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ANA CLÁUDIA SOUZA VIDAL DE NEGREIROS

ON THE PARAMETER ESTIMATION PROBLEM OF THE *q*-EXPONENTIAL DISTRIBUTION FOR RELIABILITY APPLICATIONS

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ANA CLÁUDIA SOUZA VIDAL DE NEGREIROS

"ON THE PARAMETER ESTIMATION PROBLEM OF THE q-EXPONENTIAL DISTRIBUTION FOR RELIABILITY APPLICATIONS"

ÁREA DE CONCENTRAÇÃO: PESQUISA OPERACIONAL

A comissão examinadora, composta pelos professores abaixo, sob a presidência do(a) primeiro(a), considera o(a) candidato(a) **ANA CLÁUDIA SOUZA VIDAL DE NEGREIROS, APROVADO(A).**

Recife, 23 de fevereiro de 2018.

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Prof. FRANCISCO CRIBARI NETO, PhD (UFPE)

À minha mãe (Eliane).

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ABSTRACT

This work involved the q-Exponential distribution, which can be used to model each of the three phases of the bathtub curve and is an alternative to the Weibull distribution. The q-Exponential has two parameters (q – shape; η – scale) and it stems from the Tsallis' non-extensive entropy. This model does not have the limitation of a constant hazard rate like the Exponential one, thus allowing the modeling of either system improvement $(1 < q < 2)$ or degradation $(q < 1)$. Besides, it has more flexibility regarding the decay of the Probability Density Function (PDF) curve and it can model very well data sets with extreme values (power law characteristic). This feature is interesting in the reliability context because many equipment can work for long time until the first failure. However, when data sets are related to the degradation phase of systems, the application of the q-Exponential distribution becomes difficult due to convergence problems in the estimation process via the maximum likelihood (ML) method. This difficulty is due to the monotone behavior of the q-Exponential log-likelihood function when $q < 1$, which is generally known as "monotone likelihood problem". Because of that, it is almost impossible to obtain good estimates for the parameters considering the original log-likelihood function. In this sense, this research applied the Firth's penalization method to solve this problem. We also verified that one of the regularity conditions imposed by the ML method is not satisfied by the q-Exponential distribution. Then, with the objective of satisfying this condition, it was also proposed a variable change, which partially solved just the problems of this distribution. Nevertheless, the Firth's method yielded satisfactory results even for small samples. Comparisons of the results were performed via Monte Carlo simulations for the original and penalized q-Exponential distribution. Additionally, bootstrap confidence intervals were constructed for the parameters and comparisons were made between the fit provided by the q-Exponential and Weibull distributions. Application examples involving failure data of complex equipment using the Firth's penalization method are presented and discussed. The obtained results indicate that the penalized log-likelihood enables the use of the q-Exponential distribution in the modeling of data sets related to degrading systems.

Keywords: q-Exponential distribution. Reliability. Monotone likelihood. Firth's method.

RESUMO

Este trabalho envolveu a distribuição q-Exponencial, a qual pode ser usada para modelar as três fases da curva da banheira e é uma alternativa para a distribuição Weibull. A distribuição q-Exponencial tem dois parâmetros (q – forma; η – escala) e é oriunda da entropia não-extensiva de Tsallis. Este modelo não tem a limitação de uma taxa de falhas constante como a distribuição Exponencial, assim permite modelar tanto a fase de melhoramento $(1 < q < 2)$ quanto a de degradação $(q < 1)$. Além disso, tem mais flexibilidade quanto ao decaimento da curva da Função Densidade de Probabilidade (FDP) e consegue modelar muito bem conjuntos de dados com grandes valores (característica de power law). Esta característica é interessante no contexto de confiabilidade porque muitos equipamentos podem trabalhar por muito tempo até que ocorra a primeira falha. No entanto, quando os conjuntos de dados estão relacionados à fase de degradação dos sistemas, a aplicação da distribuição q-Exponencial se torna difícil devido a problemas de convergência no processo de estimação pelo método da máxima verossimilhança (MV). Este problema acontece por causa de uma condição chamada de "verossimilhança monótona". Por causa disso, é praticamente impossível obter estimativas plausíveis para os parâmetros através da função de verossimilhança original. Neste sentido, esta pesquisa aplicou o método de penalização de Firth para corrigir este problema. Também foi verificado que uma condição de regularidade imposta pelo método de MV não é satisfeita pela distribuição q-Exponencial. Então, com o objetivo de satisfazer também esta condição, uma mudança de variável foi proposta, a qual solucionou apenas parcialmente os problemas desta distribuição. Todavia, o método de Firth produziu resultados satisfatórios mesmo para amostras pequenas. Comparações dos resultados foram realizadas através de simulações Monte Carlo para as distribuições q-Exponencial original e penalizada. Além disso, intervalos de confiança bootstrap foram construídos para os parâmetros e comparações foram feitas entre o ajuste alcançado pelas distribuições q-Exponencial e Weibull. Aplicações envolvendo dados de falhas de equipamentos complexos usando o método de penalização de Firth são apresentadas e discutidas. Os resultados obtidos indicam que a log-verossimilhança penalizada permite o uso da distribuição q-Exponencial na modelagem de dados de falhas na fase de degradação dos sistemas.

Palavras-chave: Distribuição q-Exponencial. Confiabilidade. Verossimilhança monótona. Método de Firth.

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LIST OF ACRONYMS

CDF – CUMULATIVE DISTRIBUTION FUNCTION

GRP - GENERALIZED RENEWAL PROCESS

MLE – MAXIMUM LIKELIHOOD ESTIMATES

MRI - MAGNETIC RESONANCE IMAGING

MTBF – MEAN TIME BETWEEN FAILURES

NM – NELDER-MEAD

PDF – PROBABILITY DENSITY FUNCTION

RF – RADIO FREQUENCY

TBF – TIME BETWEEN FAILURES

SUMMARY

1 INTRODUCTION

The reliability concept is associated to the ability of a system to operate under designated operating conditions for a designated period of time or number of cycles (MODAREES, 1999). Recently, the reliability knowledge area had a significant increase. Perhaps, this development may be explained by its importance in a company. Nowadays, reliability is linked to some crucial aspects for a good management, such as costs, customer confidence, strategic management, strategic maintenance, workplace safety, etc. In this context, some probability distributions are used to model systems' failure times to provide many important information to the company like failure probabilities, expected number of failures up to a certain time, mean time between failures (MTBF), among others. With all this information the company is able to improve their systems, to plan maintenance actions, to avoid failures etc. Among the probability models used in reliability, the Exponential and Weibull distributions are the most used ones. Recently, the q-Exponential distribution, proposed by Tsallis (1988), has emerged as an alternative. However, this probability model presents some features that should be investigated so as to enable its wide use in the reliability context.

According to Tsallis (2009) the q-Exponential distribution is obtained by maximizing the non-extensive entropy under appropriate constraints, which is associated with the probability density function (for more details about these constraints see Tsallis (2009, p.89)). As other q-distributions, it has been applied to a variety of problems in many research areas including the field of complex systems. Picoli, Mendes & Malacarne (2009) bring in their work a summary of its basic properties, like the success of q-distributions in describing some systems to be in part due to its ability of exhibit heavy-tails and model power law behavior. For instance, Malacarne, Mendes & Lenzi (2002) showed that the population of a country is well described by a q-Exponential distribution with Probability Density Function (PDF) presenting a power law behavior (PICOLI, MENDES & MALACARNE, 2003). Campo, Ferri & Roston (2009) verified that the temporal correlation function of hydrogen bonds can be modeled by a q-Exponential probabilistic model. Bercher & Vignat (2008) indicated that q-exponentials are stable by a statistical normalization operation. Besides, Sales Filho *et al*. (2016) used the q-Exponential to infer about a useful performance metric in system reliability, the index $R =$

$P(Y < X)$, where Y is the stress, X is the strength and both are supposed independent q-Exponential random variables with different parameters.

The q-Exponential distribution has two parameters: q and η, where q is the shape parameter and η is the scale parameter. As compared to the Exponential distribution that has just one parameter (η), the q-Exponential distribution has more flexibility regarding the decay of the PDF. Indeed, the Exponential probability distribution is a special case of the q-Exponential when $q \rightarrow 1$. Another feature of this distribution is that it does not have the limitation of a constant hazard rate as the Exponential one, thus allowing the modeling of either system improvement ($1 < q < 2$) or degradation ($q < 1$). Indeed, the q-Exponential distribution can model each of the three phases of the bathtub curve, which has three distinct periods: decreasing failure rate for infant mortality; constant failure rate for useful life; and increasing failure rate for wear-out. Figure 1 shows a bathtub curve.

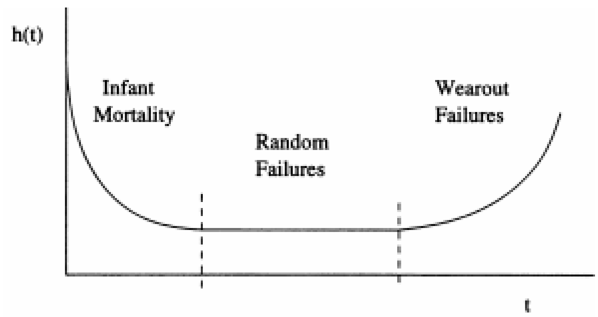

Figure 1: The classical bathtub curve.
Source: Sellito (2005)

The q-Exponential distribution can successfully model data with values of great magnitude (PICOLI, MENDES & MALACARNE, 2009). This feature is interesting on the reliability context because many equipment may work for long time until the first failure. However, an estimation problem verified in the q-Exponential distribution happens in the modeling of the degradation phase of systems (when $q < 1$). The fit of data from degrading systems is crucial in reliability engineering and, in order to use the q-Exponential model in this case, the corresponding estimation problem must be solved.

For a given sample with values that have great order of magnitude, the q-Exponential distribution is expected to adjust the data well. In cases like these, the parameter q lies within the interval (1, 2) and the corresponding q-Exponential PDF presents power law behavior (PICOLI, MENDES & MALACARNE, 2009). The maximum likelihood estimation of the q-Exponential parameters when $1 < q < 2$ presents no difficulties. Nevertheless, it has been observed in Sales Filho *et al*. (2016) that, when $q < 1$, the techniques used to obtain the maximum likelihood estimates either provide poor results or fail to converge. In those cases, the q-Exponential log-likelihood function seems to be monotonically increasing, which renders the estimation task theoretically impossible. A function is characterized as monotone when it preserves the relation of order. As the parameters' values increase, the function's value also increases. According to Pianto & Cribari-Neto (2011) the called "monotone likelihood" occurs when the log-likelihood obtains its maximum for infinite parameter values. Heinze & Schemper (2001) affirm that the monotone likelihood is noted in the fitting process of a Cox model if the likelihood converges to a finite value, while at least one parameter estimate diverges to ±∞.

The q-Exponential distribution has the following PDF:

$$f_q(t) = \frac{(2-q)\left[1-\frac{(1-q)t}{\eta}\right]^{1/1-q}}{\eta}, \text{ for } t \geq 0, \tag{1.1}$$

$q < 2$ and $\eta > 0$,

when $q < 1$, the PDF of Eq. (1.1) has a limited support with an upper bound that depends on the parameters η and q:

$$t \in \begin{cases} [0;\infty), & 1 < q < 2 \\ \left[0, \frac{\eta}{1-q}\right], & q < 1 \end{cases}. \tag{1.2}$$

Some authors have studied in the problem of the monotone likelihood. There are some methods in the literature to solve this problem. However, the approaches used to correct this problem are different from author to author. For example, Firth (1993) developed a method based on an approach for bias reduction that does not depend on finiteness of $\hat{\theta}$. The author worked with the exponential families. Loughin (1998) considered a bootstrap method that can be used to correct this problem by using the Cox proportional hazards model. Heinze & Schemper (2001) proposed an adaptation of a procedure by Firth (1993). Cribari-Neto, Frery &

Silva (2002) suggested a method to correct the likelihood function also based on resampling, they used the $\mathcal{G}_A^0(\alpha, \gamma, n)$ distribution.

Other way to handle the q-Exponential likelihood function is by applying a variable change or a reparameterization. According to Cordeiro (1999), one of the regularity conditions to apply the maximum likelihood method refers to the independence of the PDF support with respect to its parameters. This condition is not verified with q-Exponential model as its support depends on the value of parameters q and η, as can be seen in Equation (1.2).

In this work, the Firth's penalization method will be applied in order to penalize the q-Exponential log-likelihood function. This method was chosen because of its efficiency and simplicity of implementation. However, a variable change will be implemented before the Firth's method as an attempt to comply with the regularity condition. If this change of variable solves the q-Exponential problem, results will be compared.

The log-likelihood function related to the q-Exponential distribution will be derived and analyzed to verify whether it presents the monotone likelihood problem. The Nelder-Mead (1965) optimization method will be used for function maximization because it presented a better result compared with the particle swarm optimization (PSO) method using the q-Exponential distribution (SALES FILHO, 2016). A change of variable will be performed, and the Firth's penalization method will be applied in the q-Exponential log-likelihood function. Additionally, the original and penalized log-likelihoods will be compared through numerical experiments and using reliability-related data sets.

1.1 Objectives

1.1.1 General objective

The general objective of this work is to use the Firth's penalization method to correct the q-Exponential distribution log-likelihood function to obtain good estimates for its parameters. The proposed method will be applied to fit reliability-related data of engineered equipment.

1.1.2 Specific objectives

The specific objectives of this work are the following:

- Identification if there is any combination of parameters that turns the *q*-Exponential log-likelihood into a monotone function;
- Investigation of reparameterizations of the *q*-Exponential distribution that enable parameter estimation via the maximum likelihood method;
- Investigation if the change of variables can correct the *q*-Exponential log-likelihood function and satisfy the regularity conditions;
- Investigation of methods to correct the monotone log-likelihood of the *q*-Exponential distribution, if necessary;
- Application of a variable change and of the Firth's penalization method to try solving the monotone likelihood problem of the *q*-Exponential log-likelihood function;
- Comparison of the results provided by the original and corrected *q*-Exponential log-likelihoods.
- Development of bootstrap confidence intervals for the parameters of the *q*-Exponential distribution;
- Application of the *q*-Exponential distribution to reliability-related data and comparison of the *q*-Exponential results with the ones obtained by the Weibull model.

