	3.366	3.850	17.044	0.397	0.142	0.118	0.677
HIM	12.470	5.625	1.446	23.494	3.807	0.979	1.889	5.725	0.085	0.016	0.053	0.117
TYM	5.165	1.860	1.518	8.811	0.504	0.105	0.299	0.709	0.094	0.044	0.008	0.180
SPD	5.515	2.929	0.000	11.257	0.745	0.119	0.511	0.979	1.793	0.364	1.081	2.506
SPN	1.798	0.179	1.447	2.149	0.737	0.092	0.557	0.917	0.693	0.121	0.457	0.930

Table 5.8: Comparison of mean BA concentrations among various fish species using methods for censored distributions with statistic (3.5) (p-value p_{W}), and the replacement method with statistic (3.6) (p-value p_{rep}). Comparison of distributions of BA concentrations using the likelihood ratio test (3.4) (p-value p_{LR}).

	Atlantic salmon vs. Atlantic cod			Atlantic salmon vs. Striped catfish			Atlantic cod vs. Striped catfish		
	p_{W}	p_{rep}	p_{LR}	p_{W}	p_{rep}	p_{LR}	p_{W}	p_{rep}	p_{LR}
TRM	0.53	0.53	0.52	0.20	0.16	0.18	0.50	0.46	0.49
PHE	0.82	0.46	0.57	0.90	0.89	0.40	0.95	0.48	0.06
PUT	0.86	0.85	$< 0.01^*$	0.38	0.30	0.54	0.13	0.02^*	$< 0.01^*$
CAD	0.51	0.65	0.50	$< 0.01^*$	0.01^*	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$
HIM	$< 0.01^*$	0.13	$< 0.01^*$	$< 0.01^*$	0.03^*	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$
TYM	$< 0.01^*$	0.01^*	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$
SPD	$< 0.01^*$	0.10	$< 0.01^*$	0.04^*	0.21	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	0.01^*
SPN	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	$< 0.01^*$	0.74	0.77	0.17

* - rejection of the hypothesis at the significance level of 0.05

method was not able to reveal the difference between mean BA concentrations. One of the reasons for that could be a low power of the asymptotic test caused by the small sample sizes or a high skewness of the data. Moreover, there is a high variability of the estimate of the mean HIM concentration in Atlantic salmon (see standard deviations in Table 5.7) which can affect the test results. In case of Atlantic cod and striped catfish for PUT, the high variability of mean concentration estimates (see standard deviations in Table 5.6) has a significant influence on values of the test statistics (3.5) which results into non-significant differences between the means.

Another part of the analysis was to compare distributions of BA concentrations among various species. It was found out that all tests (the likelihood ratio test, the Lagrange multiplier test, and the Wald test) give similar results. On that account, only results for the likelihood ratio test are presented in Table 5.8. It can be seen that the results are very similar to the comparison of mean BA concentrations with one exception. There is a significant difference in distributions of PUT concentrations between Atlantic cod and the other species, even though the mean concentrations among species are similar (see Fig. 5.3a). In case of SPN, there is a clear difference in distributions between Atlantic salmon and the other species. Nevertheless, the difference in distributions between Atlantic cod and striped catfish is not significant enough to warrant rejection of the null hypothesis at the significance level of 0.05 (see Fig. 5.3b).

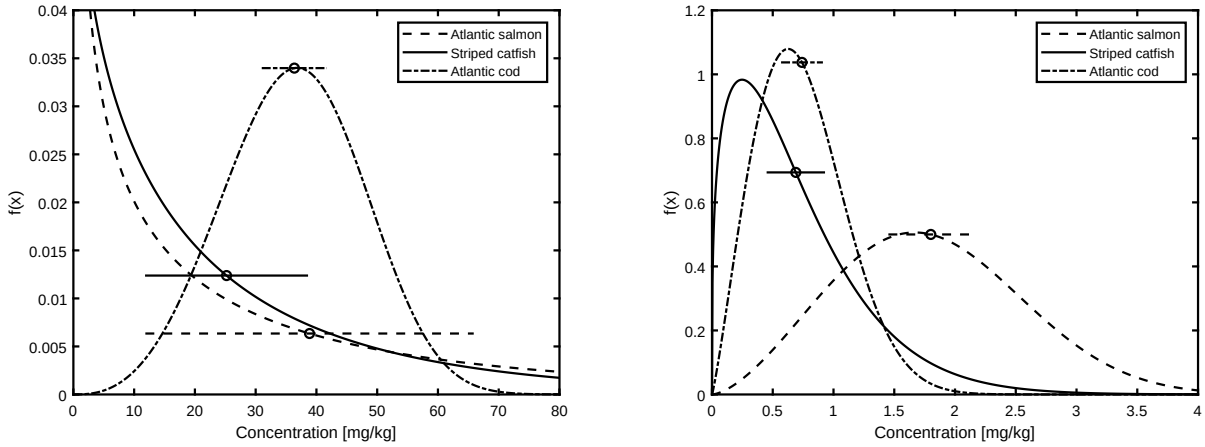


Figure 5.3: Probability density functions of a) PUT, b) SPN concentrations with mean values (circle) and their confidence intervals (horizontal line).

