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Sample Plans Comparisons for Shelf Life Estimation Using Sensory Evaluation Scores.

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Abstract

Sensory evaluations to determine the shelf life of food products are routinely conducted in food experimentation. In such experiments, trainned panelists are asked to judge food attributes by reference to a scale of numbers (scores varying from 0 to 6 for example). The "failure time" associated to a product unit under test is usually defined as the time required to reach a cutt-off point previously defined by the food company. Important issues associated with the planning and execution of this kind of testing are total sampling size, frequency of sample withdrawals, panel design, and statistical analysis of the panel data, to list a few. Different approaches have been proposed for the analysis of this kind of data. In particular, Freitas, Borges and Ho (2001) proposed an alternative model based on a dichotomization of the score data and a Weibull as the underlying distribution for the time to failure. The model was applied to a real situation. The authors evaluated also through a simulation study, the bias and mean square error of the estimates obtained for percentiles and fraction defectives. The simulation study used only the same sample plan implemented in the real situation. In this paper we focus on the planning issues associated with these experiments. Sample plans are contrasted and compared in a simulation study, through the use of the approach proposed by Freitas, Borges and Ho (2001).
KEY WORDS: *left censored; right censored; sample plans; sensory evaluations; shelf life; Weibull.*

1 Introduction

Food technologists use the term *shelf life* when they speak of the *length of time required for the product to be unfit for human consumption.* During this finite shelf life, the product is in a state of satisfactory quality in terms of nutricional value, taste, texture, and appearance.

The shelf lives of food products vary, but they are determined routinely for each particular product by its manufacturer or processor. Major areas involved in a food's shelf life include:

- **loss of nutrient value** such as vitamin loss and protein breakdown;
- **spoilage by microorganisms**, enzymatic action, or insect infestation;
- **loss of functional properties** such as thickening power in sauce mixes, ou the "set" in instant puddings;
- **loss of aesthetic qualities** such as color, flavor, aroma, texture, or general appearance.

As one can see, chemical, physical, microbiological, and nutritional analyses are fundamental, but equally important are sensory evaluations to determine the shelf life.

In such experiments, a sample of product units is stored and periodically, at preespecified evaluation times, a sample of units is collected from the ones stored and subjected to sensory evaluations by a trained panel. Each panelist is asked to judge each product's attribute by reference to a rating scale, for instance, a seven point rating scale varying from 0 to 6. Because of the destructive nature of the evaluations, units that have already been evaluated at a given time cannot be restored to be evaluated later on. The *failure time* of a given unit is then defined as the time required for that unit to get a score equal to the cutt-off point previously chosen by the food company. For a unit evaluated at a preestablished time, one of the two situations can happen: the score is either less than ou equal to the cut-off point or greater than the cut-off point. In the former case the "failure time" is somewhere between the start of the experiment and the present time of evaluation. In the latter case, the product is still good for consumption and its "failure" will take place sometime after evaluation. Thus, this kind of procedure generates data either right or left censored (Lawless, 1989).

A number of authors have discussed and proposed different statistical approaches to the problem of shelf life estimation based on data with the characteristics just mentioned. A good discussion can be found in the recent work by Freitas, Borges and Ho (2001). In that work the authors have also proposed an alternative statistical model which incorporates both the information of the right and left censored data and uses a Weibull as the underlying distribution for the failure time. The model was applied to the data coming from a real situation. A small simulation study was implemented considering only the basic sample plan used in the real experiment.

In this paper the purpose is to gain more insight into the problems related to the *design* of these studies. It is important to emphasize that conventional experimental designs as presented in many statistical texts (Montgomery, 2000) have been used in food experimentation. But when we talk about studies that concentrate in *the length of time required for the product to achieve the limit of acceptable sensory qualities (taste, appearence, etc.)* not much can be found in the literature. Due to the destructive nature of the sampling procedure, the problem has been to develop designs for shelf life studies with a reasonable sample size.

Gacula (1975) addresses this question and states that "... a possible approach to the problem is to concentrate the majority of samples in the experimental periods where the maximum information is desired. This time is the period where the units are likely to fail or are approaching the limit of acceptable quality." He also proposes that in combination with this approach, one may suspend observation at the early part of the experimental period. These designs were called "staggered designs".

In this paper, the purpose is to expand the simulation study implemented in the previous work by Freitas, Borges and Ho (2001). Using the same modeling approach, the simulation study will focus on the effect of the below listed items on the "quality" of percentiles and fraction defectives estimates:

- storage conditions: the number of variables included and at what levels (for instance, temperature, humidity, packing material, etc.);
- total sample size: the total number of units that will be under test;
- the proportion of alocation: how many units will be stored at each condition (if one is interested to study more than one condition);
- the number of evaluation times and the frequency: for example, evaluations could be done once a week for 20 weeks ou twice a week for 20 weeks, every two weeks for 24 weeks, etc.

The paper is organized as follows. First, we briefly present the modeling approach as in Freitas, Borges and Ho (2001). In Section 3, we present the results of the simulation study with no covariates. In Section 4, we present the results of the simulation study for the model with two covariates.

2 A Statistical Model for Sensory Data using the Weibull as the Underlying Distribution.

Freitas, Borges and Ho (2001) have developed the following model. Suppose a sample of $N = \sum_{i=1}^{k} n_i$ food product units is taken from the production line and stored under a given environmental condition. These units will be evaluated by a trained panel at prestablished evaluation times in order to determine its shelf life.

Let τ_i $(i = 1, ..., k)$ be the evaluation times (fixed). Then, at the evaluation time τ_1, n_1 units are sampled from the total N and subjected to a sensory evaluation by n_1 panelists who score each attribute (odor, flavor, appearance) using a 7 point rating scale (for instance, 0 to 6).

The evaluation is destructive, consequently these n_1 units can no longer be followed in time. Next at τ_2, n_2 units are sampled from the $N - n_1$ units left and evaluated by n_2 painelists. This process is repeated through the last evaluation time τ_k when the remaining n_k units are finally evaluated.

Let Z_{ij} be the score assigned to the j^{th} product unit ($j = 1, ..., n_i$) evaluated at the time τ_i ($i = 1, ..., k$).