1.2 Methodology

This work is characterized as an applied research, because it is conducted to solve a specific problem of literature and to a practical methodology implementation. It presents an application of the Firth's penalization method to correct the *q*-Exponential log-likelihood function in order to apply the *q*-Exponential distribution in reliability analyses.

Additionally, this research can be classified as qualitative and quantitative. It is qualitative because it makes use of a literature review to understand and analyze the specific problem treated in this work. On the other hand, it is quantitative given that computational programs and statistical methods are used to find and understand solutions for the analyzed problem.

This research was divided into the following steps:

- Step 1: initially, it was made an investigation about the topics considered in this work. The topics were: the features of the *q*-Exponential distribution; the monotone likelihood problem; the methods that can be used to solve this problem; parameter estimation; methods for function optimization to be used in the maximization of the *q*-Exponential log-likelihood function; reliability-related data from literature to be used to demonstrate the penalized function results.

- Step 2: then, a change of variable was applied to the *q*-Exponential PDF as an attempt to satisfy regularity conditions and to solve the monotone likelihood problem. However, only the regularity conditions are met, since the new function did not produce good parameters' estimates. This is an indication that, in spite of the change of variable, the monotone likelihood problem persists.

- Step 3: next, study of the possible methods that could solve the *q*-Exponential problem and application of the Firth's penalized method in the *q*-Exponential log-likelihood function. Tests were made using the software R.

- Step 4: then, numerical experiments were implemented and performed;

- Step 5: finally, the *q*-Exponential penalized function was applied to two application examples from literature.

1.3 Structure of the work

This research contains six chapters, including this introduction. Chapter 2 provides the theoretical background: the *q*-Exponential distribution, important concepts and methods used over the work, such as Maximum Likelihood Estimation, bootstrap confidence intervals, Firth's penalization method and Nelder-Mead optimization method. Chapter 3 presents an investigation of the *q*-Exponential distribution behavior depending on its parameters' values. It also includes some reparameterizations and change of variables applied in an attempt to satisfy regularity conditions and to directly obtain the maximum likelihood estimates for its parameters. In Chapter 4, a penalization method is applied to the *q*-Exponential log-likelihood function. In this chapter there are tables with comparisons between the results obtained with the original and the penalized functions. Chapter 5 brings two examples to show the applicability of the penalized function; it also presents comparisons with the fit provided by the Weibull distribution. And, finally, Chapter 6 provides the work's conclusion.

2 THEORETICAL BACKGROUND

In this chapter, the theoretical background that is necessary to this study is presented.

2.1 Characterization of q-Exponential distribution

The q-Exponential distribution has the PDF presented in Equation (1.1). The parameter q determines the density shape and is known as entropic index, and η is the scale parameter. In the limit $q \to 1$, Equation (1.1) recovers the usual Exponential distribution.

Figure 2 shows the behavior of the q-Exponential PDF for η constant and three possible values of q. As it is possible to see through Equation (1.2) the support of the q-Exponential function is limited for $q < 1$. Figure 2 shows, for example, that when the $q = 0.5$ and $\eta = 3$ the support is limited by 6.

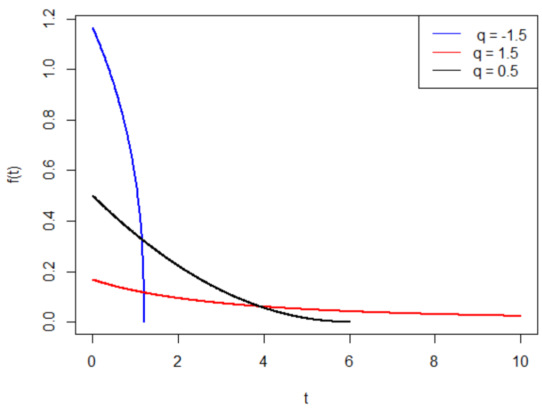

Figure 2: q-Exponencial PDF for η=3 and some values of q.
Source: This research (2018)

The q-Exponential has the following Cumulative Distribution Function (CDF):

$$F(t) = 1 - \left[1 - (1-q)\left(\frac{t}{\eta}\right)\right]^{\frac{2-q}{1-q}}, t \geq 0 \tag{2.1}$$

By definition, the hazard rate is $h(t) = \frac{f(t)}{R(t)}$ (MODARRES, KAMINSKIY & KRIVTSOV, 1999), where $R(t)$ is the reliability function with $R_q(t) = 1 - F(t)$. Thus, it is possible write:

$$h(t) = \frac{\frac{(2-q)\left[1-\frac{(1-q)t}{\eta}\right]^{\frac{1}{1-q}}}{\eta}}{\left[1-\frac{(1-q)t}{\eta}\right]^{\frac{2-q}{1-q}}} = \frac{(2-q)}{\eta}\left[1-\frac{(1-q)t}{\eta}\right]^{-1}. \tag{2.2}$$

Differently from the Exponential distribution, the q-Exponential hazard rate can be monotone increasing, monotone decreasing or constant for $q < 1$, $1 < q < 2$ and $q \to 1$, respectively. Indeed, this is an important characteristic of the q-Exponential distribution, especially in the reliability context because this feature enables the q-Exponential to model the three phases of the bathtub curve. Figure 3 presents the behavior of the q-Exponential hazard rate and of the q-Exponential CDF. For $\eta = 3$ and $q = 1.5$ the hazard rate is decreasing.

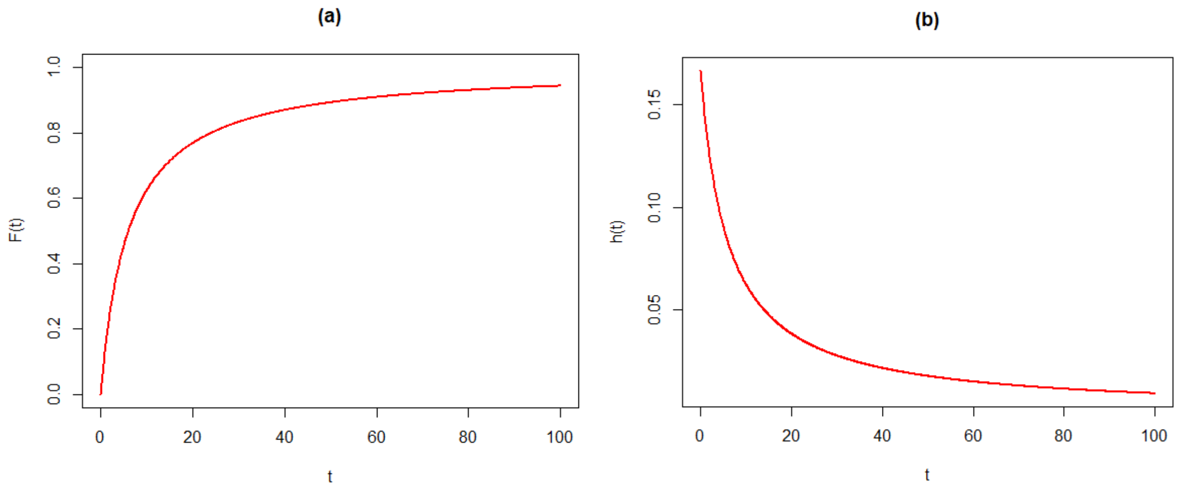

Figure 3: q-Exponential CDF with $\boldsymbol{\eta} = \mathbf{3}$ *and* $\boldsymbol{q} = \mathbf{1.5}$*; b) q-Exponential* $\boldsymbol{h}(\boldsymbol{t})$
with $\boldsymbol{\eta} = \mathbf{3}$ *and* $\boldsymbol{q} = \mathbf{1.5}$.
Source: This research (2018)

The conditional reliability function (MODARRES, KAMINSKIY & KRIVTSOV, 1999) is

$$R(t|t_0) = \frac{\left[1-(1-q)\left(\frac{t+t_0}{\eta}\right)\right]^{\frac{2-q}{1-q}}}{\left[1-(1-q)\left(\frac{t_0}{\eta}\right)\right]^{\frac{2-q}{1-q}}}. \tag{2.3}$$

This function calculates the reliability of an additional time period (t) when the item has worked for a time period (t_0). Figure 4 presents the conditional reliability of the q-Exponential for $t_0 = 2$h and for $t_0 = 5$h. Figure 4 represents the case which the hazard rate is decreasing, $1 < q < 2$.

Figure 5 illustrates the conditional reliability of the q-Exponential for $t_0 = 80$h and for $t_0 = 100$h. Besides, Figure 5 represents the case which the hazard rate is growing, $q < 1$.

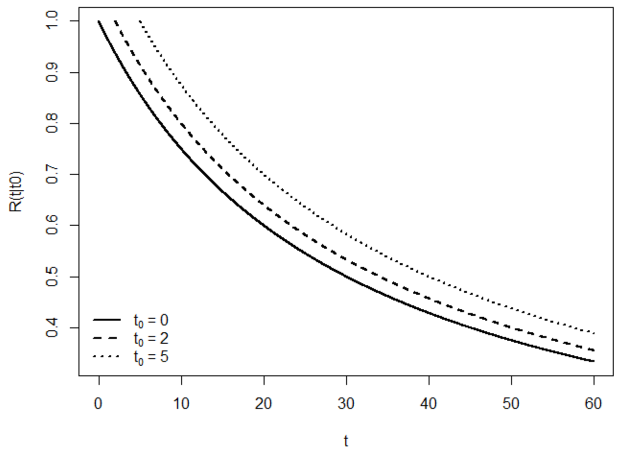

Figure 4: Conditional reliability of the q-Exponential function with $\boldsymbol{\eta = 15}$, $\boldsymbol{q = 1.5}$
Source: This research (2018)

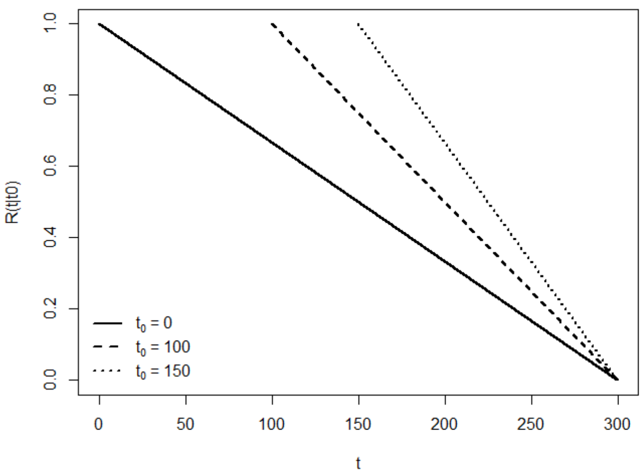

Figure 5: Conditional reliability of the q-Exponential function with $\boldsymbol{\eta = 150}$, $\boldsymbol{q = 0.5}$
Source: This research (2018)

2.2 Estimation of parameters

2.2.1 Maximum likelihood estimation

There are some ways to estimate the parameters of a probabilistic model, but the maximum likelihood method is one of the most used techniques. Considering the uniparametric case, assume a random sample of the random variable T with size n: $T_1, T_2, \dots, T_n$. It is the PDF of the random variable T, $f(t|\theta)$, with $\theta \in \Theta$, where Θ is the parametric space. Thus, the likelihood function of Θ, for the considered sample, can be written as presented by Bolfarine & Sandoval (2000):

$$L(\theta|t) = \prod_{i=1}^{n} f(t_i|\theta). \tag{2.4}$$

The value that maximizes the likelihood function is the maximum likelihood estimator of θ, and it is represented by $\hat{\theta}$ and $\hat{\theta} \in \Theta$.

In general, maximizing the natural logarithm of the likelihood function is easier than maximizing directly the likelihood function. The log-likelihood function is defined as

$$l(\theta|T) = \ln[L(\theta|T)]. \tag{2.5}$$

Thus, the maximum likelihood estimate for θ is obtained by calculating the root of the first derivative of the log-likelihood function, that is

$$\frac{dl(\theta|T)}{d\theta} = 0. \tag{2.6}$$

In situations in which the solution of Eq. (2.6) is very difficult to obtain analytically, it can be provided by numerical procedures or by heuristics.

In the specific case of the q-Exponential distribution, the likelihood function is

$$L(q,\eta|T) = \prod_{i=1}^{n} \frac{(2-q)\left[1-\frac{(1-q)t_i}{\eta}\right]^{1/1-q}}{\eta} = \frac{(2-q)^n}{\eta^n} \prod_{i-1}^{n} \left[1 - \frac{(1-q)t_i}{\eta}\right]^{1/1-q} \tag{2.7}$$

and the corresponding log-likelihood function is

$$l(q,\eta|T) = \ln\left(\frac{(2-q)^n}{\eta^n}\prod_{i=1}^{n}\left[1-\frac{(1-q)t_i}{\eta}\right]^{1/1-q}\right) =$$

$$= n\ln\left(\frac{2-q}{\eta}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\ln\left(1-\frac{(1-q)t_i}{\eta}\right). \tag{2.8}$$

The transformation above can be used because it is a monotonic transformation. In other words, it preserves the order of the numbers. Thus, the values that maximize Eq. (2.7) are the same that maximize Eq. (2.8).

To obtain the Maximum Likelihood Estimates (MLEs) for the parameters the log-likelihood function is maximized. This can be done by setting the first derivative of l with respect to each parameter to zero. The q-Exponential score equations are the following:

$$0 = \frac{\partial l}{\partial q} = -\frac{n}{2-q} + \frac{1}{(1-q)^2}\sum_{i=1}^{n}\ln\left(1-\frac{(1-q)t_i}{\eta}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\frac{t_i}{\eta\left(1-\frac{(1-q)t_i}{\eta}\right)}, \tag{2.9}$$

$$0 = \frac{\partial l}{\partial \eta} = -\frac{n}{\eta} - \frac{1}{1-q}\sum_{i=1}^{n}\frac{(1-q)t_i}{\eta^2\left(1-\frac{(1-q)t_i}{\eta}\right)}. \tag{2.10}$$

It is possible to obtain a simplified expression for Equation (2.10), as
$n = -\frac{1}{(1-q)}\sum_{i=1}^{n}\frac{(1-q)t_i}{\eta-(1-q)t_i}$.