Risk Probabilities

Once the model distributions of BA concentrations are stated and the unknown parameters in the model are estimated, probabilities of exceeding certain limit values of BA concentrations can be calculated. The risk probability R of exceeding the limit value LV can be approximated using formula

$$R = P(X > LV) \doteq 1 - F(x, \widehat{\lambda}, \widehat{\tau}),$$

where $F(x, \lambda, \tau)$ is cdf (2.1).

In general, it is difficult to select a specific limit value of BA concentrations that could seriously harm consumers' health. In fact, every BA has its own physiological effect on human body; additionally, each body reacts to exposure to BAs (and other biologically active substances) in a slightly different way. Based on our opinion and also recommendations regarding the food safety in other studies, four limit values of BA concentrations were selected, specifically 3, 10, 22 and 100 mg/kg. According to Halász et al. (1994), Shalaby (1996) and Ten Brink et al. (1990), the limits of 3 and 10 mg/kg are very important especially for PHE and HIM. Higher concentrations can cause vasodilation effects (affect blood pressure and heart activity), headache and/or breathing problems. More serious problems can be expected with increased alcohol consumption and/or when antihistamins are used. Table 5.9 shows that HIM concentration in Atlantic salmon exceeds the limit value of 3, 10 and 22 mg/kg with probabilities 0.79, 0.45 and 0.17. Additionally, PUT and CAD concentrations over 20 mg/kg can increase the effects of HIM, TYM and PHE on the human body (Halász et al., 1994; Shalaby, 1996; Ten Brink et al., 1990). Table 5.9 shows that PUT concentration exceeds the limit value of 22 mg/kg with probabilities 0.38 for striped catfish, 0.44 for Atlantic salmon, and 0.89 in case of Atlantic cod. CAD

Table 5.9: Probabilities of exceeding limit values (LV) of BA concentrations for Atlantic salmon (AS), Atlantic cod (AC), and striped catfish (SC).

LV [mg/kg]	3			10			22			100		
	AS	AC	SC	AS	AC	SC	AS	AC	SC	AS	AC	SC
TRM	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
PHE	0.03	0.05	0.03	< 0.01	< 0.01	0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
PUT	0.81	1.00	0.84	0.62	0.99	0.61	0.44	0.89	0.38	0.10	< 0.01	0.03
CAD	0.70	0.75	< 0.01	0.30	0.38	< 0.01	0.07	0.12	< 0.01	< 0.01	< 0.01	< 0.01
HIM	0.79	0.45	< 0.01	0.45	0.07	< 0.01	0.17	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
TYM	0.56	< 0.01	< 0.01	0.14	< 0.01	< 0.01	0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
SPD	0.48	< 0.01	0.17	0.15	< 0.01	< 0.01	0.03	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
SPN	0.07	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

concentration exceeds 22 mg/kg with probabilities 0.07 for Atlantic salmon, and 0.12 for Atlantic cod. The limit of 100 mg/kg is the generally accepted limit for evaluation of food safety not only for individual BAs, but also for the total amount of BA concentrations (Benkerroum, 2016; EFSA, 2011; Halász et al., 1994; Kalač, 2014; Ten Brink et al., 1990). The limit value of 100 mg/kg is exceeded only in case of PUT concentration in Atlantic salmon with probability 0.1, and in striped catfish with probability 0.03.

Conclusion

This thesis described and analyzed statistical methods that can be used when dealing with Type I multiply left-censored data with the Weibull distribution. The maximum likelihood method was used for estimation of the unknown parameters. It was shown using simulations that the estimates of parameter λ have lower bias for higher values of parameter τ, i.e. for a lower skewness of the sample distribution. The estimates of parameter τ are similar bias-wise for various values of τ. Moreover, in order to describe variability of the parameters' estimates, the expected Fisher information matrix should be preferred, especially for small sample sizes. In addition, confidence intervals for the expected value of the censored Weibull distribution were investigated. Despite the fact, that in case of high number of censored values confidence intervals based on the maximum likelihood method are much wider than confidence intervals obtained using the bootstrap, the maximum-likelihood-based confidence intervals have better coverage probabilities. Moreover, there were described statistical tests for comparison of expected values and/or distributions of two independent censored samples from Weibull distribution. When we want to compare more than two samples, Bonferroni correction (or other types of corrections like Holm-Bonferroni or Šidák's correction etc.) can be applied to control the family-wise error rate, i.e. the probability of making at least one Type I error when performing multiple hypotheses tests. In addition, statistical tests for testing reduction of the censored Weibull distribution to the exponential submodel were proposed, because the Weibull distribution can sometimes be unnecessarily complicated for modelling of real data. Since all methods described in this thesis assume that the censored data have Weibull distribution, several goodness-of-fit tests were assessed. It was shown using simulations that the Anderson-Darling test has the best performance in most cases.