Each of the n_i units evaluated at a given time will be considered as *unfit for consumption* (regarding a particular attribute) depending on the score assigned by the panelist. Let us refer for a moment to the real situation described in Section 2. In that case, the j^{th} unit evaluated at time τ_i will be considered unfit for consumption (regarding the attribute being evaluated) if Z_{ij}=0,1,2 or 3. If, on the other hand, $Z_{ij} > 3$ then the attribute "failure" will occur sometime in the future but we will not be able to know when at the present time. It should be enfasized that it is possible to have a unit being considered "unfit" regarding its flavor but "fit for consumption" regarding its appearance.

We can define a new random variable Y_{ij}, given by

$$Y_{ij} = \begin{cases} 1 & \text{if } Z_{ij} < 4 \text{ (i.e., if score } < 4) \\ 0 & \text{if } Z_{ij} \geq 4 \text{ (i.e., if score } \geq 4). \end{cases}$$

Therefore, at each fixed time τ_i we have a random sample of size n_i from a random variable Y_{ij} where Y_{ij} is Bernoulli distributed with probabiity p_i given by

$$p_i = P(Y_{ij} = 1) = P(0 < T_{ij} \leq \tau_i)$$

,

where T_{ij} is the failure time of the j^{th} unit evaluated at τ_i.

Thus, in a equivalent way, Y_{ij} can be defined as

$$Y_{ij} = \begin{cases} 1 & \text{if } 0 < T_{ij} \leq \tau_i \\ 0 & \text{if } T_{ij} > \tau_i. \end{cases}$$

Or

$$\begin{aligned} P(Y_{ij} = s_{ij}) &= P(0 < T_{ij} \leq \tau_i) = 1 - R(\tau_i), \text{ if } s_{ij} = 1 \\ &= P(T_{ij} > \tau_i) = R(\tau_i), \text{ if } s_{ij} = 0, \end{aligned} \tag{1}$$

where R(.) in (1) is the **reliability function** (Nelson, 1990).

The main purpose here is to estimate the shelf life of a food product, taking into account some sensory quality characteristics. If we take a better look at this problem, we see that in fact the shelf life itself is a random variable whose behavior for each attribute follows some underlying distribution. One way to tackle this problema is to estimate percentiles of each shelf life distribution (considering each attribute separately) and then pick one for each attribute to represent the "attributes' shelf life". If the manufacturer decides to have only one value reported as a shelf life for the product, the minium value could be chosen.

Freitas, Borges and Ho assumed that the failure time T_{ij} of the j^{th} unit evaluated at time τ_i (fixed) has a Weibull distribution, with parameters α_j and $\delta \geq 1$, and

- the parameters α_j and δ are defined by

$$\begin{aligned} \alpha_j &= \exp\{\boldsymbol{X_j \beta}\} = \exp\{X_j^0\ \beta_0 + X_j^1\ \beta_1 + \ \dots \ + X_j^q\ \beta_q\}, \\ (\ j &= 1, 2, \dots, n_i\ ) \quad \text{and} \quad \delta = \exp(\gamma) \quad \gamma \geq 0 \end{aligned} \tag{2}$$

- $\boldsymbol{X_j} = (X_j^0, X_j^1, \dots, X_j^q)$ is a (q+1) vector of covariates related to the j^{th} unit evaluated at τ_i
- $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_q)'$ is a (q+1) vector of parameters associated to the covariates.

Now using the fact that for a Weibull distribution with parameters α and δ, $R(t) = \exp\{-(\alpha\ t)^\delta\}$ and Y_{ij} has a Bernoulli distribution with probability p_i given by (1), the likelihood function is given by

$$\begin{aligned} L(\boldsymbol{\theta}) &= \prod_{i=1}^{k} \prod_{j=1}^{n_i} \left\{ \left[e^{-(\tau_i\ \alpha_j)^\delta} \right]^{1-s_{ij}} \quad \left[1 - e^{-(\tau_i\ \alpha_j)^\delta} \right]^{s_{ij}} \right\} \\ &= \prod_{i=1}^{k} \prod_{j=1}^{n_i} \left\{ \left[e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}} \right]^{1-s_{ij}} \quad \left[1 - e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}} \right]^{s_{ij}} \right\}, \end{aligned} \tag{3}$$

where $\boldsymbol{\theta'} = (\boldsymbol{\beta'}; \delta)$.

Maximum likelihood estimates are obtained by direct maximization of the logaritmum of expression (3). The expressions of the first derivatives are:

$$\left[\frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right]_{(q+2)\times 1} = \begin{bmatrix} \frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \boldsymbol{\beta}} \\ \frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \gamma} \end{bmatrix}, \tag{4}$$

where:

$$\begin{aligned} \frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \boldsymbol{\beta}} &= \sum_{i=1}^{k} \sum_{j=1}^{n_i} \boldsymbol{X_j'} \left\{ -(1-s_{ij}) e^\gamma (\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma} + \frac{s_{ij} e^\gamma e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}} (\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}{\left[1 - e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}} \right]} \right\}, \\ \frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \gamma} &= \sum_{i=1}^{k} \sum_{j=1}^{n_i} \left\{ e^\gamma (\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma} \ln(\tau_i e^{\boldsymbol{X_j\beta}}) \left[-(1-s_{ij}) + \frac{s_{ij} e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}}{\left(1 - e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}} \right)} \right] \right\}. \end{aligned}$$