However, the system formed by Equations (2.9) and (2.10) does not have a closed solution. Thus, numerical methods can be used to obtain parameters' estimates. However, these methods may fail to converge and may yield poor parameters' estimates, possibly because of the monotone likelihood problem.

2.2.2 Observed and expected information

To define observed and expected information is important before define the score function. Let $l(\theta|T)$ be the log-likelihood function. The vector score is defined as

$$U(\theta|T) = \left(\frac{\partial l(\theta|T)}{\partial \theta_1}, \cdots, \frac{\partial l(\theta|T)}{\partial \theta_d}\right)^T; \tag{2.11}$$

it is the gradient vector of the log-likelihood function.

The observed information matrix (Fisher's information) can be defined as

$$I_O(\theta|T) = \begin{bmatrix} -\frac{\partial^2 l(\theta|T)}{\partial \theta_1^2} & \cdots & -\frac{\partial^2 l(\theta|T)}{\partial \theta_1 \partial \theta_d} \\ \vdots & \ddots & \vdots \\ -\frac{\partial^2 l(\theta|T)}{\partial \theta_d \partial \theta_1} & \cdots & -\frac{\partial^2 l(\theta|T)}{\partial \theta_d^2} \end{bmatrix}.$$

and the matrix of expected information (Fisher's information) can be defined as

$$I_E(\theta|T) = \begin{bmatrix} E\left[-\frac{\partial^2 l(\theta|T)}{\partial \theta_1^2}\right] & \cdots & E\left[-\frac{\partial^2 l(\theta|T)}{\partial \theta_1 \partial \theta_d}\right] \\ \vdots & \ddots & \vdots \\ E\left[-\frac{\partial^2 l(\theta|T)}{\partial \theta_d \partial \theta_1}\right] & \cdots & E\left[-\frac{\partial^2 l(\theta|T)}{\partial \theta_d^2}\right] \end{bmatrix}.$$

An important property of $I_O(\hat{\theta}|T)$ and $I_E(\hat{\theta}|T)$ is that they measure the observed/expected curvature in the log-likelihood surface (RIBEIRO JR *et al.*, 2012).

2.2.3 Bootstrap confidence intervals

Bootstrap is a computer intensive statistical technique based on resampling (EFRON, 1993). The principal idea is to create a number of samples based on the available data set. The bootstrap method can be used to construct percentile confidence intervals for the parameters and also to estimate an estimator's distribution.

There are two types of bootstrap for the construction of confidence intervals: the parametric and the non-parametric bootstrap. The description below is based in Efron, (1993):

Parametric Bootstrap:

- Step 1: From a first sample for the variable $T = \{t_1, t_2 \cdots t_n\}$, estimate the parameters by maximizing the log-likelihood function;

- Step 2: A new sample for T is generated using the estimates obtained in the previous step and a number generator for variable T. Based on this new sample, compute the bootstrap sample estimate of θ, say θ^*, by maximizing the log-likelihood function of the variable T;

- Step 3: Repeat step 2 for N times;

- Step 4: By using N values of θ^* and by adopting α as significance level, find the percentiles $\theta^*_{\alpha/2}$ and $\theta^*_{1-(\alpha/2)}$. Thus, it is possible to determine an approximate confidence interval, with confidence equal to $100^*(1-\alpha)\%$, for the parameter θ, as:

$$C.I.= \left(\theta^*_{\alpha/2}, \theta^*_{1-(\alpha/2)}\right). \tag{2.11}$$

Non-Parametric Bootstrap:

- Step 1: From the original sample for the variable $T = \{t_1, t_2 \cdots t_n\}$, generate a new sample for T by sampling with replacement. Based on this new sample, compute the estimate of θ, θ^*, by maximizing the log-likelihood function of the variable T;

- Step 2: Repeat step 1 for N times.

- Step 3: By using N values of $\theta^*$and by adopting a α significance level, the percentiles $\theta^*_{\alpha/2}$ and $\theta^*_{1-(\alpha/2)}$ are obtained; they determine an approximate confidence interval for the parameter with confidence level equal to $100^*(1-\alpha)\%$, using Equation (2.11).

2.3 Bootstrapped Kolmogorov-Smirnov test (K-S Boot)

According to Blain (2014), in practice, applying the one-sample Kolmogorov-Smirnov test (K-S test) is not very useful because it requires a simple null hypothesis, i.e., the distribution must be completely specified with all parameters known beforehand. A bootstrapped version of a K-S test was proposed as an alternative to overcome this problem (STUTE, MANTEIGA & QUINDIMIL, 1993). This method results in precise asymptotic approximations of the *p*-values (CASTRO, 2013) and has the following steps:

- Step 1: From an initial sample from the variable $= (t_1, t_2, \cdots, t_n)$, estimate the parameters $\Theta = (\theta_1, \theta_2, \cdots, \theta_n)$ and compute the theoretical CDF: $F_n(T, \hat{\theta})$.

- Step 2: Compute $D_0 = max_{1 \le i \le n} \left| \left| \hat{F}_n(t_i) - F_n(t_i, \hat{\Theta}) \right|, \left| \hat{F}_n(t_{i-1}) - F_n(t_i, \hat{\Theta}) \right| \right|$, where $\hat{F}_n(T)$ is the empirical CDF.

- Step 3: Use the estimates obtained in the first step to create new samples for T, *i.e.*: $\{t^*_{1,j}, t^*_{2,j}, \cdots, t^*_{n,j}\}$. Based on these new samples, compute the bootstrap sample of $\hat{\Theta}$, say $\Theta^*_j = \{\theta^*_{1j}, \theta^*_{2j}, \cdots, \theta^*_{kj}\}$, $j = (1, 2, \cdots, N)$.

- Step 4: Repeat step 3 for N times.

- Step 5: Compute

$$D^*_j = max_{1 \le i \le n} \left| \left| \hat{F}^*_{n,j}(t^*_{i,j}) - F^*_{n,j}(t^*_{i,j}, \hat{\Theta}^*) \right|, \left| \hat{F}^*_{n,j}(t^*_{i,j}) - F^*_{n,j}(t^*_{(i-1),j}, \hat{\Theta}^*) \right| \right|.$$

The null hypothesis is rejected if $D_0 > D^*_{(N(1-\alpha)+1)}$ at significance level α. An approximate *p*-value can be computed using:

$$p = \frac{\#\{D^*_j \ge D_0\} + 1}{N+1},$$

where $\#\{D^*_j \ge D_0\}$ indicates the number of times that D^*_j $(j = 1, 2, \cdots, N)$ is bigger than D_0.

2.4 Regularity conditions

The maximum likelihood method is one of the most used approaches methods to obtain estimates of the parameters of a probabilistic model. However, there are some regularity conditions that must be satisfied to guarantee the asymptotic properties of the maximum likelihood estimates of consistency, unity, normality, efficiency and sufficiency (CORDEIRO, 1999).

Let $t_i's$ be realizations of one random variable T characterized by P_θ distributions that belong to one determined class P and this class depends on one vector θ of dimension p, $\theta \in \Theta$. Let $f(t;\theta)$ and $L(\theta) = \prod f(t_i;\theta)$ be the density and likelihood functions, respectively.

The following regularity conditions are required (CORDEIRO, 1999):

i. P_θ are identifiable, i.e., $\theta \neq \theta' \in \Theta$ implies $P_\theta \neq P_{\theta'}$;

ii. P_θ distributions have the same support for all $\theta \in \Theta$, i.e., $A = \{t; f(t;\theta) > \theta\}$ does not depend on θ;

iii. There is an open set Θ_1 in Θ that has θ_0 such that the density function $f(t;\theta)$, for almost every t, admits all derivatives until the third order in relation to θ, for all $\theta \in \Theta_1$;

iv. $E_\theta\{U(\theta)\} = 0$ and the information matrix $0 < I(\theta) < \infty$ for all $\theta \in \Theta_1$;

v. There are functions $M_{ijk}(t)$ independent of θ such that, for $i, j, k = 1, \cdots, p$,

$$\left|\frac{\partial^3 \log f(t;\theta)}{\partial\theta_i \partial\theta_j \partial\theta_k}\right| < M_{ijk}(t) \tag{2.12}$$

for all $\theta \in \Theta_1$, where $E_{\theta_0}\{M_{ijk}(t)\} < \infty$.

One of the problems verified in the q-Exponential distribution is that it does not satisfy the second regularity condition shown above, i.e., the function's support depends on the parameters of the probability distribution. Then, this work applied a change of variable in order to try correct this problem.

2.5 Change of variable

When a function g is invertible, it is possible to obtain an expression for the density function of $Y = g(T)$ using Theorem 1(FARIAS, KUBRUSLY & SOUZA, 2014):

Theorem 1: Jacobian method

Let X be a continuous random variable with density function f_T. Let also $g: \mathbb{R} \rightarrow \mathbb{R}$ be a strictly monotone and differentiable function in the $lm(T)$ set. If $Y = g(T)$, then:

i. $lm(T) = g\big(lm(T)\big) = \{y \in \mathbb{R} \mid \exists\, t \in lm(Y) \text{ with } y = g(t)\}$;

ii. Y is a random variable;

iii. $f_Y(y) = f_T\big(g^{-1}(y)\big)\left|\frac{d}{dy}g^{-1}(y)\right|$, if $y \in lm(Y)$.

where $lm(Y)$ is a data set that can be finite or infinite.

Demonstration of (iii) is presented below, the other demonstrations can be found in Farias Kubrusly & Souza (2014):

To demonstrate item (iii) the Distribution Function Method is used. It is required to find $F_Y(y) = P(Y \leq y)$. It is important to divide the case that g is strictly increasing and strictly decreasing.

If g is strictly increasing, g^{-1} can be obtained and it is also a strictly increasing function. Then, in this case:

$$F_Y(y) = P(Y \leq y) = P(g(T) \leq y) = P\big(T \leq g^{-1}(y)\big) = F_T\big(g^{-1}(y)\big). \tag{2.13}$$

Then, deriving with respect to y, it was found the relation between f_Y and f_T:

$$f_Y(y) = \frac{d}{dy}F_T\big(g^{-1}(y)\big) = f_T\big(g^{-1}(y)\big)\frac{d}{dy}g^{-1}(y). \tag{2.14}$$

If g is strictly decreasing, g^{-1} can be obtained and it is also a strictly decreasing function. Then, in this case:

$$F_Y(y) = P(Y \leq y) = P(g(T) \leq y) = P\big(T \geq g^{-1}(y)\big) = 1 - F_T\big(g^{-1}(y)\big). \tag{2.15}$$

Then, deriving in relation to y, the relation between f_Y and f_T is obtained:

$$f_Y(y) = \frac{d}{dy}\Big(1 - F_T\big(g^{-1}(y)\big)\Big) = -f_T\big(g^{-1}(y)\big)\frac{d}{dy}g^{-1}(y). \tag{2.16}$$

In case that g is strictly increasing $\frac{d}{dy}g^{-1}(y) > 0$ for all y, then it is possible to write

$$\frac{d}{dy}g^{-1}(y) = \left|\frac{d}{dy}g^{-1}(y)\right|. \tag{2.17}$$

And in case that g is strictly decreasing $\frac{d}{dy}g^{-1}(y) < 0$ for all y, it is possible to write

$$\frac{d}{dy}g^{-1}(y) = -\left|\frac{d}{dy}g^{-1}(y)\right|. \quad (2.18)$$

Thus, for any g strictly monotone:

$$f_Y(y) = f_X\left(g^{-1}(y)\right)\left|\frac{d}{dy}g^{-1}(y)\right|. \quad (2.19)$$

2.6 Nelder-Mead optimization method

The Nelder–Mead method is a numerical approach frequently applied to nonlinear optimization. It is also known as Downhill Simplex method. This method is used to find the minimum or maximum of an objective function in a multi-dimensional space. It is a method fairly used in unconstrained optimization problem of a function of n variables. This numerical approach has been used in many studies with the aim of maximizing the log-likelihood function and to estimate the parameters of various probability distributions in many areas, as reliability, statistics, economy, etc.

According to Gonçalves (2013), the Nelder-Mead method has the following characteristics:

- Ease of computational implementation;
- Calculations of the derivatives of the objective function are not necessary;
- Few evaluations of the objective function are necessary;
- The value of the objective function quickly decreases in the first iterations.

The Nelder-Mead uses the concept of a simplex, which is a polytope with $n + 1$ vertices in n dimensions.

Consider the problem of unconstrained minimization:

$$\min_{t \in \mathfrak{R}^n} f(t), \text{ where } f : \mathfrak{R}^n \longrightarrow \mathfrak{R}. \quad (2.20)$$

In this work, $f(t)$ is the negative of the q-Exponential log-likelihood.

In one iteration of this method, the $n+1$ vertices of the simplex, $t_1, t_2, \cdots, t_{n+1}$ belonging to $\Re^n$ are required according to the growth of the values of f, i.e:

$$f(t_1) \leq f(t_2) \leq \cdots \leq f(t_{n+1}), \tag{2.21}$$

where t_{n+1} is the worst vertex and t_1 is the best vertex.

The repositioning of these vertices takes into consideration four coefficients:

- Reflection coefficient (ρ)
- Expansion coefficient (χ)
- Contraction coefficient (γ)
- Reduction coefficient (σ)

Nelder and Mead (1965) explain that these coefficients must satisfy the following restrictions:

$$\rho > 0, \chi > 1, 0 < \gamma < 1 \text{ and } 0 < \sigma < 1.$$

The Nelder-Mead method attempts to exchange the worst vertex of the simplex by another one with better value. The new vertex is obtained by reflection, expansion or contraction of the worst vertex along the line through this vertex and the centroid of the best n vertices. The worst vertex is replaced by a new vertex or the simplex is reduced around the better vertex at each iteration.