Statistical methods described in this thesis were applied in modelling of real data. Specifically, for assessing the impact of the wastewater treatment plant on musk compounds concentrations in fish, for the comparison of biogenic amines concentrations in various fish species, and for modelling of elemental carbon concentrations in Mbengue et al. (2018). Because of the flexibility of the Weibull distribution, more applications could be found in other areas. In addition, Type I left-censored distributions were also applied in the extreme value theory for estimation of the extremal index (Holešovský and Fusek, 2020), see Appendix B for more details.

All methods used in this thesis were implemented in Matlab (version R2022b) and are available from the author upon request.

Appendices

Appendix A

Derivation of the Expected FIM

The expected FIM (2.8) is calculated using formula

$$\boldsymbol{J}_n(\lambda,\tau) = n\boldsymbol{J}(\lambda,\tau) = n\begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} = \begin{bmatrix} -\mathrm{E}\frac{\partial^2 l}{\partial\lambda^2} & -\mathrm{E}\frac{\partial^2 l}{\partial\lambda\partial\tau} \\ -\mathrm{E}\frac{\partial^2 l}{\partial\tau\partial\lambda} & -\mathrm{E}\frac{\partial^2 l}{\partial\tau^2} \end{bmatrix},$$

where

$$\begin{aligned} nJ_{11} = & -\sum_{i=1}^{k}\mathrm{E}\left(N_i\right)\left\{\frac{\left(d_i^{\tau}\lambda^{\tau}\tau^2 + d_i^{\tau}\lambda^{\tau}\tau - d_i^{2\tau}\tau^2\right)\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}\right. \\ & -\frac{\left(d_{i-1}^{\tau}\lambda^{\tau}\tau^2 + d_{i-1}^{\tau}\lambda^{\tau}\tau - d_{i-1}^{2\tau}\tau^2\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}} \\ & \left.-\frac{\tau^2\left\{d_{i-1}^{\tau}\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - d_i^{\tau}\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}{\lambda^{2\tau+2}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}\right\} \\ & -\mathrm{E}\left(N_0\right)\frac{\tau}{\lambda^2} + \frac{\tau^2+\tau}{\lambda^{\tau+2}}\mathrm{E}\left(\sum_{i=n-N_0+1}^{n} X_{(i)}^{\tau}\right), \end{aligned} \tag{A.1}$$

$$\begin{aligned} nJ_{22} = & -\sum_{i=1}^{k}\mathrm{E}\left(N_i\right)\left\{\frac{\left(d_i^{\tau}\lambda^{\tau} - d_i^{2\tau}\right)\left[\log\left(\frac{d_i}{\lambda}\right)\right]^2\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}}\right. \\ & -\frac{\left(d_{i-1}^{\tau}\lambda^{\tau} - d_{i-1}^{2\tau}\right)\left[\log\left(\frac{d_{i-1}}{\lambda}\right)\right]^2\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right]}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}} \\ & \left.-\frac{\left\{d_{i-1}^{\tau}\log\left(\frac{d_{i-1}}{\lambda}\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - d_i^{\tau}\log\left(\frac{d_i}{\lambda}\right)\exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}{\lambda^{2\tau}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^{\tau}\right] - \exp\left[-\left(\frac{d_i}{\lambda}\right)^{\tau}\right]\right\}^2}\right\} \end{aligned} \tag{A.2}$$

$$
\begin{aligned}
&+\frac{\mathrm{E}\left(N_0\right)}{\tau^2}+\frac{\left[\log(\lambda)\right]^2}{\lambda^\tau}\mathrm{E}\left(\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\right)-\frac{2\log(\lambda)}{\lambda^\tau}\mathrm{E}\left[\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\log\left(X_{(i)}\right)\right]\\
&+\frac{1}{\lambda^\tau}\mathrm{E}\left\{\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\left[\log\left(X_{(i)}\right)\right]^2\right\},
\end{aligned}
$$