The elements of the Fisher Information matrix I($\boldsymbol{\theta}$) ($(q+2) \times (q+2)$) are given by

$$I(\boldsymbol{\theta}) = E\left\{-\left[\frac{\partial^2\mathcal{L}(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta'}}\right]\right\}_{(q+2)\times(q+2)} = \left[\begin{array}{cc} I_{11} & I_{12} \\ I'_{12} & I_{22} \end{array}\right], \tag{5}$$

where:

$$I_{11} = E\left\{-\left[\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{\beta}\partial\boldsymbol{\beta'}}\right]\right\} = \sum_{i=1}^{k}\sum_{j=1}^{n_i}(\boldsymbol{X'_j X_j})\left\{\frac{e^{2\gamma}e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}(\tau_i e^{\boldsymbol{X_j\beta}})^{2e^\gamma}}{\left(1-e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}\right)}\right\},$$

$$I_{12} = E\left\{-\left[\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{\beta}\partial\gamma}\right]\right\} = \sum_{i=1}^{k}\sum_{j=1}^{n_i}\boldsymbol{X'_j}\left\{\frac{e^{2\gamma}e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}(\tau_i e^{\boldsymbol{X_j\beta}})^{2e^\gamma}\ln(\tau_i e^{\boldsymbol{X_j\beta}})}{\left(1-e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}\right)}\right\},$$

$$I_{22} = E\left\{-\left[\frac{\partial^2\mathcal{L}}{\partial\gamma^2}\right]\right\} = \sum_{i=1}^{k}\sum_{j=1}^{n_i}\left\{\frac{e^{2\gamma}e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}(\tau_i e^{\boldsymbol{X_j\beta}})^{2e^\gamma}[\,\ln(\tau_i e^{\boldsymbol{X_j\beta}})\,]^{\,2}}{\left(1-e^{-(\tau_i e^{\boldsymbol{X_j\beta}})^{e^\gamma}}\right)}\right\},$$

with I_{11}, I_{12} and I_{22} with dimensions $(q+1)\times(q+1)$, $(q+1)\times 1$ and 1×1 respectively.

Maximum likelihood estimator is obtained by implementing numeric optimization methods such as the well known Newton-Raphson algorithm. In this work we have used a minor adjustment to the Newton-Raphson procedure, sometimes used in statistical problems, called Fisher's Score (McCullagh and Nelder, 1989).

If $\hat{\boldsymbol{\theta}} = (\hat{\beta}_0, \hat{\beta}_1, ..., \hat{\beta}_q, \hat{\gamma})'$ is the maximum likelihood estimator of $\boldsymbol{\theta} = (\beta_0, \beta_1, ..., \beta_q, \gamma)'$ then

- for a given set of covariates $\boldsymbol{X_j} = (X_j^0, X_j^1, ..., X_j^q)$, the maximum likelihood estimate of the percentile $t_{p(j)}$ is given by

$$\hat{t}_{p(j)} = \frac{1}{\hat{\alpha}_j}\,[-\ln(1-p)\,]^{\frac{1}{\hat{\delta}}},$$

  where, $\hat{\alpha}_j = \exp\{\boldsymbol{X_j}\widehat{\boldsymbol{\beta}}\}$ and $\hat{\delta} = \exp\{\hat{\gamma}\}$

- using maximum likelihood large sample theory (asymptotic normality) and the delta method(Cox and Hinkley, 1974), it is possible to find the expression of the asymptotic variance estimator

$$\widehat{Var}(\hat{t}_{p(j)}) \doteq Z'\,I^{-1}(\boldsymbol{\theta})\,Z\;_{\left\{\text{para } \boldsymbol{\theta} = \widehat{\boldsymbol{\theta}}\right\}}, \tag{6}$$

  where Z is a vector of dimension (q+2) $\times$ 1 given by

$$Z = \left[\begin{array}{c} \left(\frac{-(-\ln(1-p)\,)^{\frac{1}{e^\gamma}}}{e^{\boldsymbol{X_j\beta}}}\right)\boldsymbol{X'_j} \\ -\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,- \\ \frac{-[-\ln(1-p)\,]^{\frac{1}{e^\gamma}}\,[\,e^{-\gamma}\ln(-\ln(1-p)\,)\,]}{e^{\boldsymbol{X_j\beta}}} \end{array}\right]. \tag{7}$$

Therefore, 95% confidence interval (asymptotic) for $t_{p(j)}$ is

$$UB = \hat{t}_{p(j)} + (1,96)\left\{\widehat{Var}(\hat{t}_{p(j)})\right\}^{1/2}, \quad (8)$$

$$LB = \hat{t}_{p(j)} - (1,96)\left\{\widehat{Var}(\hat{t}_{p(j)})\right\}^{1/2} \quad (9)$$

- equivalently, for a given set of covariates $\boldsymbol{X_j} = (X_j^0, ..., X_j^q)$, the maximum likelihood estimator of the fraction defective in t_0, $F_j(t_0)$, is given by

$$\hat{F}_j(t_0) = 1 - \hat{R}_j(t_0) = 1 - e^{-(t_0 e^{\boldsymbol{X_j}\widehat{\boldsymbol{\beta}}})^{e^{\hat{\gamma}}}} \quad (10)$$

- making use of the asymptotic normality property of the maximum likelihood estimator and the delta method (Cox e Hinkley, 1974) we get the expression of the 95% confidence interval for the fraction defective $\hat{F}_j(t_0) = 1 - \hat{R}_j(t_0)$:

$$UB = 1 - \left\{\hat{R}_j(t_0)\right\}^{\exp\left\{1{,}96\ [\widehat{Var}(\hat{\phi})]^{1/2}\right\}}, \quad (11)$$

$$LB = 1 - \left\{\hat{R}_j(t_0)\right\}^{\exp\left\{-1{,}96\ [\widehat{Var}(\hat{\phi})]^{1/2}\right\}}, \quad (12)$$

where $\hat{\phi}$ and $\widehat{Var}(\hat{\phi})$ in (11) and (12) are given by

$$\hat{\phi} = \ln(-\ln\ \hat{R}_j(t_0)\ ), \quad (13)$$

$$\widehat{Var}(\hat{\phi}) \doteq Z'\ I^{-1}(\boldsymbol{\theta})\ Z_{\left\{\text{para } \boldsymbol{\theta} = \widehat{\boldsymbol{\theta}}\right\}}, \quad (14)$$

and Z is a vector of dimension (q+2) $\times$ 1 given by

$$Z = \begin{bmatrix} e^{\gamma}\ \boldsymbol{X_j'} \\ -------- \\ e^{\gamma}\ \ln(t_0\ e^{\boldsymbol{X_j\beta}}\ ) \end{bmatrix}. \quad (15)$$

We point out that expressions (11) and (12) were calculated applying the asymptotic normal distribution to the tranformation ϕ (expression [15])for which the range is unrestricted. Then, the confidence interval for the fraction defective is found applying the inverse transformation. This procedure suggested by Kalbfleisch and Prentice (1980; page 15) prevents the occurence of limits outside the range [0,1].