Below is presented a set of steps that corresponds to an iteration of the Nelder-Mead algorithm (Nelder & Mead, 1965):

- **Step 1 - Rank:** Rank the $n+1$ vertices:

$$f(t_1) \leq f(t_2) \leq \cdots \leq f(t_{n+1});$$

- **Step 2- Centroid:** Calculate the centroid of the n best vertices:

$$\bar{t} = \sum_{i=1}^{n} \frac{t_i}{n}.$$

- **Step 3- Reflection:** Calculate the reflected vertex (t_r):

$$t_r = \bar{t} + \rho(\bar{t} - t_{n+1}).$$

If $f(t_1) \leq f(t_r) \leq f(t_n)$, then do $t_{n+1} = t_r$ and finalize the iteration.

- **Step 4- Expansion:** If $f(t_r) \leq f(t_1)$, calculate the expanded vertex (t_e):

$$t_e = \bar{t} + \chi(t_r - \bar{t}).$$

If $f(t_e) \leq f(t_r)$, then do $t_{n+1} = t_e$ and end the iteration, else $t_{n+1} = t_r$ and end the iteration.

- **Step 5- Contraction:** If $f(t_r) \geq f(t_n)$

5.1 External:
If $(t_n) \leq f(t_r) \leq f(t_{n+1})$, calculate the external contraction vertex (t_{ce}) :

$$t_{ce} = \bar{t} + \gamma(t_r - \bar{t}).$$

If $f(t_{ce}) \leq f(t_r)$, then do$t_{n+1} = t_{ce}$ and end the iteration, otherwise go to step 6.

5.2 Internal:
If $f(t_n) \geq f(t_n)$, calculate the internal contraction vertex(t_{ci}):

$$t_{ci} = \bar{t} - \gamma(\bar{t} - t_{n+1}).$$

If $f(t_{ci}) \leq f(t_{n+1})$, then do $t_{n+1} = t_{ci}$ and end the iteration, else go to step 6.

- **Step 6- Reduction:** Calculate vectors $v_i = t_1 + \sigma(t_i - t_1)$, $i = 2, \cdots, n+1$. The vertices (not ordered), for the next iteration are: $t_1, v_2, \cdots, v_{n+1}$.

Nelder & Mead (1965) explain that given a tolerance Δ_{tol}, the following stop criterion takes into account the function value in the simplex vertices:

$$\sqrt{\sum_{i=1}^{n+1} \frac{\left(f(t_i) - f(\bar{t})\right)^2}{n}} < \Delta_{tol}. \quad (2.22)$$

2.7 Firth's penalization method

A method to penalize the log-likelihood function in order to reduce the bias of the MLE was proposed by Firth (1993). Actually, the idea behind his method is that since the parameter estimate may not exist it is safer to modify the estimation equations for bias correction prior to estimation. Then, let $U^*(\theta)$ be the modified score function. For the exponential family model, the rth component of the modified score equation is given by

$$U_r^*(\theta) = U_r(\theta) + A_r(\theta), \tag{2.23}$$

in which $A_r(\theta)$ is the rth part of $A(\theta) = -I(\theta)B_1(\theta)/n\,, r = 1, \cdots,$ dim(θ). $B_1(\theta)$ is denoted here as the first order term in the bias expansion on the MLE: $B(\theta) = B_1(\theta)/n + B_2(\theta)/n + \cdots$.

In the case of an exponential family in canonical form, the observed information (Fisher's information) does not depend on the data, and it follows that

$$A_r(\theta) = \frac{\partial}{\partial\theta_r}\left\{\frac{1}{2}\log|I(\theta)|\right\}. \tag{2.24}$$

The correction of the likelihood function is applied as follows

$$L^*(\theta|T) = L(\theta|T)|K(\theta)|^{1/2}, \tag{2.25}$$

where the penalization term $|K(\theta)|^{1/2}$ is the determinant of the Fisher information matrix and it is the Jeffreys (1946) invariant prior. Equivalently, estimation can be executed by maximizing

$$l^*(\theta|T) = l(\theta|T) + \frac{1}{2}\log|K(\theta)|. \tag{2.26}$$

Note that the method proposed by Firth (1993) can be more easily applied in canonical exponential models. The exponential family in the canonical mode is defined as

$$f(t;\theta) = h(t)exp\big(\eta(\theta)u(t) - b(\theta)\big) \tag{2.27}$$

where the functions $h(t), \eta(\theta), u(t)$ and $b(\theta)$ assume real values. However, even when applied to functions that are not members of this group, this penalty method yields great results, as in Fonseca & Cribari-Neto (2016) that used it with a bimodal Birbaun-Saunders model.

3 INVESTIGATION AND CHANGES IN THE q-EXPONENTIAL LOG-LIKELIHOOD FUNCTION

This chapter will show an investigation about the behavior of the q-Exponential log-likelihood function and changes in its PDF as an attempt to correct its monotone behavior.

3.1 Behavior of the q-Exponential log-likelihood function

The following steps are applied to find an expression of the log-likelihood as a function of either η or q, so as to ease the identification of situations in which the log-likelihood is monotone increasing. First, we will show an evaluation of the arguments of the logarithms of

$$l(T|q,\eta) = n\ln\left(\frac{2-q}{\eta}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\ln\left(1 - \frac{(1-q)t_i}{\eta}\right)$$

in order to establish the criteria that the q-Exponential parameters must satisfy to preserve the validity of the log-likelihood function:

- For $1 < q < 2$, there is no problem, all arguments are valid.
- For $0 < q < 1$, the argument of the logarithms in the second part of Eq. (2.8) must satisfy the following inequality:

$$\frac{(1-q)t_i}{\eta} < 1, \forall\, i. \tag{3.1}$$

  Otherwise, the logarithm function would become indefinite, as its argument would be smaller or equal to zero.
- For $q \leq 0$, the same inequality in Eq. (3.1) must be satisfied.

Through inequality (3.1), t_i can be expressed as

$$t_i < \frac{\eta}{(1-q)}, \tag{3.2}$$

which has to be true for all i, including t_{max}^{o}, the largest observed value in the sample. Thus, t_{max}^{o} should be strictly smaller than the term of the right side, which will be called t_{max}:

$$t_{max}^{o} < \frac{\eta}{(1-q)} = t_{max}. \tag{3.3}$$

Also, δ is defined as the difference between t_{max} and t_{max}^{o}:

$$t_{max} - t_{max}^{o} = \delta. \tag{3.4}$$

Parameter η can be isolated from the equality in Eq. (3.3) and, by using Eq. (3.4), it can be written as a function of q, t_{max}^{o} and δ:

$$\eta = (1-q)t_{max} = (1-q)(t_{max}^{o} + \delta). \tag{3.5}$$

Thus, η in Eq. (2.8) can be replaced by the second equality of Eq. (3.5) and the following expression of the log-likelihood is obtained:

$$n\ln\left(\frac{1}{t_{max}^{o}+\delta}\right) + n\ln\left(\frac{2-q}{1-q}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\left(1 - \frac{t_i}{t_{max}^{o}+\delta}\right). \tag{3.6}$$

Notice that Eq. (3.6) is the log-likelihood function of Eq. (2.8) in terms of the parameter q, the sample value t_{max}^{o} and the constant δ. Parameter η is implicitly present in this equation.

Once Eq. (3.6) is obtained, we can write the following limit for $q \to -\infty$:

$$\lim_{q\to-\infty}\left[n\ln\left(\frac{1}{t_{max}^{o}+\delta}\right) + n\ln\left(\frac{2-q}{1-q}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\left(1 - \frac{t_i}{t_{max}^{o}+\delta}\right)\right] = n\ln\left(\frac{1}{t_{max}^{o}+\delta}\right). \tag{3.7}$$

Therefore, the log-likelihood function has $n\ln\left(\frac{1}{t_{max}^{o}+\delta}\right)$ as asymptote when $q \to -\infty$. This also happens to be an upper bound for the maximum value for the log-likelihood function that is practically never reached, since the more negative the parameter q the ligher the of the log-likelihood towards the asymptote. In this way, optimization techniques used to estimate the q-Exponential parameters when q is lower than 1 may present convergence difficulties as they tend to reach huge negative estimates for q. This behavior of the estimation procedures is indeed expected, since the function to be maximized is monotone increasing as $q \to -\infty$ (SALES FILHO, 2016). Such a convergence failure is reflected in the construction of confidence intervals, which tend to be large and practically useless.

Now we will be isolate the parameter q and will manipulate the log-likelihood function in order to set it in terms of η and the observed sample values. Thus, inequality (3.1) can be written as

$$q > -\left(\frac{\eta}{t_i}\right) + 1. \tag{3.8}$$

Then, we can replace the value of q in the first term of Eq. (2.8) by $-\left(\frac{\eta}{t^0_{max}+\delta}\right) + 1$, the parameter δ must be added to t^o_{max}because the theoretic t_{max} is larger than the observed t^0_{max}. In this way, the first term of Eq. (2.8) is

$$n \ln\left(\frac{1}{\eta} + \frac{1}{t_{max}+\delta}\right) = n \ln\left(\frac{(t_{max}+\delta)+\eta}{\eta(t_{max}+\delta)}\right). \tag{3.9}$$

The second term of Eq. (2.8) can be written as

$$\ln\left(\left[1 - \frac{t_i}{t_{max}+\delta}\right]^{(t_{max}+\delta)/\eta}\right). \tag{3.10}$$

Thus, Eq. (2.8) also can be written as follows

$$l(t|q,\eta) = n \ln\left(\frac{1}{\eta} + \frac{1}{t_{max}+\delta}\right) + \sum_{i=1}^{n} \ln\left(\left[1 - \frac{t_i}{t_{max}+\delta}\right]^{(t_{max}+\delta)/\eta}\right). \tag{3.11}$$

Once Eq. (3.11) is obtained, we can write the following limit for $\eta \to \infty$:

$$\lim_{\eta\to\infty} n \ln\left(\frac{1}{\eta} + \frac{1}{t_{max}+\delta}\right) + \sum_{i=1}^{n} \ln\left(\left[1 - \frac{t_i}{t_{max}+\delta}\right]^{(t_{max}+\delta)/\eta}\right) = n \ln\left(\frac{1}{t_{max}+\delta}\right). \tag{3.12}$$

The results found in Eq. (3.7) and Eq. (3.12) are the same.

It is important to notice that the sample size is constant. Experiments with some different samples were made, and these tests showed that, when the value of q decreases, the log-likelihood function increases. In other words, the called monotone likelihood is verified. Figure 6 shows this behavior. The red line represents an asymptote, which is the limit when $q \to -\infty$. However, even the limit of the function when $q \to -\infty$ being a finite a real number (Eq. (3.7)), this just happens in the infinite. In other words, it does not happen in practice. In this way, the green curve will always get closer to the asymptote but will never reach it.

The behavior verified in Figure 6 is analogous as the one observed in Figure 7. The first shows the behavior of the log-likelihood function presented in Eq. (3.6) when $q \to -\infty$. And the latter illustrates the behavior of the log-likelihood presented in Eq. (3.11) as η increases.

Both graphics were constructed with $n = 50$, $q = -1000$, $\eta = 4000$ and $\delta = 0.0001$. The asymptote represented by the red line in both graphics was calculated by the result of Eq. (3.7), which is the same as the result of Eq. (3.12). These asymptotes have the exactly same value when the sample is the same, as their value only depends on sample size, on the maximum sample value and on the value of δ. The asymptote value presented in the Figure 6 and in Figure 7 is -80.2470.

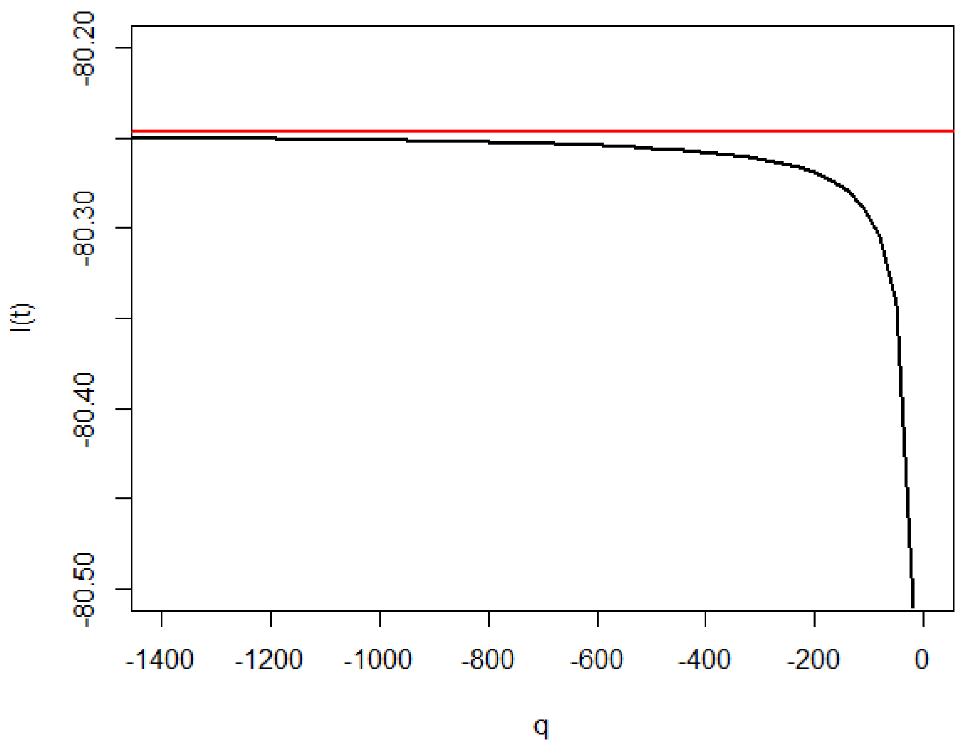

Figure 6: Behavior of the log-likelihood function when the parameter q decreases. Source: This research (2018)