$$
\begin{aligned}
nJ_{12}=nJ_{21}=-\sum_{i=1}^{k}\mathrm{E}\left(N_i\right)\Bigg\{&\frac{\left[d_i^{2\tau}\tau\log\left(\frac{d_i}{\lambda}\right)-d_i^\tau\lambda^\tau\tau\log\left(\frac{d_i}{\lambda}\right)-d_i^\tau\lambda^\tau\right]\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}}\\
&-\frac{\left[d_{i-1}^{2\tau}\tau\log\left(\frac{d_{i-1}}{\lambda}\right)-d_{i-1}^\tau\lambda^\tau\tau\log\left(\frac{d_{i-1}}{\lambda}\right)-d_{i-1}^\tau\lambda^\tau\right]\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}}\\
&+\frac{\tau\left\{d_{i-1}^\tau\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-d_i^\tau\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2}\\
&\times\frac{\left\{d_{i-1}^\tau\log\left(\frac{d_{i-1}}{\lambda}\right)\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-d_i^\tau\log\left(\frac{d_i}{\lambda}\right)\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}}{\lambda^{2\tau+1}\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\}^2}\Bigg\}\\
&+\frac{\mathrm{E}\left(N_0\right)}{\lambda}+\frac{\tau\log(\lambda)-1}{\lambda^{\tau+1}}\mathrm{E}\left(\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\right)-\frac{\tau}{\lambda^{\tau+1}}\mathrm{E}\left[\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\log\left(X_{(i)}\right)\right].
\end{aligned}
\tag{A.3}
$$

Considering the Type I censoring, the random vector $(N_0, N_1, \ldots, N_k)$ has multinomial distribution $\mathrm{Mu}_{k+1}(n, \theta_0, \theta_1, \ldots, \theta_k)$, where

$$
\theta_i=\begin{cases}F(d_i,\lambda,\tau)-F(d_{i-1},\lambda,\tau) & \text{for } i=1,\ldots,k,\\ 1-F(d_k,\lambda,\tau) & \text{for } i=0,\end{cases}
$$

and $n = N_0 + N_1 + \cdots + N_k$. Since the marginal frequencies N_i, $i = 0, \ldots, k$ have binomial distribution, their expectations are

$$
\mathrm{E}\left(N_i\right)=n\theta_i=\begin{cases}n\left\{\exp\left[-\left(\frac{d_{i-1}}{\lambda}\right)^\tau\right]-\exp\left[-\left(\frac{d_i}{\lambda}\right)^\tau\right]\right\} & \text{for } i=1,\ldots,k,\\ n\exp\left[-\left(\frac{d_k}{\lambda}\right)^\tau\right] & \text{for } i=0.\end{cases}
\tag{A.4}
$$

It remains to derive the expectations

$$
\mathrm{E}\left(\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\right),\quad \mathrm{E}\left[\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\log\left(X_{(i)}\right)\right],\quad \mathrm{E}\left\{\sum_{i=n-N_0+1}^{n}X_{(i)}^\tau\left[\log\left(X_{(i)}\right)\right]^2\right\}.
\tag{A.5}
$$

It follows from the law of total expectation that

$$\mathrm{E}(X) = \mathrm{E}\left[\mathrm{E}(X|N_0)\right] = \sum_{n_0} \mathrm{E}(X|N_0 = n_0)\mathrm{P}(N_0 = n_0) \tag{A.6}$$

for random variables X, N_0. Since $N_0 \sim \mathrm{Bi}(n, \theta_0)$, it follows from (A.6) that

$$\begin{aligned}
\mathrm{E}\left(\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau}\right) &= \sum_{n_0=0}^{n} \mathrm{E}\left(\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau} | n_0\right) \mathrm{P}(N_0 = n_0) \\
&= \sum_{n_0=0}^{n} \left[\sum_{i=n-n_0+1}^{n} \mathrm{E}\left(X_{(i)}^{\tau}\right)\right] \binom{n}{n_0} \theta_0^{n_0} (1-\theta_0)^{n-n_0} \\
&= \sum_{n_0=0}^{n} \left[\sum_{i=n-n_0+1}^{n} \mathrm{E}\left(X_{(i)}^{\tau}\right)\right] \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau}\right] \\
&\quad \times \left\{1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\right\}^{n-n_0},
\end{aligned} \tag{A.7}$$

and analogically

$$\begin{aligned}
\mathrm{E}\left[\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau} \log\left(X_{(i)}\right)\right] &= \sum_{n_0=0}^{n} \left\{\sum_{i=n-n_0+1}^{n} \mathrm{E}\left[X_{(i)}^{\tau} \log\left(X_{(i)}\right)\right]\right\} \\
&\quad \times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau}\right] \left\{1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\right\}^{n-n_0},
\end{aligned} \tag{A.8}$$

$$\begin{aligned}
\mathrm{E}\left\{\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau} \left[\log\left(X_{(i)}\right)\right]^2\right\} &= \sum_{n_0=0}^{n} \left\{\sum_{i=n-n_0+1}^{n} \mathrm{E}\left\{X_{(i)}^{\tau} \left[\log\left(X_{(i)}\right)\right]^2\right\}\right\} \\
&\quad \times \binom{n}{n_0} \exp\left[-n_0 \left(\frac{d_k}{\lambda}\right)^{\tau}\right] \left\{1 - \exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\right\}^{n-n_0}.
\end{aligned} \tag{A.9}$$