3 Simulation Study # 1: the case of the Weibull model with no covariates

This section presents simulation results for the Weibull model with no covariates:

$$\begin{aligned} \boldsymbol{X_j} &= (X_j^0, ..., X_j^q) = (X_j^0) \equiv (1) \quad \text{(fixed) and,} \\ \boldsymbol{\beta} &= (\beta_0, \beta_1, ..., \beta_q)' \equiv (\beta_0). \end{aligned}$$

Therefore,

$$\begin{aligned} \alpha_j &= \exp(X_j^0 \beta_0) = \exp(\beta_0) = \alpha, \\ \text{and } \delta &= \exp(\gamma) \text{ for all } j = 1, 2, ..., n_i \text{ and } i = 1, 2, ..., k. \end{aligned}$$

Consequently, $\boldsymbol{\theta} = (\beta_0, \gamma)'$ is the vector of parameters to be estimated by maximum likelihood.

3.1 Description of the Simulation Study

Some basic questions had to be answered in order to implement the study:

1) Which values of α and δ (and consequently of β_0 and γ) should be used in the simulations?

Our main purpuse was to study the "quality" or "performance" of the estimates obtained by the model proposed in situations which imitate the real data available as close as possible. Our emphasis was in getting good estimates of percentiles and fraction of defectives. As measures of "quality" or "performance", we used:

- the absolute bias B= $\{(\sum_{i=1}^{N} \hat{u}_i)/N\} -$ (real value of u) where $\hat{u}_i$ are the estimated parameter values for each of the N samples generated;
- the relative bias RB={(absolute value of B)/(real value of u)}x100%;
- the standard deviation (SD) and the mean square error (MSE).

To get a first guess of the range of values to be used in the simulation, the model proposed was fitted to the real data set presented in Freitas, Borges and Ho (2001). The parameters estimates are summarized in Table 2.

For each storage condition, the average value of the estimates obtained for α ($\bar{\hat{\alpha}}$) where 0.019, 0.0298 and 0.0619 for storage conditions room temperature and humidity, chamber 1 and 2 respectively. Simulations were implemented using $\alpha =$ 0.020, $\alpha = 0.035$ and $\alpha = 0.065$. δ values ranged from 1.2 to 2, with incremets of size $\triangle$ =0.2. Note that the values presented in Table 2 are included in this range.

2) Which sample plans should be implemented in the simulation study?

Table 1: Parameters estimates for the Weibull model applied to the real data

	attribute					
	odor		flavor		appearance	
storage condition	$\hat{\alpha}$	$\hat{\delta}$	$\hat{\alpha}$	$\hat{\delta}$	$\hat{\alpha}$	$\hat{\delta}$
room temp.and humidity	0.0191	1.3	0.0181	1.2	0.0193	1.9
environmental chamber 1	0.0302	1.6	0.0358	1.4	0.0233	2
environmental chamber 2	0.0596	1.6	0.0659	1.4	0.0602	2

By "sample plan" we mean: the number of weeks of follow-up (nw), the number of panelists allocated to each week (np) and the total number of product units under test ($N = nw \times np$).

Once again the idea was also to mimic the scenarios found in the real data set. Tables 2, 3 and 4 summarize the sample plans used. Sample plans labelled "I" in Tables 2, 3 and 4 are exactly the ones implemented in the sensory evaluations of the dehidrated product mentioned in Freitas, Borges and Ho (2001).

Table 2: Scenarios considered in the simulation study: α =0.02 and δ = 1.2 to 2, increments of 0.2

	characteristics of each sample plan		
sample plan	$N^{(1)}$	$nw^{(2)}$	$np^{(3)}$
I	357	51	7
II	714	51	14
III	280	40	7
IV	560	40	14
V	504	36	14
VI	224	32	7
VII	448	32	14
VIII	168	24	7
IX	336	24	14

(1): number of units; (2): number of follow-up weeks;
(3): number of panelists assigned to each week.

3) Which steps will be followed in the simulation study?

In the proposed model, the underlying distribution of the failure time is a Weibull but in a real test situation, in fact what is observed is the score assigned by the panelist to a given product unit. In the model proposed in Section 3, the results are dichotomized according to the cut-off point stablished by the company. In other words, the result is either zero or one depending on the "failure" time (T) be located before ou after the evaluation time (τ).

In the simulation study we assumed that the evaluations were implemented weekly. In addition, the total follow-up time is nw weeks and np panelists are requested weekly to compose the laboratory panel.

The main steps followed are given below:

Table 3: Scenarios considered in the simulation study: α =0.035 and δ = 1.2 to 2, incremetns of size 0.2

	characteristics of each sample plan		
sample plan number	$N^{(1)}$	$nw^{(2)}$	$np^{(3)}$
I	252	36	7
II	504	36	14
III	448	32	14
IV	392	28	14

(1): number of units; (2): number of follow-up weeks ;
(3): number of panelists assigned to each week.

Table 4: Scenarios considered in the simulation study: α =0.065 and δ = 1.2 to 2, increments of size 0.2

	characteristics of each sample plan		
sample plan number	$N^{(1)}$	$nw^{(2)}$	$np^{(3)}$
I	126	18	7
II	252	18	14
III	168	12	14

(1): number of units; (2): number of follow-up weeks;
(3): number of panelists assigned to each week.

- **step 1**: choose a set of parameters values α and δ, and one of the sample plans listed in Tables 3, 4 and 5;
- **step 2**: generate a random sample of size N=nw× np of failute times t, from a Weibull (α, δ) were $\alpha = e^{\beta}$ and $\delta = e^{\gamma}$; values of α and δ were choosen in step 1;
- **step 3**: dichotomize the results and store them in a vector (Y). The dichotomization is done by comparing each of the N failure times t with the N evaluation times τ (τ assumes values from 1 to *nw* weeks). If t> τ then Y=0, otherwise Y=1 (failure has already occured);
- **step 4**: calculate the maximum likelihood estimator of β and γ (or, α and δ) using the dichotomized data and expression (3);
- **step 5**: using the parameters estimates calculated in step 4, find the estimates of percentiles and fraction of defectives;
- **step 6**: store the values calculated in 5;
- **step 7**: generate another random sample as in step 2 and repeat steps 3 to 6;
- **step 8**: steps 2 to 7 should be repeated until 1000 samples have been generated. Then, based on the 1000 random samples, calculate for each percentile and fraction of defective of interest:

- the average of the 1000 values estimated;
- the standard deviation (SD) based on the 1000 values;
- the absolute bias (B); the relative bias (RB) and the MSE (mean square error).