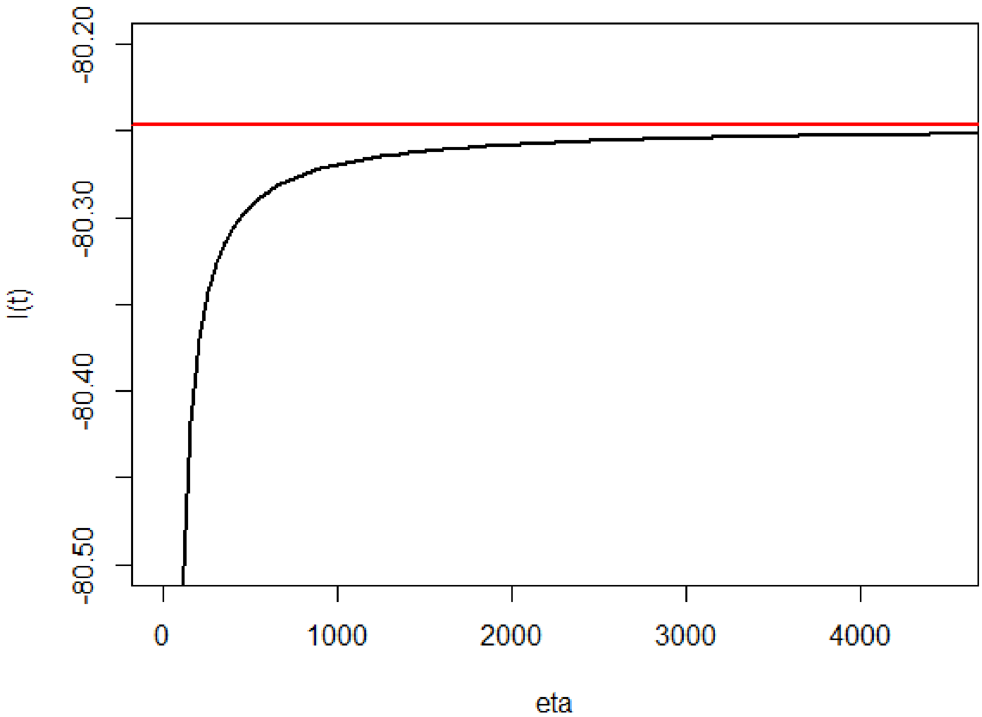

Figure 7: Behavior of the log-likelihood function when the parameter $\boldsymbol{\eta}$ *increases.*
Source: This research (2018)

3.2 Change of variable of the *q*-Exponential probability model

As discussed in the previous section, the *q*-Exponential distribution presents the called monotone likelihood, which concerns a behavior that makes the likelihood function increase as the parameters' values increase in module. However, this is not the only problem verified in this distribution. There are some regularity conditions that must be satisfied to guarantee the properties of the maximum likelihood estimators, as shown in Sub-section 3.3. In fact, the regularity condition that treats the independence of the function's support in relation to the parameters is not satisfied for the *q*-Exponential distribution.

With the goal to correct the log-likelihood function of the *q*-Exponential to satisfy the regularity condition, was applied a change of variable. The description of the change of variable is below.

Initially, the variable Y is defined as a function of the random variable $T \sim q - \text{Exp}$ as follows:

$$Y = \frac{t}{t_{max}}. \tag{3.13}$$

With this change, necessarily the function's support will be between 0 and 1, because the variable T has been divided by the theoretic maximum value. Thus, the regularity condition problem was solved, and the function's support does not depend on the distribution parameters anymore.

Using the results showed in (2.22), it follows

$$g^{-1}(T) = T = Yt_{max}, \tag{3.14}$$

$$\frac{dg^{-1}(T)}{dy} = t_{max}, \tag{3.15}$$

where

$$t_{max} = \frac{\eta}{1-q} = t_{max}^{0} + \delta. \tag{3.16}$$

Then,

$$f_y = f_t[Yt_{max}]t_{max}.$$

then,

$$f(y) = \frac{2-q}{1-q}(1-y)^{\frac{1}{1-q}}, \tag{3.17}$$

where

$$Y = \frac{t}{t_{max}^{0}+\delta}. \tag{3.18}$$

Eq. (3.17) is the new q-Exponential PDF; in other words, it is the reparametrized function of the q-Exponential distribution. The new density function now can be a function composed just by the parameters q and δ, but it is possible to obtain the parameter η with Eq. (3.16) presented above.

The new q-Exponential log-likelihood function defined only by the parameters q and δ is given as follows

$$l(y,q,\eta) = n\ln\left(\frac{2-q}{1-q}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\ln(1-y_i). \tag{3.19}$$

And the limit for $q \to -\infty$ is the following:

$$\lim_{q\to-\infty} n\ln\left(\frac{2-q}{1-q}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\ln(1-y_i) = \lim_{q\to-\infty} n\ln\left(1+\frac{1}{1-q}\right) + \frac{1}{1-q}\sum_{i=1}^{n}\ln(1-y_i) = 0$$
(3.20)

The limit $q \to -\infty$ goes equals zero and no larger depends on the sample length as is verified with the original log-likelihood function. Figure 10 shows the curve behavior with the log-likelihood function after the reparameterization with the parameters q and δ.

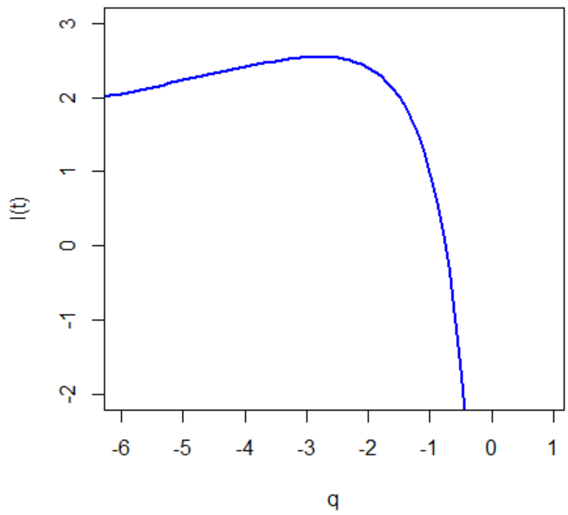

Figure 8: Behavior of the log-likelihood function after the change of variable with just the parameter q
Source: This research (2018)

Differently from Figure 6, by visual inspection of Figure 8 we see that now there is a value of parameter q that maximizes the log-likelihood function.

Then, is calculated the log-likelihood function just with the parameter η. To that end, it was necessary use the following equality:

$$q = -\left(\frac{\eta}{t_{max}}\right) + 1.$$

Thus, it was obtained the new q-Exponential log-likelihood function just with the parameter η:

$$l(y) = n\ln\left(\frac{2+\left(\frac{\eta}{t_{max}}\right)-1}{1+\left(\frac{\eta}{t_{max}}\right)-1}\right) + \frac{1}{1+\left(\frac{\eta}{t_{max}}\right)-1}\sum_{i=1}^{n}\ln(1-y_i) = n\ln\left(\frac{1+\left(\frac{\eta}{t_{max}}\right)}{\left(\frac{\eta}{t_{max}}\right)}\right) + \frac{1}{\left(\frac{\eta}{t_{max}}\right)}\sum_{i=1}^{n}\ln(1-y_i) = n\ln\left(1+\frac{t_{max}}{\eta}\right) + \frac{t_{max}}{\eta}\sum_{i=1}^{n}\ln(1-y_i).$$

And the limit for $\eta \to \infty$ is the following:

$$\lim_{\eta\to\infty} n\ln\left(1+\frac{t_{max}}{\eta}\right) + \frac{t_{max}}{\eta}\sum_{i=1}^{n}\ln(1-y_i) = 0. \quad (3.21)$$

The limit of the q-Exponential log-likelihood function as $\eta \to \infty$ is also zero, just like the result obtained in Eq. (3.20).

Eq. (3.19) can be written just in terms of the parameters q and δ through the Eq. (3.16). Thus, it is important to know the behavior of the parameter δ too. Indeed, δ is an auxiliary parameter, and it will be used to obtain the original parameters of the q-Exponential distribution. Figure 9 presents the behavior of the log-likelihood with respect to δ.

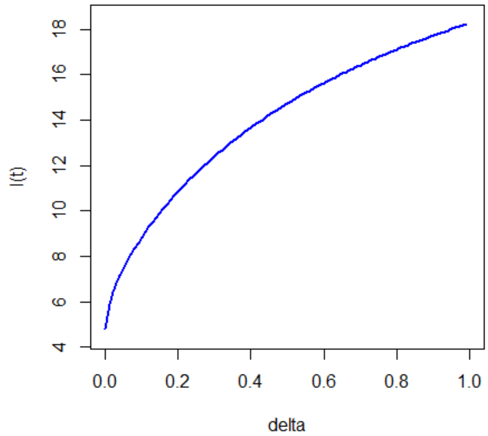

Figure 9: Behavior of the parameter $\boldsymbol{\delta}$*.*
Source: This research (2018)

It is possible to note that, differently from the new behavior of the parameter q, Figure 9 indicates that the monotone likelihood problem still exists. Figure 10 presents the behavior of the q-Exponential log-likelihood function with both parameters together (q and δ) and we clearly observe that the monotonic behavior of the log-likelihood function is still verified.

3.2.1 Characterization of the modified q-Exponential distribution

The new q-Exponential CDF and reliability function are as follows:

$$F(y) = \int_{-\infty}^{y} \frac{2-q}{1-q}(1-y)^{\frac{1}{1-q}}\,dy = 1-(1-y)^{\frac{2-q}{1-q}}, \tag{3.23}$$

$$R(y) = (1-y)^{\frac{2-q}{1-q}}. \tag{3.24}$$

Thus, the new q-Exponential hazard rate is:

$$h(y) = \frac{\frac{2-q}{1-q}(1-y)^{\frac{1}{1-q}}}{(1-y)^{\frac{2-q}{1-q}}} = \frac{(2-q)}{(1-q)}(1-y)^{\frac{q-1}{1-q}}. \tag{3.25}$$

Figure 11 presents the behavior of the new q-Exponential distribution hazard rate. The graphic shows an increasing curve. Thus, the properties of the q-Exponential, for $q < 1$, are preserved. The distribution is still able to model data in the degradation phase of the bathtub curve.

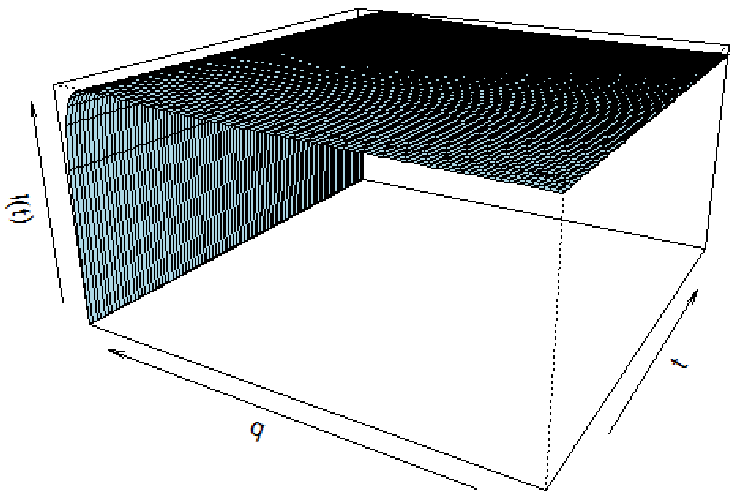

Figure 10: Graphic for the log-likelihood in function of q and t.
Source: This research (2018)

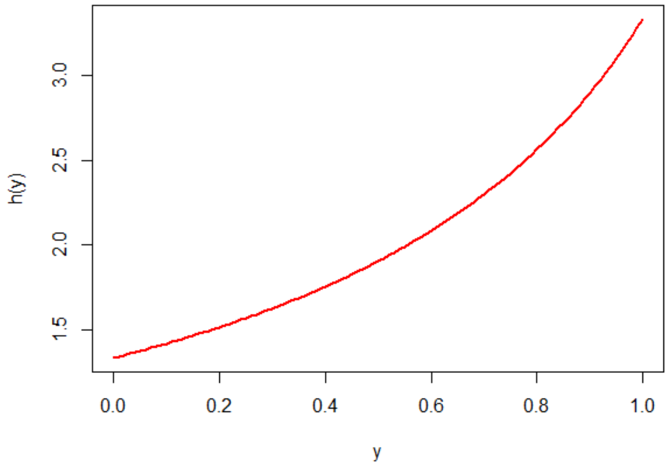

Figure 11: New q-Exponential hazard rate to $\boldsymbol{q = -2}$ *and* $\boldsymbol{\delta = 0.1}$

Source: This research (2018)

Although this change of variable solved partially the regularity condition related to the function's support, and preserved properties of the q-Exponential probability model, such as an increasing hazard rate for $q < 1$, as shown in Figure 11, this function does not produce good estimates for the parameters. Then, was applied the penalization Firth's method in this function, this correction was implemented in the software R, but it did not solve the problem because the correction did not produce good parameter estimates. Indeed, the implementation made in R could not turn back any results for this situation, the function implemented just turn back computational errors.

Therefore, it was decided to maintain this modification in this work, even though it does not solve the monotone log-likelihood problem. However, it is possible to think about other change of variables or any reparameterization for the q-Exponential log-likelihood function in future works or even find other method to correct this modified function.

4 PENALIZED q-EXPONENTIAL LOG-LIKELIHOOD

In this chapter, Firth's method is applied to penalize the q-Exponential log-likelihood function. A slight modification of the method was required and it will be described in what follows. This method was chosen to penalize the q-Exponential log-likelihood function basically for two reasons; the first respects to the efficiency obtained with the application, as it is possible see in Fonseca & Cribari-Neto (2018); and the second can be explained by the simplicity of this method.