Another step is to derive the expectations

$$\mathrm{E}\left(X_{(i)}^{\tau}\right), \quad \mathrm{E}\left[X_{(i)}^{\tau} \log\left(X_{(i)}\right)\right], \quad \mathrm{E}\left\{X_{(i)}^{\tau} \left[\log\left(X_{(i)}\right)\right]^2\right\}. \tag{A.10}$$

The pdf of variable $X_{(i)}$ is (see Hogg et al., 2005)

$$f_{(i)}(x) = n\binom{n-1}{i-1} f(x) \left[F(x)\right]^{i-1} \left[1 - F(x)\right]^{n-i}, i = 1, 2, \ldots, n,$$

which after substitution of cdf (2.1) and pdf (2.2) leads to

$$f_{(i)}(x) = n\binom{n-1}{i-1} \frac{\tau}{\lambda^{\tau}} x^{\tau-1} \sum_{j=0}^{i-1} (-1)^j \binom{i-1}{j} \exp\left[-\left(\frac{x}{\lambda}\right)^{\tau} (n-i+j+1)\right].$$

Using (see Abramowitz and Stegun, 1964)

$$\int_0^\infty x\mathrm{e}^{-x}\mathrm{d}x = \Gamma(2) = 1, \quad \int_0^\infty x\log(x)\,\mathrm{e}^{-x}\mathrm{d}x = \Gamma'(2) = 1-\gamma_e,$$

$$\int_0^\infty x\left[\log(x)\right]^2\mathrm{e}^{-x}\mathrm{d}x = \Gamma''(2) = \frac{\pi^2}{6} - 2\gamma_e + \gamma_e^2,$$

with Euler-Mascheroni constant $\gamma_e \doteq 0.57722$, the expectations (A.10) are

$$\begin{aligned}\mathrm{E}\left(X_{(i)}^\tau\right) &= \int_0^\infty x^\tau f_{(i)}(x)\mathrm{d}x \\ &= n\binom{n-1}{i-1}\lambda^\tau\sum_{j=0}^{i-1}(-1)^j\binom{i-1}{j}(n-i+j+1)^{-2},\end{aligned} \tag{A.11}$$

$$\begin{aligned}\mathrm{E}\left[X_{(i)}^\tau\log\left(X_{(i)}\right)\right] &= \int_0^\infty x^\tau\log(x)f_{(i)}(x)\mathrm{d}x \\ &= n\binom{n-1}{i-1}\frac{\lambda^\tau}{\tau}\sum_{j=0}^{i-1}(-1)^j\binom{i-1}{j}(n-i+j+1)^{-2} \\ &\quad\times\left[\log\left(\frac{\lambda^\tau}{n-i+j+1}\right)+1-\gamma_e\right],\end{aligned} \tag{A.12}$$

$$\begin{aligned}\mathrm{E}\left\{X_{(i)}^\tau\left[\log\left(X_{(i)}\right)\right]^2\right\} &= \int_0^\infty x^\tau\left[\log(x)\right]^2 f_{(i)}(x)\mathrm{d}x \\ &= n\binom{n-1}{i-1}\frac{\lambda^\tau}{\tau^2}\sum_{j=0}^{i-1}(-1)^j\binom{i-1}{j}(n-i+j+1)^{-2} \\ &\quad\times\left\{\left[\log\left(\frac{\lambda^\tau}{n-i+j+1}\right)\right]^2 + 2\log\left(\frac{\lambda^\tau}{n-i+j+1}\right)(1-\gamma_e)\right. \\ &\quad\left.+\frac{\pi^2}{6} - 2\gamma_e + \gamma_e^2\right\}.\end{aligned} \tag{A.13}$$

Details of the derivation can be found in Fusek (2013). The substitution of (A.11)–(A.13) into (A.7)–(A.9) leads to

$$\begin{aligned}\mathrm{E}\left(\sum_{i=n-n_0+1}^{n}X_{(i)}^\tau\right) &= n\lambda^\tau\sum_{n_0=0}^{n}\sum_{i=n-n_0+1}^{n}\binom{n-1}{i-1}\sum_{j=0}^{i-1}(-1)^j\binom{i-1}{j} \\ &\quad\times(n-i+j+1)^{-2}\binom{n}{n_0}\exp\left[-n_0\left(\frac{d_k}{\lambda}\right)^\tau\right] \\ &\quad\times\left\{1-\exp\left[-\left(\frac{d_k}{\lambda}\right)^\tau\right]\right\}^{n-n_0},\end{aligned} \tag{A.14}$$

$$\mathrm{E}\left[\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau}\log\left(X_{(i)}\right)\right] = n\frac{\lambda^{\tau}}{\tau}\sum_{n_0=0}^{n}\sum_{i=n-n_0+1}^{n}\binom{n-1}{i-1}\sum_{j=0}^{i-1}(-1)^{j}\binom{i-1}{j} \tag{A.15}$$
$$\times (n-i+j+1)^{-2}\left[\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right)+1-\gamma_e\right]$$
$$\times \binom{n}{n_0}\exp\left[-n_0\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\left\{1-\exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\right\}^{n-n_0},$$