These steps were implemented for each one of the sample plans listed in Tables 3, 4 and 5.

3.2 Simulation Results

Tables 6 and e 7 present the simulation results for percentiles of a Weibull (α;δ), with $\alpha = 0.02$ and $\delta = 1.2$ and 1.6 respectively.

All the comparisons were done taking sample plan "I" as the reference, since that was the sample plan used in the real data set.

For the Weibull (0.02; 1.2) plans II, V e IV presented better results than plan I, considering all the performance measures(SD; RB and MSE).

The results obtained with plan II where expected since the sample size for this case was doubled. On the other hand, plans IV and V generated results much more precise and with smaller bias. In other words, the test could have been implemented with a shorter follow-up time (40 ou 36 weekes). But the price one would have to pay is to alocate 14 instead of 7 panelists each week.

For the Weibull(0.02; 1.6) the results are practically the same. Here, plans IV and V invert positions. Plans II, IV and V have better measures of performance (once compared to plan I) when we estimate percentiles.

Similar results where found for other values of δ, for instance $\delta = 1.4$, 1.8 and 2.

Table 8 shows the results of the simulation study considerig a Weibull with $\alpha = 0.02$ and $\delta = 1.2$. The quantities estimated were fractions of defectives calculated at different points in time.

Here, it is not possible to identify sample plans with better peformance than plan I for all measures calculated. For instance, for a Weibull (0.02; 1.2) plans II, IV and V are better than plan I when we take into account the SD and MSE (one exception is plan V for $t_0 = 32$ weeks).

For the Weibull (0.02; 1.6) plan II has better performance than plan IV and V. But, plans IV and V are not better than plan I when all measures of performance are compared. For instance, for plan IV, the bias associated with the estimate of $t_0 = 4$ and 32 weeks and the relative bias for 32 weeks are both larger than the ones obtained for plan I.

Therefore, when the quantity to be estimated is the fraction of defectives, the results have shown that for the Weibull (0.02; δ) plan II has the best performance regarding all performance measures. Plans IV and V have also good performance but it depends also on the indicator choosen for the comparison.

The results for other values of δ (1.4;1.8 and 2) are very similar to the ones just described.

Table 5: Simulation results (1000 samples)- percentiles t_p of a Weibull with $\alpha = 0.02$ and $\delta = 1.2$

plan	p	true value	estimate	SD(1)	bias(2)	RB(3) (%)	MSE
N=357	10^{-6}	0.0005	0.0015	0.0038	0.0010	201	1.5×10^{-5}
nw=51	10^{-5}	0.0034	0.0072	0.0128	0.0039	114	0.0002
np=7	10^{-4}	0.0232	0.0372	0.0459	0.0140	60	0.0023
I	10^{-3}	0.1582	0.2029	0.1698	0.0447	28	0.0308
	10^{-2}	1.0817	1.1866	0.6110	0.1049	10	0.3843
N=714	10^{-6}		0.0009	0.0012 (-68)(4)	0.0004 (-60)	86 (-57)	1.5×10^{-6}
nw=51	10^{-5}		0.0052	0.0054 (-58)	0.0018 (-54)	54 (-52)	3×10^{-5}
np=14	10^{-4}		0.0305	0.0240 (-48)	0.0073 (-48)	32 (-47)	0.0006
II	10^{-3}		0.1840	0.1033 (-39)	0.0258 (-94)	16 (-43)	0.0110
	10^{-2}		1.1531	0.4094 (-33)	0.0713 (-32)	7 (-30)	0.1738
N=280	10^{-6}		0.0020	0.0045	0.0015	295	2.2×10^{-5}
nw=40	10^{-5}		0.0089	0.0154	0.0055	161	2.7×10^{-4}
np=7	10^{-4}		0.0425	0.0545	0.0193	83	0.0033
III	10^{-3}		0.2176	0.1958	0.0594	38	0.0419
	10^{-2}		1.2142	0.6810	0.1324	12	0.4814
N=560	10^{-6}		0.0013	0.0022 (-42)	0.0008 (-20)	155 (-23)	5.2×10^{-6}
nw=40	10^{-5}		0.0066	0.0085 (-34)	0.0031 (-21)	92 (-19)	8.3×10^{-5}
np=14	10^{-4}		0.0351	0.0343 (-25)	0.0119 (-15)	51 (-15)	0.0013
IV	10^{-3}		0.1978	0.1372 (-19)	0.0397 (-11)	25 (-11)	0.0204
	10^{-2}		1.1806	0.5125 (-16)	0.0989 (-6)	9 (-10)	0.2724
N=504	10^{-6}		0.0012	0.0020 (-47)	0.0007 (-30)	142 (-29)	4.3×10^{-6}
nw=36	10^{-5}		0.0062	0.0080 (-38)	0.0028 (-28)	83 (-27)	7.2×10^{-5}
np=14	10^{-4}		0.0336	0.0331 (-28)	0.0104 (-26)	45 (-25)	0.0012
V	10^{-3}		0.1903	0.1346 (-21)	0.0321 (-28)	20 (-29)	0.0191
	10^{-2}		1.1489	0.5064 (-17)	0.0672 (-36)	6 (-40)	0.2610
N=224	10^{-6}		0.0034	0.0081	0.0029	574	7.4×10^{-5}
nw=32	10^{-5}		0.0133	0.0253	0.0099	290	7.4×10^{-4}
np=7	10^{-4}		0.0560	0.0809	0.0328	141	0.0076
VI	10^{-3}		0.2560	0.2619	0.0978	62	0.0781
	10^{-2}		1.3003	0.8265	0.2185	20	0.7308
N=448	10^{-6}		0.0018	0.0034	0.0013	255	1.3×10^{-5}
nw=32	10^{-5}		0.0082	0.0125	0.0048	142	0.0002
np=14	10^{-4}		0.0405	0.0466	0.0173	74	0.0025
VII	10^{-3}		0.2122	0.1726	0.0541	34	0.0327
	10^{-2}		1.2057	0.5993	0.1240	11	0.3745
N=168	10^{-6}		0.0082	0.0260	0.0077	1537	7.4×10^{-4}
nw=24	10^{-5}		0.0252	0.0627	0.0218	640	0.0044
np= 7	10^{-4}		0.0846	0.1563	0.0614	264	0.0282
VIII	10^{-3}		0.3170	0.4049	0.1588	100	0.1892
	10^{-2}		1.3835	1.0676	0.3018	28	1.2308
N=336	10^{-6}		0.0034	0.0087	0.0029	583	$8,5 \times 10^{-5}$
nw=24	10^{-5}		0.0132	0.0259	0.0098	287	7.6×10^{-4}
np=14	10^{-4}		0.0546	0.0794	0.0314	135	0.0073
IX	10^{-3}		0.2480	0.2497	0.0898	57	0.0704
	10^{-2}		1.2677	0.7566	0.1860	17	0.6071