Under regularity conditions and for large samples, $\hat{\theta} \sim N_3(\theta, I(\theta)^{-1})$ approximately, where $I(\theta)$ is Fisher's (expected) information matrix:

$$I(\theta) = E\left[\frac{\partial l(\theta)}{\partial \theta} \quad \frac{\partial l(\theta)}{\partial \theta^T}\right].$$

The score function of the q-Exponential log-likelihood is presented in Equations (2.9) and (2.10). In general, $I(\theta) = E[J(\theta)]$ is easier to compute, where $J(\theta) = -\partial^2 l(\theta)/\partial\theta\partial\theta^T$ is the observed information. For the q-Exponential model, we obtain

$$J(\theta) = \begin{bmatrix} J_{qq} & J_{q\eta} \\ J_{\eta q} & J_{\eta\eta} \end{bmatrix},$$

where

$$J_{qq} = -\frac{n}{(2-q)^2} + \frac{2}{(1-q)^3}\sum_{i=1}^{n} \ln\left(1 - \frac{(1-q)t_i}{\eta}\right) + \frac{2}{(1-q)^2}\sum_{i=1}^{n} \frac{t_i}{\eta\left(1-\frac{(1-q)t_i}{\eta}\right)} + \frac{1}{(1-q)}\sum_{i=1}^{n} \frac{t_i^2}{\eta^2\left(1-\frac{(1-q)t_i}{\eta}\right)}, \quad (4.1)$$

$$J_{\eta\eta} = \frac{n}{\eta^2} + \frac{1}{(1-q)}\sum_{i=1}^{n}\left(-\frac{2(1-q)t_i}{\eta^2\left(1-\frac{(1-q)t_i}{\eta}\right)} - \frac{t_i^2(1-q)^2}{\eta^4\left(1-\frac{(1-q)t_i}{\eta}\right)}\right), \quad (4.2)$$

$$J_{q\eta} = J_{\eta q} = \frac{1}{(1-q)^2}\sum_{i=1}^{n} \frac{(1-q)t_i}{\eta^2\left(1-\frac{(1-q)t_i}{\eta}\right)} + \frac{1}{(1-q)}\sum_{i=1}^{n} -\frac{t_i}{\eta^2\left(1-\frac{(1-q)t_i}{\eta}\right)} - \frac{t_i^2(1-q)}{\eta^4\left(1-\frac{(1-q)t_i}{\eta}\right)}. \quad (4.3)$$

Thus, as previously presented, the original idea of this method involves the utilization of the matrix of the expected or the observed information (Fisher's information), but in some cases the expected information it is not easily to be obtained. In these cases, the matrix of the observed information can be used as an approximation of the expected information. The penalization is obtained by the Equation 2.26 (Firth's penalization method).

Table 1 presents the results of a Monte Carlo simulation ran with the original q-Exponential log-likelihood function and with the penalized q-Exponential log-likelihood function for η constant and three values of q. This simulation was performed by the function Optim of the computational software R with 10000 replications for five sample sizes (20, 50, 100, 500, 1000) and the numerical method utilized to do the maximizations was the Nelder-Mead.

Table 1: Point Estimation and Relatives Bias for parameters $\boldsymbol{q}$ and $\boldsymbol{\eta}$ with $\boldsymbol{\eta}$ constant

For $q = -20$ and η = 5	$\hat{q}$	**Rel. Bias $\hat{q}$**	$\hat{\eta}$	**Rel. Bias $\hat{\eta}$**
Original function, n=20	-141900356	7095017	31963831	6392765
Penalized function, n=20	-8.2962	-0.5851	2.0913	-0.5817
Original function, n=50	-50594075	2529703	11797129	2359425
Penalized function, n=50	-8.6269	-0.5686	2.2415	-0.5516
Original function, n=100	-22844008	1142199	5377958	1075591
Penalized function, n=100	-8.8741	-0.5562	2.3236	-0.5352
Original function, n=500	-2213100	110654	525524.8	105104
Penalized function, n=500	-9.8777	-0.5061	2.5832	-0.4833
Original function, n=1000	-535200.5	26759.03	127240.5	25447.09
Penalized function, n=1000	-10.7615	-0.4619	2.7966	-0.4406
For $q = -2$ and η = 5	$\hat{q}$	**Rel. Bias $\hat{q}$**	$\hat{\eta}$	**Rel. Bias $\hat{\eta}$**
Original function, n=20	-98051761	49025880	146483739	29296747
Penalized function, n=20	-4.4989	1.2494	8.24302	0.6486
Original function, n=50	-16157679	8078839	25362689	5072537
Penalized function, n=50	-4.3327	1.1663	8.4486	0.6897
Original function, n=100	-1600956	800476.8	2558381	511675.2
Penalized function, n=100	-4.2796	1.1398	8.5361	0.7072
Original function, n=500	-2.8395	0.4197	6.3609	0.2721
Penalized function, n=500	-3.6188	0.8094	7.6328	0.5265
Original function, n=1000	-3.2317	0.6158	7.0284	0.4056
Penalized function, n=1000	-3.5828	0.7914	7.6010	0.5202
For $q = 0.5$ and η = 5	$\hat{q}$	**Rel. Bias $\hat{q}$**	$\hat{\eta}$	**Rel. Bias $\hat{\eta}$**
Original function, n=20	-4928221	-9856444	28659849	5731969
Penalized function, n=20	0.3891	-0.2216	7.6341	0.5268
Original function, n=50	-24925.44	29591.83	147964.1	-24925.44
Penalized function, n=50	0.8546	0.7092	4.7675	-0.0464
Original function, n=100	0.3610	-0.2779	5.7856	0.1571
Penalized function, n=100	0.9645	0.9290	4.4141	-0.1171
Original function, n=500	0.4720	-0.0559	5.1602	0.0320
Penalized function, n=500	0.6298	0.2597	4.9724	-0.0055
Original function, n=1000	0.4781	-0.0437	5.1462	0.0292
Penalized function, n=1000	0.4948	-0.0102	5.0114	0.0022

Source: This research (2018)

By analyzing the results showed in the Table 1, it is verified that the penalized q-Exponential log-likelihood presented better parameter estimates compared to the original function, even for small sizes of sample as 20 and 50 observations.

For $q = -20$ and $\eta = 5$ the original q-Exponential log-likelihood function did not yield any good estimate for the parameters. Meanwhile the larger absolute relative bias that the penalized function reached for the parameter q was -0.5851 and the larger absolute relative bias for the parameter η was -0.5817, *i.e.*, the corrected function achieved a bias lower than 60% for the smallest sample size. This bias drops to lower than 50% as the size of sample is 1000 observations.

For $q = -2$ and $\eta = 5$, the original function did not produce good results for the sample sizes 20, 50 and 100 realizations. Indeed, for these sample sizes the estimates are very poor. However, for these parameters values, starting of samples with 500 observations the original q-Exponential log-likelihood function yields reliable estimates for the parameters. On the other hand, for both values of parameters, the corrected function produces good estimates for all sample sizes. However, it is important to make it clear that for great sample sizes (500 and 1000, for example) the original function did produce slightly results than the penalized function.

For $q = 0.5$ and $\eta = 5$, the results for this combination of parameters were similar at the previous case. The original function produced good estimates for the parameters just for samples with a larger number of observations (100, 500 and 1000 realizations). And the penalized function yielded very good estimates for all the sample sizes, which means that the penalty in the q-Exponential log-likelihood function worked very well. The largest absolute relative bias verified with the corrected function was 0.9290 for the parameter q and 0.5268 for the parameter η. Meanwhile, the largest absolute relative bias that the original function produced was -9856444 for the parameter q and 5731969 for the parameter η.

Table 2 present the results of a Monte Carlo simulation ran with the original and penalized q-Exponential log-likelihood for q constant and three values of η. This simulation was also performed by the function Optim of the computational software R with 10000 replications for five sample sizes (20, 50, 100, 500, 1000) and the numerical method utilized to do the maximizations was the Nelder-Mead.

Table 2: Point Estimation and Relatives Bias for parameters $\boldsymbol{q}$ and $\boldsymbol{\eta}$ with $\boldsymbol{q}$ constant

For $q = -2$ and $\eta = 50$	$\hat{q}$	**Rel. Bias** $\hat{q}$	$\hat{\eta}$	**Rel. Bias** $\hat{\eta}$
Original function, n=20	-19770436	9885217	295654300	5913085
Penalized function, n=20	-3.6797	0.8398	70.2032	0.4040
Original function, n=50	-3206861	1603430	50337273	1006744
Penalized function, n=50	-3.4177	0.7088	69.9918	0.3998
Original function, n=100	-309689.9	154844	4951017	99019.33
Penalized function, n=100	-3.3334	0.6667	70.0970	0.4019
Original function, n=500	-2.4841	0.2420	57.7073	0.1541
Penalized function, n=500	-3.1803	0.5901	69.0548	0.3810
Original function, n=1000	-2.4325	0.2162	57.0019	0.1400
Penalized function, n=1000	-3.0389	0.5194	66.9627	0.3392
For $q = -2$ and $\eta = 500$	$\hat{q}$	**Rel. Bias** $\hat{q}$	$\hat{\eta}$	**Rel. Bias** $\hat{\eta}$
Original function, n=20	-10294098	5147048	1540086511	3080172
Penalized function, n=20	-3.6346	0.8173	695.8656	0.3917
Original function, n=50	-1664069	832033.6	261186838	522372.7
Penalized function, n=50	-3.4038	0.7019	697.7501	0.3955
Original function, n=100	-159733	79865.48	25527798	51054.6
Penalized function, n=100	-3.3228	0.6614	699.3281	0.3986
Original function, n=500	-2.4983	0.2491	579.2700	0.1585
Penalized function, n=500	-3.2385	0.6192	700.2667	0.4005
Original function, n=1000	-2.3246	0.1623	552.0839	0.1041
Penalized function, n=1000	-3.2141	0.6070	698.7303	0.3970
For $q = -2$ and $\eta = 1000$	$\hat{q}$	**Rel. Bias** $\hat{q}$	$\hat{\eta}$	**Rel. Bias** $\hat{\eta}$
Original function, n=20	-8970900	4485449	2686290200	2686289
Penalized function, n=20	-3.6472	0.8236	1394.5930	0.3945
Original function, n=50	-1409583	704790.3000	442743701	442742.7000
Penalized function, n=50	-3.4039	0.7019	1395.3930	0.3953
Original function, n=100	-134713.4000	67355.7100	43027614	43026.6100
Penalized function, n=100	-3.3165	0.6582	1396.4650	0.3964
Original function, n=500	-2.5063	0.2531	1161.0870	0.1610
Penalized function, n=500	-3.2282	0.6141	1397.1590	0.3971
Original function, n=1000	-2.3050	0.1525	1097.6210	0.0976
Penalized function, n=1000	-3.2128	0.6064	1397.0850	0.3970

Source: This research (2018)

For $q = -2$ and $\eta = 50$, the original function did not produce good results for the sample sizes 20, 50 and 100 realizations. For this sample sizes the estimates are very poor. However, for these parameters values, starting of samples with 500 observations the original *q*-Exponential log-likelihood function yields good estimates for the parameters. On the other hand, for these both values of parameters, the corrected function still to produces good estimates of the parameters for all sample sizes.

For $q = -2$ and $\eta = 500$, for this combination of parameters, once again the original q-Exponential log-likelihood function only yielded good results for larger sample sizes (500 and 1000 observations, for example). And once more the penalized function maintains good results (small biases) even for small sample sizes (20 and 50 observations, for example).

For $q = -2$ and $\eta = 1000$, the corrected function remained consistent, *i.e.* the results obtained with this function were still good even for small samples, just as for the other combinations of parameters. On the other hand, the original function only starts to produce good results for samples with at least 500 observations.

The results presented in Tables 4.1 and 4.2 show that the penalized function is consistent and effective even for small sizes samples since it is possible to obtain good results in these cases. On the other hand, the original function proved to be more effective for big sizes sample. However, as the parameter q increases in module, the original function does not yield good results even for larger sample sizes, as it is possible to see in the Table 1, for $q = -20$ and $\eta = 5$. Other tests with values of the parameter q higher in module were made and the results obtained by the original log-likelihood were not good.

In practice, it is not viable to obtain samples with a big number of realizations, sometimes there are not financing to get this or just it is not possible. Thus, it is possible to affirm that the original function is not a good choice, because it only showed good results in specific cases. Moreover, as the parameter q increases in module, the original function does not produce good results at all.

4.1 Confidence intervals based on bootstrap methods

In what follows, the parametric and non-parametric bootstrap methods will be applied to construct the confidence intervals for the parameters q and η of the q-Exponential distribution.

4.1.1 Confidence intervals based on parametric bootstrap for the q-Exponential parameters

The sequence showed below presents the way used to construct the confidence intervals based on parametric bootstrap for the q-Exponential parameters, q and η:

1. Obtain estimates for q and η for the q-Exponential distribution by maximizing Equation (2.10).

2. By using the estimates obtained in the first step and using

$$T = \frac{\eta\left[1 - U^{\left(\frac{1-q}{2-q}\right)}\right]}{1 - q}$$

obtained by means of the inversion method, it is possible to generate a new sample T^*, *i.e.*, $\{t_1^*, t_2^*, \cdots, t_n^*\}$. Based on this new sample, the bootstrap estimates must be computed for q and η, say q^* and η^*, by maximizing Equation (2.10).

3. Then, repeat the step 2 for N times.

4. Next, by using the N values of q^* and η^*, obtained in the step 3, and by adopting α as significance level, the quantiles $\alpha/2$ and $1-\alpha/2$ for q^* and η^* are obtained. Finally, it is possible to obtain approximate confidence intervals for the parameters q and η with confidence of $100(1-\alpha)\%$ by the following equations:

$$CI[q;\ 100(1-\alpha)\%] = \left[q^*_{\alpha/2}, q^*_{1-\alpha/2}\right], \quad (4.4)$$

$$CI[\eta;\ 100(1-\alpha)\%] = \left[\eta^*_{\alpha/2}, \eta^*_{1-\alpha/2}\right]. \quad (4.5)$$

Simulations were made in order to assess the coverage of 95% of the confidence intervals provided by the bootstrap method. The nominal level of significance was set to $\alpha = 0.05$. The idea was to count how many times the true parameter value of q and η were within the confidence interval. For this experiment the penalized function was used, a Monte Carlo simulation experiment was performed with 5000 replications, for three sample sizes ($n = 20$, $n = 50$ and $n = 100$) and for four parameter combinations, as shown in Table 3.