$$\mathrm{E}\left\{\sum_{i=n-n_0+1}^{n} X_{(i)}^{\tau}\left[\log\left(X_{(i)}\right)\right]^2\right\} = n\frac{\lambda^{\tau}}{\tau^2}\sum_{n_0=0}^{n}\sum_{i=n-n_0+1}^{n}\binom{n-1}{i-1}\sum_{j=0}^{i-1}(-1)^{j}\binom{i-1}{j} \tag{A.16}$$
$$\times (n-i+j+1)^{-2}\left\{\left[\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right)\right]^2\right.$$
$$\left.+\,2\log\left(\frac{\lambda^{\tau}}{n-i+j+1}\right)(1-\gamma_e)+\frac{\pi^2}{6}-2\gamma_e+\gamma_e^2\right\}$$
$$\times \binom{n}{n_0}\exp\left[-n_0\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\left\{1-\exp\left[-\left(\frac{d_k}{\lambda}\right)^{\tau}\right]\right\}^{n-n_0}.$$

Moreover, substituting (A.4) and (A.14)–(A.16) into (A.1)–(A.3), the elements of the expected FIM (2.8) are obtained.

Appendix B

Estimation of the Extremal Index Using Censored Distributions

Traditional extreme value theory is based on independent and identically distributed variables. When dealing with extreme events in time series, this assumption is often violated, and the dependence in data is reflected in occurrence of extremes close to each other, which is described by a clustering parameter. In order to create series that can be considered independent, block or runs declustering is usually applied (see, for example, Fawcett and Walshaw, 2012; Holešovský et al., 2016). Such a preprocessing usually leads to a significant data reduction, which may result in higher variation of the estimates. Consequently, it is more suitable to deal with the original time series and estimate the clustering parameter, and thereby the dependence at extremal levels.

Let $X_1, X_2, \ldots$ be a strictly stationary sequence with marginal cumulative distribution function (cdf) F, right end-point $x^* = \sup\{x : F(x) < 1\}$, and denote $M_n = \max\{X_1, \ldots, X_n\}$. Furthermore, let us have a sequence of independent variables $X_1^*, X_2^* \ldots$ with the same marginal distribution F, and denote $M_n^* = \max\{X_1^*, \ldots, X_n^*\}$. The fundamental extreme value theorem states that given some constants $a_n > 0$, b_n and under appropriate regularity conditions, the variable $(M_n^* - b_n)/a_n$ converges in distribution to generalized extreme value (GEV) distribution with cdf G^*. At the same time, if the series $X_1, X_2, \ldots$ satisfies the $D(u_n)$ condition of Leadbetter et al. (1983) with a suitable threshold $u_n = a_n x + b_n$ for all $x > 0$, the limiting distribution of $(M_n - b_n)/a_n$ is again GEV with cdf G (see e.g. Beirlant et al., 2004). The $D(u_n)$ condition limits the long-range dependence at extreme levels, and hence provides asymptotic independence between far apart extreme observations. The limiting distributions are related to each other by $G = [G^*]^\theta$, where $0 < \theta \leq 1$ is the extremal index. When $\theta < 1$, the extremes tend to cluster. If $X_1, \ldots, X_n$ are independent, then $\theta = 1$. Conversely, if $\theta = 1$, the asymptotic behaviour of M_n^* and M_n is identical, even though $X_1, \ldots, X_n$ may be dependent. The extremal index is the key measure of short-range dependence at extreme values, and governs clustering of extremes of a univariate series. Various papers discuss many extremal

index estimators; for example, the cluster size (runs and blocks) estimators (Hsing, 1991; Smith and Weissman, 1994); the maxima methods (Ancona-Navarrete and Tawn, 2000; Gomes, 1993; Northrop, 2015); the two-threshold estimator (Laurini and Tawn, 2003); the intervals estimator (Ferro and Segers, 2003); the iterative weighted least squares estimator (Süveges, 2007); the gap estimator (Süveges, 2007) and its generalization, the K-gaps estimator (Süveges and Davison, 2010). Assessment of several estimators can be found in Ancona-Navarrete and Tawn (2000); different blocks estimators are compared in Holešovský et al. (2014), and Holešovský (2017). Here we propose a new approach to the extremal index estimation based on the artificial censoring.