(1) standard deviation; (2) estimate - real value; (3) relative bias =(abs.value(bias)/real)×100%
(4) % improvement to plan I= ((plan Y - plan I)/(plan I)) × 100%

Table 6: Simulation results (1000 samples) - percentiles t_p of a Weibull with $\alpha = 0.02$ and $\delta = 1.6$

plan	p	true value	estimate	SD(1)	bias(2)	RB(3) (%)	MSE
N=357	10^{-6}	0.0089	0.0170	0.0211	0.0081	91	0.0005
nw=51	10^{-5}	0.0375	0.0590	0.0590	0.0215	57	0.0039
np=7	10^{-4}	0.1581	0.02116	0.1640	0.0535	34	0.0298
I	10^{-3}	0.6670	0.7848	0.4417	0.1178	18	0.2090
	10^{-2}	2.8205	3.0236	1,0872	0.2030	7	1.2232
N=714	10^{-6}		0.0120	0.0105 (-50)(4)	0.0032 (-60)	35 (-62)	0.0001
nw=51	10^{-5}		0.0461	0.0324 (-45)	0.0086 (-60)	23 (-60)	0.0011
np=14	10^{-4}		0.1795	0.0984 (-40)	0.0213 (-60)	13 (-62)	0.0101
II	10^{-3}		0.7122	0.2854 (-35)	0.0452 (-62)	7 (-61)	0.0835
	10^{-2}		2.8896	0.7425 (-46)	0.0691 (-66)	2 (-71)	0.5560
N=280	10^{-6}		0.0221	0.0343	0.0132	149	0.0014
nw=40	10^{-5}		0.0706	0.0879	0.0331	88	0.0088
np=7	10^{-4}		0.2348	0.2258	0.0767	48	0.0057
III	10^{-3}		0.8205	0.5691	0.1536	23	0.3474
	10^{-2}		3.0446	1.3190	0.2241	8	1.7899
N=560	10^{-6}		0.0143	0.0165 (-22)	0.0054 (-33)	61 (-33)	0.0003
nw=40	10^{-5}		0.0518	0.0470 (-20)	0.0143 (-33)	38 (-33)	0.0024
np=14	10^{-4}		0.1925	0.1328 (-19)	0.0343 (-36)	22 (-35)	0.0188
IV	10^{-3}		0.7367	0.3622 (-18)	0.0698 (-41)	10 (-44)	0.1360
	10^{-2}		2.9184	0.8875 (-18)	0.0979 (-52)	3 (-57)	0.7972
N=504	10^{-6}		0.0162	0.0230 (9)	0.0073 (-10)	82 (-10)	0.0006
nw=36	10^{-5}		0.0562	0.0600 (2)	0.0187 (-13)	50 (-12)	0.0040
np=14	10^{-4}		0.2019	0.1589 (-3)	0.0438 (-18)	28 (-18)	0.0272
V	10^{-3}		0.7538	0.4139 (-6)	0.0869 (-26)	13 (-28)	0.1788
	10^{-2}		2.9397	0.9784 (-10)	0.1191 (-41)	4 (-43)	0.9714
N=224	10^{-6}		0.0329	0.0697	0.0240	270	0.0054
nw=32	10^{-5}		0.0936	0.1475	0.0561	150	0.0025
np=7	10^{-4}		0.2818	0.3245	0.1237	78	0.1206
VI	10^{-3}		0.9063	0.7268	0.2393	36	0.5855
	10^{-2}		3.1596	1.5415	0.3391	12	2.4911
N=448	10^{-6}		0.0188	0.0269	0.0099	112	0.0008
nw=32	10^{-5}		0.0624	0.0703	0.0249	66	0.0056
np=14	10^{-4}		0.2150	0.1843	0.0569	36	0.0372
VII	10^{-3}		0.7749	0.4721	0.1078	16	0.2345
	10^{-2}		2.9485	1.0886	0.1280	5	1.2015
N=168	10^{-6}		0.0629	0.1627	0.0540	607	0.0294
nw=24	10^{-5}		0.1463	0.2943	0.1088	290	0.0984
np=7	10^{-4}		0.3668	0.4493	0.2087	132	0.3453
VIII	10^{-3}		1.0125	1.0530	0.3455	52	1.2282
	10^{-2}		3.1924	1.9606	0.3718	13	3.9820
N=336	10^{-6}		0.0288	0.0546	0.0200	224	0.0034
nw=24	10^{-5}		0.0839	0.1205	0.0464	124	0.0167
np=14	10^{-4}		0.2583	0.2737	0.1002	63	0.0849
IX	10^{-3}		0.8499	0.6225	0.1830	27	0.4210
	10^{-2}		3.0402	1.2932	0.2196	8	1.7206

(1) standard deviation; (2) estimated - real; (3) relative bias =(abs.value(bias)/real value)×100%