From the analysis of the results reported in Table 3, it can be inferred that, in general, the results were satisfactory because the coverages obtained for the confidence intervals were, in general, close to the tested quantile (90% and 95%). However, for small samples (for example, $n = 20$), for some cases, the performance of the parametric bootstrap were worst compared with the performance provided by larger samples.

Table 3: Confidence Intervals Coverage obtained by the Parametric Bootstrap Simulations

Sample Size	Parameter value	Coverage	Sample Size	Parameter value	Coverage
$n = 20$	$q = -2$	0.840	$n = 20$	$q = -5$	0.426
	$\eta = 5$	0.558		$\eta = 50$	0.640
$n = 50$	$q = -2$	0.982	$n = 50$	$q = -5$	0.764
	$\eta = 5$	0.976		$\eta = 50$	0.784
$n = 100$	$q = -2$	0.982	$n = 100$	$q = -5$	0.946
	$\eta = 5$	0.980		$\eta = 50$	0.946
Sample Size	**Parameter value**	**Coverage**	**Sample Size**	**Parameter value**	**Coverage**
$n = 20$	$q = -10$	0.784	$n = 20$	$q = -20$	0.840
	$\eta = 80$	0.764		$\eta = 100$	0.84
$n = 50$	$q = -10$	0.998	$n = 50$	$q = -20$	0.986
	$\eta = 80$	0.996		$\eta = 100$	0.976
$n = 100$	$q = -10$	0.998	$n = 100$	$q = -10$	0.986
	$\eta = 80$	0.998		$\eta = 100$	0.986

Source: This research (2018)

4.1.2 Confidence intervals based on non-parametric bootstrap for the q-Exponential parameters

The steps presented following shows how to build the confidence intervals based on non-parametric bootstrap for the q-Exponential parameters, q and η:

1. First, a new sample $X^* = \{x_1^*, x_2^*, \cdots, x_n^*\}$ is generated with replacement from a original sample $X = \{x_1, x_2, \cdots, x_n\}$. Based on this new sample, the estimates q^* and η^* for q and η are computed by maximizing the Equation (2.10).

2. Then, the first step must be repeated N times.

3. Finally, with the N values of q^* and η^* obtained in the step 2 and by adopting α as a significance level, the quantiles $\alpha/2$ and $1-\alpha/2$ for q and η must be found. Thus, it is possible construct by Equations (4.4) and (4.5) approximate confidence intervals for q and η, with confidence interval equals to $100(1-\alpha)\%$.

Table 4 shows the Monte Carlo simulation results made to test how robust the q-Exponential penalized function can be with respect to the non-parametric bootstrap confidence intervals. By analyzing Table 4 it is possible to note that, as the parametric bootstrap (Table 3), the non-parametric bootstrap is also satisfactory, once the probabilities reached with this method are in mostly superior than 80%. Some results were unsatisfactory, as for $q = -5$, $\eta = 50$ and $n = 20$, which for parameter q the confidence interval coverage was of 0.478 and for parameter η was of 0.490, both less than 50%, but these inferior results are the minority. On the other hand, for this same setting, when the size of the sample increases the results improve.

The next chapter brings examples with reliability-related data in which both q-Exponential log-likelihood functions, original and penalized, are applied. Besides, there is a comparison between the fit provided by the q-Exponential and Weibull distributions.

Table 4: Confidence Intervals Coverage obtained by the Non-Parametric Bootstrap Simulations

Sample Size	Parameter value	Coverage	Sample Size	Parameter value	Coverage
$n = 20$	$q = -2$	0.928	$n = 20$	$q = -5$	0.478
	$\eta = 5$	0.962		$\eta = 50$	0.490
$n = 50$	$q = -2$	0.982	$n = 50$	$q = -5$	0.622
	$\eta = 5$	0.962		$\eta = 50$	0.730
$n = 100$	$q = -2$	0.992	$n = 100$	$q = -5$	0.684
	$\eta = 5$	0.986		$\eta = 50$	0.824
Sample Size	**Parameter value**	**Coverage**	**Sample Size**	**Parameter value**	**Coverage**
$n = 20$	$q = -10$	0.518	$n = 20$	$q = -20$	0.644
	$\eta = 80$	0.83		$\eta = 100$	0.91
$n = 50$	$q = -10$	0.622	$n = 50$	$q = -20$	0.730
	$\eta = 80$	0.824		$\eta = 100$	0.962
$n = 100$	$q = -10$	0.824	$n = 100$	$q = -10$	0.824
	$\eta = 80$	0.962		$\eta = 100$	0.984

Source: This research (2018)

5 EMPIRICAL APPLICATIONS

In this chapter, two empirical applications with failure data are considered. They can be modeled by a q-Exponential distribution with $q < 1$, *i.e.*, with an increasing hazard rate (last phase of the bathtub curve).

The first case study, whose data are in Table 5, involves a magnetic resonance imaging (MRI) equipment. MRI scanners use strong magnetic fields, radio waves, and field gradients to generate images of the organs in the body to be analyzed by doctors and specialists (PEREIRA, 2017).

Figure 12 shows an exams room. According to Pereira (2017), the exams room is composed by the main part of the equipment and the patient table, the gantry, with the magneto, the gradient coil and the radio frequency (RF). The author still explain that the magneto is a big coil that needs to be refrigerated by liquid helium in order to maintain its superconductors characteristics.

Table 5: TBF of the MRI equipment (sample 1)

Number	TBF	Number	TBF	Number	TBF	Number	TBF
1	**99**	18	**66**	35	**14**	52	**3**
2	**38**	19	**25**	36	**35**	53	**46**
3	**109**	20	**4**	37	**73**	54	**17**
4	**10**	21	**8**	38	**18**	55	**7**
5	**35**	22	**26**	39	**38**	56	**75**
6	**42**	23	**98**	40	**140**	57	**58**
7	**31**	24	**11**	41	**19**	58	**102**
8	**18**	25	**87**	42	**10**	59	**6**
9	**53**	26	**11**	43	**17**	60	**53**
10	**3**	27	**54**	44	**4**	61	**47**
11	**12**	28	**22**	45	**54**	62	**26**
12	**13**	29	**13**	46	**26**	63	**87**
13	**40**	30	**54**	47	**135**	64	**6**
14	**6**	31	**19**	48	**44**	65	**13**
15	**78**	32	**47**	49	**59**		
16	**77**	33	**14**	50	**11**		
17	**24**	34	**53**	51	**18**		

Source: PEREIRA (2017)

Figure 12: Exams room of MRI
Source: PEREIRA (2017)

The second case study, whose data are in Table 6, refers to a UHT milk filling machine from the manufacturer Tetra Pak, A3 Flex version 015V (CARNAÚBA & SELLITO, 2013). The authors explain that the machine functions are: to manufacture the package, to sterilize the packing material, to pack the product and to provide the product in the final mat. Packaging machines are critical equipment for the production of dairy products and their breakdown can represent a complete stop of the entire process (SELLITO, BORCHADT & ARAÚJO, 2002). In the case studied in this dissertation a machine failure represents loss of production.

The machine shown in Figure 13 is composed by some subsystems, for which many failure modes can cause a general failure. Thus, the first subsystem that fails causes the interruption of the production process (CARNAÚBA & SELLITO, 2013). The equipment failure data were collected by the software PLMS Centre Premium, which is provided by Tetra Pak. According to Carnaúba & Sellito (2013), this software collects data directly from the machine in real time, stores them in a database and provides the results by means of spreadsheets and graphics. Figure 13 shows an illustration of a packaging machine.

Table 6: TBF of the packaging machine (sample 2)

Observation number	Time Between Failure (TBF)
1	7.492
2	7.485
3	9.449
4	3.951
5	1.748
6	2.070
7	10.628
8	4.256
9	5.262
10	3.223
11	8.376
12	12.598
13	5.303
14	1.861

Source: CARNAÚBA & SELLITO (2013)

Figure 13: Packaging machine Tetra Pak
Source: Tetra Pak (2013)

Tetra Pak recommends that this equipment receives a prior periodic review after 500 hours of work and that is made a preventive maintenance on intervals of 1000 hours of work so as to extend the equipment maturity phase. Table 7 shows the descriptive statistics of samples 1 and 2.

Table 7: Descriptive statistics for samples 1 and 2

	Mean	St. Dev.	Minimum	Maximum	Spread
Sample 1	38.4583	30.7474	3	109	106
Sample 2	5.9787	3.4368	1.748	12.598	10.85

Source: This research (2018)

5.1 Applications

Tables 5.1 and 5.2 present the samples collected by Pereira (2017) and by Carnaúba & Sellito (2013), respectively. The unity of measurement of these data is days, and it represents the time between failures (TBF). The Nelder-Mead optimization method was used for maximizing all the functions used in this work (penalized and original log-likelihood functions of the q-Exponential distribution). For these applications, it is important ratify that it has been considered a state following the repair called as good as new.

Table 8 shows the estimates obtained for sample 1. Besides, there is a comparison between the results obtained with the original and with the penalized q-Exponential log-likelihood. For parameter q, the two estimates are lower than 1, which is the case of an increasing hazard rate. Although the estimates obtained with the original function are reasonable, once the estimates have no a greater magnitude, the penalized function achieves a better result, with a greater value for the log-likelihood.

Table 8: Parameter estimates for sample 1

Distribution	$\hat{q}$	$\hat{\eta}$	Log-likelihood value
Original q-Exponential	0.6831	64.6078	-302.4141
Penalized q-Exponential	-2.9354	550.9695	-294.6075

Source: This research (2018)

Table 9 brings the parameters' estimates for the second case (sample 2). For this case, the original log-likelihood provided poor estimates, in other words, this function produced estimates values very high. The values for $\hat{q}$ and $\hat{\eta}$ are incompatible with reality because of the high order of magnitude of these, once it is expected to obtain estimates no higher than 10^4. On the other hand, the result obtained with the penalized function are at least realistic. And, once more, the value of the log-likelihood reached with the corrected function is better than the one provided by the original function. Indeed, in both Tables 5.4 and 5.5, the value obtained for the log-likelihood function is in average twice as higher as the result given by the original function.

Table 9: Parameter estimates for sample 2

Distribution	$\hat{q}$	$\hat{\eta}$	Log-likelihood value
Original q-Exponential	-6102699	76881817	-35.4695
Penalized q-Exponential	-2.8479	48.4769	-14.4215

Source: This research (2018)

After computing the parameter estimates, it was calculated the p-value for the two samples. It was used the K-S Boot test to obtain these measures. Table 6 contains the values of sample 1. For this sample the p-value was of 0.5034, *i.e.*, the null hypothesis can not be rejected, and the q-Exponential distribution can fit the data set.

Table 6 contains the values of sample 2. For this sample the p-value was of 0.9470, *i.e.*, this p-value practically represents a perfect fit of the data set. Therefore, the null hypothesis can not be rejected, and the q-Exponential distribution can fit the data set.

Tables 10 and 12 presents the non-parametric and parametric confidence intervals for the samples 1 and 2. In these tables it is possible to see that the results obtained with the original function for the two samples are worse than the results reached by the penalized function. Besides, poor results were presented for sample 2, it is not possible to make reliable predictions with them.

In Table 11, the non-parametric bootstrap confidence intervals are presented for the parameters q and η (samples 1 and 2). The width for each parameter confidence interval is also given in this table, this measure indicates the uncertainty about the true parameter value. The width of the non-parametric bootstrap confidence intervals for the sample 1 are better than for the sample 2, once that widths are lower. However, sample 1 ($n = 65$) is larger that sample 2, because of that it is expected better results with this sample. On the other hand, the widths obtained with the computed confidence intervals for sample 2 are not bad, once this sample have a small size ($n = 14$), and improved results are expected with bigger samples. The results presented in the Table 11 were obtained with the penalized q-Exponential distribution.

Table 11 presents the parametric bootstrap confidence intervals for the parameters q and η (samples 1 and 2), obtained by the penalized function. Once more, the parametric bootstrap yielded better results for the first sample, possibly due to the same previous reason (sample size). It is not clear which of the two bootstrap methods (non-parametric and parametric) is the best. This doubt occurs because in some cases the non-parametric yielded better confidence intervals, *i.e.*, with smaller widths. In other cases, the parametric bootstrap produced better confidence intervals.

Table 10: Non-parametric bootstrap confidence intervals for samples 1 and 2 (original function)

Sample 1 (90%)	90%	Lower	Upper	Width
	q	0.0380	0.8978	0.8598
	η	41.2568	123.3934	82.1366
Sample 1 (95%)	95%	Lower	Upper	Width
	q	-0.4104	0.9377	1.3481
	η	38.5087	165.4682	126.9595
Sample 2 (90%)	90%	Lower	Upper	Width
	q	-102573800	-0.3716	102573799.6
	η	18.3506	1131927000	1131926982
Sample 2 (95%)	95%	Lower	Upper	Width
	q	-118984800	0.0210	118984800
	η	13.2344	1397191000	1397190987

Source: This research (2018)

Table 11: Non-parametric bootstrap confidence intervals for samples 1 and 2 (penalized function)

Sample 1 (90%)	90%	Lower	Upper	Width
	q	-4.0580	-2.9159	1.1421
	η	547.7873	551.3321	3.5448
Sample 1 (95%)	95%	Lower	Upper	Width
	q	-4.3825	-2.9159	1.4666
	η	547.7873	551.3321	3.5448
Sample 2 (90%)	90%	Lower	Upper	Width
	q	-5.1553	-2.8479	2.3074
	η	48.4769	51.5575	3.0806
Sample 2 (95%)	95%	Lower	Upper	Width
	q	-5.1553	-2.8479	2.3074
	η	48.4769	52.2729	4.0806

Source: This research (2018)

For sample 1 the non-parametric bootstrap produced better results for the parameter η (Tables 5.6, 5.7, 5.8 and 5.9), once for this parameter the non-parametric bootstrap has small confidence intervals widths. On the other hand, the parametric bootstrap (Tables 5.6, 5.7, 5.8 and 5.9), in general, yielded better confidence intervals bootstrap for the parameter q for sample 1. For the second sample (Table 11), considering the penalized function, the non-parametric bootstrap yielded for the parameter η a confidence interval with a width of 3.0806 (90% of confidence) and a confidence interval with a width of 4.0806 (95% of confidence) against a width of 11.6204 (90% of confidence) and a width of 13.1560 (95% of confidence) produced by the parametric bootstrap (Table 13). Thus, for this situation (for the parameter η), the non-parametric yielded a better result.