B.1 Preliminaries

Let $T(u_n)$ denote a random variable corresponding to inter-exceedance times in the underlying series $X_1, X_2, \ldots$, i.e.

$$T(u_n) = \min\{j \geq 1 : X_{j+1} > u_n | X_1 > u_n\}.$$

For threshold u_n increasing with n, and under the $\Delta^*(u_n)$ condition in Süveges (2007), it holds for $x > 0$

$$P(\overline{F}(u_n)T(u_n) \leq x) \to 1 - \theta \exp(-\theta x) =: F_\theta(x) \tag{B.1}$$

as $n \to \infty$ (see Theorem 1 in Ferro and Segers (2003)). It means that as $u_n \to x^*$ for $n \to \infty$,

$$\overline{F}(u_n)T(u_n) \xrightarrow{d} T_\theta,$$

where $\xrightarrow{d}$ denotes the convergence in distribution and T_θ follows the mixture distribution

$$(1-\theta)\varepsilon_0 + \theta\mu_\theta, \tag{B.2}$$

where ε_0 is the degenerate distribution at 0 and μ_θ is the exponential distribution with expected value $1/\theta$.

Let us have a random sequence $X_1, \ldots, X_n$, a sufficiently high threshold u, and let $N = \sum_{i=1}^{n} \mathbf{1}_{[X_i > u]}$ be the number of threshold exceedances observed at times $j_1, \ldots, j_N$, where $\mathbf{1}_{[\cdot]}$ is the indicator function. The i-th interexceedance time is denoted as $T_i = j_{i+1} - j_i$, $i = 1, \ldots, N-1$. With respect to (B.1), the variables $\overline{F}(u)T_i$, $i = 1, \ldots, N-1$, can be treated as random variables drawn from the distribution with cdf F_θ from (B.1). The value $\overline{F}(u)$ is typically replaced by its estimator N/n; however, in general, it is possible to choose a different one.

As pointed out by Ferro and Segers (2003) and Süveges (2007), the interexceedance times of a stationary process are not mutually independent, and the likelihood is constructed under the assumption of independence of all the times $T_1, \ldots, T_{N-1}$. Nevertheless, although the intra-cluster times are not independent, the different sets of intra-cluster times are asymptotically independent. It was analysed in Süveges (2007), Süveges and Davison (2010), and shown using simulations in Holešovský and Fusek (2020), that under an additional restriction on the underlying process, the assumption of independence may be disregarded. This restriction lies in requirement that the underlying sequence needs to satisfy both the $D(u_n)$ condition of Leadbetter et al. (1983) and the $D^{(k)}(u_n)$ condition of Chernick et al. (1991).

The $D(u_n)$ condition is a standard mixing condition limiting the long-range dependence at extreme levels. It implies that any two rare events that are sufficiently separated are asymptotically independent (for more details see Leadbetter et al. (1983)). Moreover, we need to restrict the dependence in the sequence more locally; for this step, the following $D^{(k)}(u_n)$ condition is required.

Condition. *$D^{(k)}(u_n)$ is said to be satisfied if a stationary series $X_1, \ldots, X_n$ under the $D(u_n)$ condition of Leadbetter et al. (1983) also satisfies*

$$nP(X_1 > u_n, M_{1,k} \leq u_n < M_{k,r_n}) \to 0$$

as $n \to \infty$ with $r_n = o(n)$ and u_n as in $D(u_n)$.

Clearly, if $D^{(k_0)}(u_n)$ holds, then $D^{(k)}(u_n)$ also holds for all $k \geq k_0$. It means that within a cluster, high-threshold exceedances are asymptotically almost surely separated by at most $k-1$ observations. The $D^{(k)}(u_n)$ condition plays a crucial role in estimation of the extremal index θ. Most of available threshold-based estimators of θ are derived under the assumption of validity of a particular $D^{(k)}(u_n)$ condition or, alternatively, the order of the condition or some related quantity appear therein as auxiliary parameters.

In the following section, we discuss a new approach to the extremal index estimation based on artificial censoring.

B.2 Censored Estimator

Let $T_{(1)} \leq \cdots \leq T_{(N-1)}$ be the ordered statistics of $T_1, \ldots, T_{N-1}$. Considering type I left-censoring, for a given time censor $D \geq 0$, there are $(N - 1 - N_C^*)$ censored times $T_{(1)}, \ldots, T_{(N-1-N_C^*)} \leq D$ and N_C^* uncensored (observed) times $T_{(N-N_C^*)}, \ldots, T_{(N-1)}$. Let us recall from (B.2) that the limiting variable is $T_\theta = (1-\theta)\varepsilon_0 + \theta\mu_\theta$. Denote $p_\theta(t) = 1$ for $t = 0$ the probability mass function (pmf) of T_θ conditioned by the event $T_\theta = 0$, and $f_\theta(t) = \theta e^{-\theta t}$ for $t > 0$ the probability density function (pdf) of T_θ conditioned by $T_\theta > 0$. Hence, p_θ and f_θ are the pmf and pdf of variables ε_0 and μ_θ, respectively.