(4) % improvement to plan I= ((plan Y - plan I)/(plan I)) × 100%

Table 7: Simulation Results (1000 samples)- fraction of defectives at t_0 for a Weibull with $\alpha = 0.02$ and $\delta = 1.2$

plan	t_0	true value	estimate	SD(1)	bias(2)	RB(3) (%)	MSE
N=357	1	0.0019	0.0105	0.0064	0.0013	15	4.2×10^{-5}
nw=51	2	0.0208	0.0225	0.0109	0.0017	8	1.2×10^{-4}
np=7	4	0.0471	0.0489	0.0176	0.0018	4	3.1×10^{-4}
I	8	0.1050	0.1059	0.0254	0.0009	0.9	6.5×10^{-4}
	12	0.1651	0.1651	0.0286	7.2×10^{-6}	0.004	$8,2 \times 10^{-4}$
	16	0.2249	0.2243	0.0291	-0.0006	0.3	8.5×10^{-4}
	20	0.2832	0.2824	0.0284	-0.0008	0.3	8.1×10^{-4}
	24	0.3393	0.3386	0.0277	-0.0007	0.2	7.8×10^{-4}
	32	0.4431	0.4431	0.0300	4.6×10^{-5}	0.01	9.0×10^{-4}
N=714	1		0.0096	0.0043	0.0005	5	1.8×10^{-5}
nw=51	2		0.0213	0.0075	0.0005	2	5.7×10^{-5}
np=14	4		0.0473	0.0124	0.0002	0.4	2.0×10^{-4}
	8		0.1043	0.0180	-0.0007	0.7	0.0003
II	12		0.1637	0.0201	-0.0014	0.9	0.0004
	16		0.2231	0.0203	-0.0019	0.8	0.0004
	20		0.2812	0.0196	-0.0020	0.7	0.0004
	24		0.3374	0.0190	-0.0019	0.6	0.0004
	32		0.4417	0.0207	-0.0014	0.3	0.0004
N=280	1		0.0109	0.0077	0.0018	19	6.2×10^{-5}
nw=40	2		0.0229	0.0126	0.0021	10	1.6×10^{-4}
np=7	4		0.0491	0.0196	0.0019	4	4.0×10^{-4}
	8		0.1055	0.0270	0.0005	0.5	7.0×10^{-4}
III	12		0.1644	0.0292	-0.0006	0.4	9.0×10^{-4}
	16		0.2237	0.0291	-0.0012	0.5	8.0×10^{-4}
	20		0.2821	0.0290	-0.0011	0.4	8.0×10^{-4}
	24		0.3387	0.0309	-0.0006	0.2	0.0010
	32		0.4442	0.0420	0.0011	0.3	0.0018
N=560	1		0.0099	0.0055	0.0008	9	3.1×10^{-5}
nw=40	2		0.0217	0.0093	0.0009	4	8.8×10^{-5}
np=14	4		0.0477	0.0149	0.0005	1	2.2×10^{-4}
	8		0.1044	0.0207	-0.0005	0.5	4.3×10^{-4}
IV	12		0.1639	0.0223	-0.0012	0.7	5.0×10^{-4}
	16		0.2236	0.0218	-0.0014	0.6	$5.0 \times 10-4$
	20		0.2822	0.0211	-0.0011	0.4	4.0×10^{-4}
	24		0.3388	0.0218	-0.0005	0.1	5.0×10^{-4}
	32		0.4443	0.0294	0.0012	0.3	5.0×10^{-4}
N=504	1		0.0103	0.0058	0.0012	13	3.4×10^{-5}
nw=36	2		0.0222	0.0096	0.0014	7	9.4×10^{-5}
np=14	4		0.0484	0.0149	0.0013	3	2.2×10^{-4}
V	8		0.1053	0.0202	0.0003	0.3	4.1×10^{-4}
	12		0.1645	0.0214	-0.0006	0.4	4.6×10^{-4}
	16		0.2237	0.0213	-0.0012	0.5	4.5×10^{-4}
	20		0.2818	0.0220	-0.0014	0.5	4.9×10^{-4}
	24		0.3379	0.0250	-0.0014	0.4	6.3×10^{-4}
	32		0.4422	0.0364	-0.0009	0.2	0.0013

(1)standard deviation; (2) estimate - real value; (3) relative bias =(abs.value(bias)/real value)×100%

4 Simulation Study #2: the case of the Weibull model with covariates

Here the main purpose is to present the results of simulations with the parameter α modeled as a function of covariates. The scenario considered is an overstress testing which is the most commom form of accelerated testing.Those kind of tests consist of running a product at higher than normal levels of some accelerating stress(es) to shorten product life. The aim is to quickly obtain data which, properly modeled and analyzed, yield desired information on product life **under normal use**. In other words the failure (and censored) data obtained under accelerated conditions are modeled to estimate quantities of interest like percentiles, fraction of defectives under normal use. Therefore, the "covariates" here are actually accelerating stresses. Nelson (1990), Meeker and Escobar (1999) are both complete references of the statistical methodology for accelerated testing procedures.

This simulation study was motivated by a number of real situations associated with shelf life determination of food products, in particular, the one described in the work by Freitas, Borges and Ho (2001). The storage of food products in environmental chambers, at higher levels of temperature and humidity for example, is a common practice. The objetive is to simulate more aggressive storage conditions. The only weakness of those experiments is the use of only one level of the stress variable(s) which makes impossible the extrapolation for the normal use conditions.

The simulation study has been divided in two subcases: one and two covariates. In each case the objective is to evaluate the quality of the estimates obtainned for chosen percentiles and fraction defectives **under the use conditions**.

4.1 Simulation Study with the Weibull model with one covariate

The model considered here is a particular case of the general model presented previously (Section 2; equation [2]), where:

$$\begin{aligned} \boldsymbol{X_j} &= (X_j^0, ..., X_j^q) = (X_j^0, X_j^1) = (1, X_j^1) \text{ and} \\ \boldsymbol{\beta} &= (\beta_0, \beta_1)' \end{aligned}$$

Therefore,

$$\begin{aligned} \alpha_j &= \exp(\beta_0 + \beta_1 X_j^1) \\ \text{and } \delta &= \exp(\gamma) \text{ for all } j = 1, 2, ..., n_i \text{ and } i = 1, 2, ..., k \end{aligned}$$

The parameter $\boldsymbol{\theta} = (\beta_0, \beta_1, \gamma)'$ is the one to be estimated by maximum likelihood.

In order to implement the simulation study, the following questions had to be answered:

1) Which values of β_0, β_1 and γ (and consequently of α e δ) should be used in the simulations?