However, still for sample 2 (Table 13) and considering the penalized function, the parametric bootstrap yielded for the parameter q a confidence interval with a width of 1.5667 (90% of confidence) and a confidence interval with a width of 1.9564 (95% of confidence) against a width of 2.3074 (90% of confidence) and a width of also 2.3074 (95% of confidence) produced by the non-parametric bootstrap, which means that, in this case, the parametric bootstrap produced better results for the parameter q.

One of the specific objectives of this work was to make comparisons between the fit provided by the q-Exponential distribution and the Weibull distribution. Thus, Figure 14 illustrates the fit for sample 1 (Table 6) provided by both distributions. While the p-value reached with the q-Exponential distribution was of 0.5034 for the first sample, for this same sample the Weibull distribution could reach a p-value of 0.1358. Hence, the two distributions are able to fit this data set, however, the q-Exponential distribution is able to fit the data better than the Weibull distribution. Besides, Figure 14 ratify that, based on the sample 1, the q-Exponential distribution can model the data better than the Weibull distribution. It is possible to see, through Figure 14, that the blue curve (Weibull curve) is under of the most points and also under the red curve (q-Exponential curve). On the other hand, the red curve touch most of the points.

The p-value reached with the q-Exponential distribution was of 0.9470 for the second sample, which represents a great fit. The Weibull distribution, in turn, could reach a p-value of 0.9710, which represents a fit even better than the one obtained with the q-Exponential distribution. Figure 15 shows the fit provided by the q-Exponential and by Weibull distributions for the second sample (Table 6). Differently from the first case, this time, by only analyzing Figure 15 it is not possible to clearly see which of the two distributions better fits the data set.

Table 12: Parametric bootstrap confidence intervals for samples 1 and 2 (original function)

Sample 1 (90%)	90%	Lower	Upper	Width
	q	-0.1584	0.8955	1.0539
	η	43.4143	139.4417	96.0274
Sample 1 (95%)	95%	Lower	Upper	Width
	q	43.4143	139.4417	96.0274
	η	39.4875	159.8111	120.3236
Sample 2 (90%)	90%	Lower	Upper	Width
	q	-81011780	-3.4106	81011776.59
	η	53.6857	965083400	965083346.3
Sample 2 (95%)	95%	Lower	Upper	Width
	q	-93562950	-0.6384	93562949.94
	η	21.2318	1100491000	1100490979

Source: This research (2018)

Table 13: Parametric bootstrap confidence intervals for samples 1 and 2(penalized function)

Sample 1 (90%)	90%	Lower	Upper	Width
	q	-3.2914	-2.9302	0.3612
	η	544.8677	553.3966	8.5289
Sample 1 (95%)	95%	Lower	Upper	
	q	-3.3495	-2.9212	0.4283
	η	543.8938	554.7666	10.8728
Sample 2 (90%)	90%	Lower	Upper	Width
	q	-4.3889	-2.8222	1.5667
	η	45.8942	57.5147	11.6204
Sample 2 (95%)	95%	Lower	Upper	Width
	q	-4.7514	-2.7950	1.9564
	η	45.3651	58.5212	13.1560

Source: This research (2018)

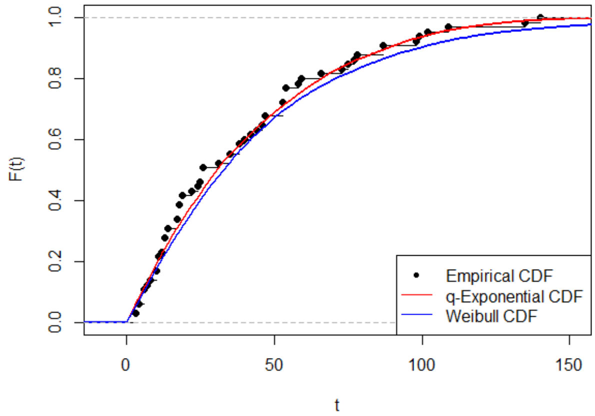

Figure 14: Theoretical (q-Exponential and Weibull) and empirical CDF's for sample 1.
Source: This research (2018)

Figure 16 shows the conditional reliability for sample 1 by the q-Exponential distribution. This measure represents the probability of the system keep working after it had worked by a determined initial time (t_0). Figure 16 brings the conditional reliability for three initial times, once for $t_0 = 0$ it has the original reliability. It is possible to infer, that the probability of the equipment work 200 days is very close to zero. Other information that this figure brings is that the last curve $(t_0 = 150)$ decays quickly, it means that the probability of the equipment work more than 150 hours is small.

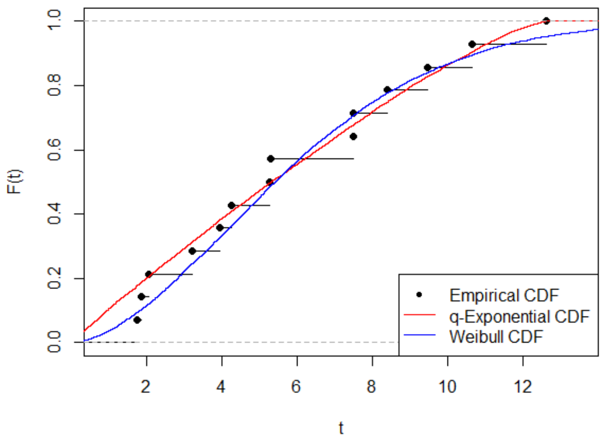

Figure 15: Theoretical (q-Exponential and Weibull) and empirical CDF's for sample 2.
Source: This research (2018)

Figure 17 shows the conditional reliability for the second sample by the q-Exponential distribution. In this case, through of the Figure 17, it is possible see that the probability of the equipment work 12 hours is already close to zero.

In summary, the two application examples showed an increasing behavior of the hazard rate, $q < 1$, however, the q-Exponential distribution had a better performance fitting the first sample, while the Weibull distribution presented a slight better result for the second sample.

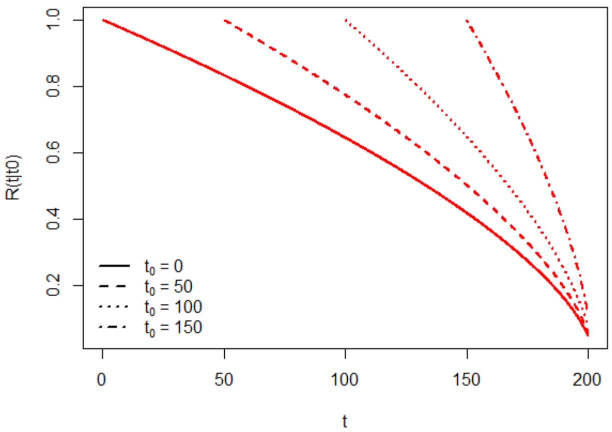

Figure 16: Conditional Reliability for sample 1
Source: This research (2018)

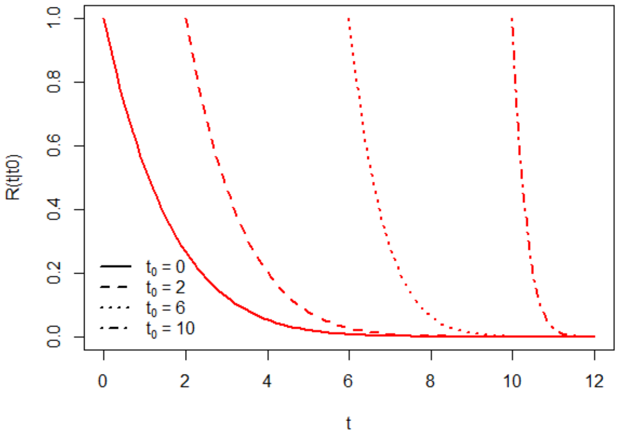

Figure 17: Conditional Reliability for sample 2
Source: This research (2018)

6 CONCLUSION

Monotone likelihood is a problem that has been studied by some authors. In fact, this corresponds to a characteristic that turns almost impossible to obtain good parameter estimates for some distributions. It happens when the increase of the parameters' values implies an increase in the log-likelihood function. In these situations plausible estimates are not obtained, once the log-likelihood function value always increases. In this work, we verified that the q-Exponential distribution presents such a monotone behavior when its shape parameter assumes values less than one.

In this context, this work applied a correction to the q-Exponential log-likelihood function based on the Firth's method, which presents the monotone behavior when $q < 1$, so that this distribution could model data sets related to increasing hazard rates (degradation phase of bathtub curve). The observed information was used instead of the expected information due to simplicity (the expected information related to the q-Exponential is very difficult or even impossible to be obtained).

The corrected q-Exponential likelihood was used in synthetic data sets and the results obtained were superior when compared with the ones provided by the original likelihood, once the corrected function achieved small biases even for small sample sizes (20 observations, for example). As expected, when the sample size increases the results get better. On the other hand, the original q-Exponential produced worse results for samples up to 100 observations. They improve when the sample is of at least 500 observations. However, when parameter q increases in absolute value, the original q-Exponential log-likelihood did not produce good results for any case, not even for large samples.

In some cases, for greater sample sizes (at least 500 observations), the original q-Exponential log-likelihood achieved slightly better results than its penalized version. But, in reliability engineering practice, it is not often possible or viable to draw large samples due to time and budget constraints. Thus, the penalized q-Exponential log-likelihood is a better option to model reliability-related data of equipment in the degrading phase of the bathtub curve $(q < 1)$.

The application examples presented two situations with the increasing hazard rate.The two data sets were modeled by an original and a penalized q-Exponential log-likelihood. For the first case (sample 1), the $\hat{q}$ and $\hat{\eta}$ estimated by the original function did not produce terrible estimates, but it is possible see that the log-likelihood value obtained for this function is almost twice than the obtained by the penalized function, which means that the penalized function produced better results. For the second sample, the estimates obtained by the original function are really bad. On the other hand, the penalized function produced plausible estimates, and, again, the log-likelihood value of two maximizations is in average twice better for the corrected distribution, which also means a better modelling.

Non-parametric and parametric bootstrap confidence intervals were constructed for the parameters q and η. In general, the confidence intervals were not very accurate. Nevertheless, the confidence intervals were made for a sample with just 14 observations (sample 2), *i.e*, for a small sample. For sample 1, which has 65 observations, the intervals presented smaller widths. In general, it is expected that results improve with a larger sample size.

Next, it was made a comparison between the fit of the data set provided by a q-Exponential distribution to that of a Weibull distribution. The results obtained for the first sample shows that the q-Exponential distribution seems be more adequate to fit the data. On other hand, for the second case (sample 2) the Weibull distribution had a fit slightly better than the q-Exponential distribution.

Finally, the penalization applied in the q-Exponential log-likelihood function is an advance for the reliability area. The Firth's penalization method enables the estimation process associated with the q-Exponential modeling of data sets from degrading systems ($q < 1$) and provides plausible results. Thus, the q-Exponential and Weibull distributions are alternative models to handle failure data related to the first phase (as commented by Sales Filho *et al.* (2016)) and to third phase of the bathtub curve.

6.1 Limitations and future works

In this research, we verified that, besides the monotone likelihood, the q-Exponential has another problem: this distribution does not satisfy the regularity condition that affirms that the function's support can not depend on the distributions parameters. This regularity condition is one of the assumptions for that the Maximum Likelihood Estimation could be used for estimating parameters satisfactorily. Even though this subject is important, some distributions are not so rigorous with this rule, as the Generalized Pareto distribution.

Therefore, in this work, a change of variable was performed in order to try to solve the mentioned regularity condition and the monotone likelihood. Just the first problem was solved for $(q < 1)$. It is important to elucidate that this change of variable just satisfy the regularity condition for $q < 1$, which represent the problematic case. However, the function found is not satisfactory because even with the Firth's penalization, it was not possible to obtain the parameter estimates. But, perhaps there are other changes of variables that could solve both problems, regularity condition and monotone likelihood. This is a subject for future researches.

Other way to solve the problem of the q-Exponential log-likelihood could be a reparameterization. Indeed, Sales Filho (2016) tried to use a reparameterization to estimate the q-Exponential parameters, and even though not having great results with this change, the author was be able to verify an improvement in the results. Thus, a reparameterization can be also a future alternative.

This research brought many questions and ideas that can be developed in future works. They are listed in the following topics:

- To investigate about some variable changes that could solve the problem of the regularity condition, and also solve the problem of the monotone likelihood of the q-Exponential distribution;

- To research some reparameterization that could solve the problem of the monotone likelihood of the q-Exponential distribution;

- To use other numerical method for function maximization and make comparisons with the results obtained with the Nelder-Mead method used in this work;

- To research about other methods used to solve the monotone likelihood problem and implement it in the q-Exponential log-likelihood function and make comparisons with the results obtained in this work;

- To extend this research for other q-distributions that presents the monotone likelihood problem and apply the corrected functions in reliability data sets;

- To develop a new method that could solve the monotone likelihood problem.
- To research about this method together with the probabilistic model named generalized renewal process (GRP);

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