Using results from Cohen (1991), the log-likelihood function of the censored sample can be written in the form of

$$\ell(\theta, D, N_C^*, \{T_{(i)}\}_{i\geq N-N_C^*}) = (N-1-N_C^*)\log F_\theta(d) + \log\frac{(N-1)!}{(N-1-N_C^*)!} + \sum_{N-N_C^*}^{N-1}\log\left\{[(1-\theta)p_\theta(t_{(i)})]^{\mathbf{1}_{[t_{(i)}=0]}}\cdot[\theta f_\theta(t_{(i)})]^{\mathbf{1}_{[t_{(i)}>0]}}\right\},$$

where $t_{(i)} = \overline{F}(u)T_{(i)}$ is considered to be ordered statistic drawn from F_θ and $d = \overline{F}(u)D$. Hence

$$\ell(\theta, D, N_C^*, \{T_{(i)}\}_{i\geq N-N_C^*}) = (N-1-N_C^*)\log(1-\theta e^{-\theta d}) + \log\frac{(N-1)!}{(N-1-N_C^*)!} + 2N_C^*\log\theta - \theta\sum_{i=N-N_C^*}^{N-1}\overline{F}(u)T_{(i)}. \tag{B.3}$$

The ML estimate $\widehat{\theta}_{\mathrm{C}}$ is obtained by maximizing the log-likelihood function (B.3).

We can estimate variability of the estimate $\widehat{\theta}_{\mathrm{C}}$ using the sample FIM

$$\widetilde{J}_{N-1} = -\frac{\mathrm{d}^2\ell}{\mathrm{d}\theta^2} = (N-1-N_C^*)\frac{e^{-\theta d}(\theta d^2 - 2d + e^{-\theta d})}{(1-\theta e^{-\theta d})^2} + \frac{2N_C^*}{\theta^2}.$$

The sample FIM $\widetilde{J}_{N-1}$ is an unbiased estimator of the expected FIM J_{N-1} and $\widetilde{J}_{N-1}(\theta) \to J_{N-1}(\theta)$ in probability for $N \to \infty$.

Considering the type I censoring, the random variable N_C^* has binomial distribution $\mathrm{Bi}(N-1, \phi)$, where $\phi = 1 - F_\theta(d)$. Therefore, $\mathrm{E}N_C^* = (N-1)\phi = (N-1)\theta e^{-\theta d}$, and the expected FIM is

$$J_{N-1} = \mathrm{E}\widetilde{J}_{N-1} = (N-1)e^{-\theta d}\left[\frac{\theta d^2 - 2d + e^{-\theta d}}{1-\theta e^{-\theta d}} + \frac{2}{\theta}\right]. \tag{B.4}$$

Considering the asymptotic properties of the ML estimator $\widehat{\theta}_{\mathrm{C}}$ (Lehmann and Casella, 1998), $\sqrt{N-1}(\widehat{\theta}_{\mathrm{C}} - \theta)$ has asymptotically normal distribution $\mathrm{N}(0, \sigma_\theta^2)$, where $\sigma_\theta^2 = (J_{N-1}/(N-1))^{-1}$.

An important point for the censored estimator $\widehat{\theta}_{\mathrm{C}}$ to work properly is the choice of the censor D. If D is too low, larger intra-cluster times are assigned to the exponential part of F_θ, and $\widehat{\theta}_{\mathrm{C}}$ is biased towards independence. The independence assumption in log-likelihood (B.3) may also be violated in this case. On the other hand, if D is too high, it leads to a higher level of uncertainty in the model, and to higher variability of the estimate. A proper choice of D is related to validity of the $D^{(k)}(u_n)$ condition with $D = k-1$, see Holešovský and Fusek (2020) for more details. Note that it can be difficult to prove validity of the $D^{(k)}(u_n)$ condition when analyzing real data. Several approaches have been proposed,

for example, the graphical diagnostics of anti-$D^{(k)}(u_n)$ events (Ferreira and Ferreira, 2018; Süveges, 2007). Nevertheless, the graphical approach generally leads to subjective conclusions. Other two methods are the information matrix test and its extensions (Ferreira, 2018b; Fukutome et al., 2015, 2019; Süveges and Davison, 2010), and the stability analysis of the runs estimator (Cai, 2022). Both of them are, however, based on estimators that are rather sensitive to the selection of the auxiliary parameters, including the threshold itself. Additional methods are proposed in Holešovský and Fusek (2024).

Properties of the censored estimator together with the intervals estimator of Ferro and Segers (2003) and the K-gaps estimator of Süveges and Davison (2010) were assessed using simulations in Holešovský and Fusek (2020). It was shown that, in comparison to the other two estimators, the censored estimator has better stability with respect to the threshold selection, and it is not much sensitive to the choice of the parameter D. In addition, the censored estimator was used for the extremal index estimation for July daily maximum temperatures at Uccle, Belgium (see Holešovský and Fusek (2020) for more details).

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