Once again, the real situation described Freitas, Borges and Ho (2001)was the basis for the choice of the parameter values used in the simulations.

In the experimental chamber 1, temperature and humidity levels were controlled at 30^oC and 80 % respectively and units were stored for 36 weeks. On the other hand, units stored in the experimental chamber 2 were kept for 18 weeks at 37^oC (the humidity was recorded but not controlled). In addition, the Weibull model fitted to each of the experimental data indicated that the temperature alone, at the chosen level of 37^oc was much more efficient as an accelerated stress (Freitas, Borges and Ho; 2001). Consequently, the reference stress condition chosen was the one set for chamber 2:

- temperature: 37^oC (humidity was not controlled);
- number of weeks (nw): 18;
- number of judges allocated to each week (nj): 7
- total number of specimens on test (N): 126.

We used three stress levels (equally spaced), which is the minimum required for extrapolations purposes (Nelson, 1980; Meeker and Escobar, 1998). The conditions are given below:

- test stress levels (assuming *temperature* as the stress variable): 37^oC, 41^oC e 45^oC;
- number of follow up weeks: 18 weeks (for each of the three conditions above);
- number of judges allocated to each week: 7 (for each of the three stress conditions);
- total number of specimens under test: $N = 378$ (126 specimens per condition);
- chosen values for the characteristic life:
  - for 37^oC (test condition [1]): $t_{0,63212} = 16$ weeks
  - for 41^oC (test condition [2]): $t_{0,63212} = 13$ weeks

Inicial values for the parâmeters β_0 and β_1 were obtained, solving the equations written for the characteristic life of the Weibull distribution ($t_{0,63212} = \frac{1}{\alpha}$). They are given bellow:

$$
\begin{aligned}
t_{0,63212} = 16 \quad &\Rightarrow \quad 16 \exp(\beta_0 + \beta_1 \, 37) = 1 \\
t_{0,63212} = 13 \quad &\Rightarrow \quad 13 \exp(\beta_0 + \beta_1 \, 41) = 1
\end{aligned}
$$

Solving the sistem for β_0 and β_1, we obtain:

$$\hat{\beta}_0 = -4,69325 \quad \text{e} \quad \hat{\beta}_1 = 0,05191$$

for any value of δ.

Therefore,

- for $45^oC \Rightarrow t_{0,63212} = 10,5625$ (test condition [3]).

Table 8 presents a summary of the parameters values:

Table 8: Reference values to be used in the simulations

condition	chosen values	estimated parameter values		
	$t_{0,63212}$	$\hat{\beta}_0$	$\hat{\beta}_1$	$\hat{\alpha}$
37^oC	16	-4,69325	0,05191	0,06250
41^oC	13	-4,69325	0,05191	0,07692
$45^oC^{(*)}$	10,5625	-4,69325	0,05191	0,09467

(*) for 45^oC, $t_{0,63212}$ was estimated

Finally, Table 9 presents the actual parameter values used in the simulations.

Table 9: Parameter values (β_0, β_1 and δ, used in the simulations

β_0	β_1	δ	(γ)
-4,4	0,03	1,2	(0,19)
-4,7	0,05	1,4	(0,34)
-5,0	0,07	1,6	(0,47)
		1,8	(0,59)
		2,0	(0,69)

(a total of 45 combinations)

2) Which sample plans will be used?

The "standard" sample plan is the one used in the experiment for chamber 1: nw = 8 weeks; nj=7 judges allocated each week (a total of 126 specimens under test).

The same sample plan will be used for each test stress level and an equal number of specimens will be allocated to each level (proportion 1:1:1). So, 126 specimens will be allocated to each test stress level.

The main purpose of the simulation study is to verify the performance of the estimates obtained for percentiles and fraction defectives for "normal storage condition", assumed to be 28^oC.

We have also implemented the allocation 4:2:1 suggested by Meeker e Hahn (1985). This allocation was suggested by the author in order to get better estimates of small percentiles.

Table 10 sumarizes the sample plans used in the simulation study.

3) Which steps will be followed in the simulation study

We assumed a follow up time of 18 weeks (nw=18) and that the evaluations were done weekly. The number of judges allocated to each week (nj) depends on the proportion of allocation, for instance 1:1:1 or 4:2:1 (see Table 10).

The steps followed in the simulation study were basically the ones listed below.

Table 10: Sample plans implemented in the simulation study for each of the 45 scenarios of Table 9

		allocation proportion					
		1:1:1			4:2:1		
characteristics		test stress levels			test stress levels		
		37^oC	41^oC	45^oC	37^oC	41^oC	45^oC
N^*=378	n^*	126	126	126	216	108	54
	nj^*	7	7	7	12	6	3
	nw^*	18	18	18	18	18	18
N=756	n	252	252	252	432	216	108
	nj	14	14	14	24	12	6
	nw	18	18	18	18	18	18

(*) N= total number of specimens; n=number of specimens allocated; nj=number of judges allocated to each week; nw= number of follow up weeks

- **step 1**: choose a set o parameter values β_0, β_1 and δ (or γ) from Table 9;
- **step 2**: generate three random samples of failure time data t, from each of the three Weibull (α, δ) distributions, where $\alpha = \exp\beta_0 + \beta_1\, 37$, $\alpha = \exp\beta_0 + \beta_1\, 41$, $\alpha = \exp\beta_0 + \beta_1\, 45$, $\delta = e^\gamma$, with β_0, β_1, δ chosen in step 1. The sample sizes for each test stress level $(37^oC, 41^oC, 45^oC)$depends on the allocation plan: 1;1;1 or 4:2:1 (see Table 10);
- **step 3**: dichotomize the results and store them in a vector (Y). The dichotomization is done by comparing each failure time t (generated according to each Weibull distribution) with the evaluation times τ (τ assumes vaules 1 to 18 weeks). If $t > 0$ then Y=0, otherwise Y=1 (failure has already ocurred);
- **step 4**: calculate the maximum likelihood estimator of β_0, β_1 and γ (or, equivalently, α e δ) using the dichotomized data;
- **step 5**: using the parameters estimates calculated in step 4, find the estimates of percentiles and fraction of defectives **for the storage condition** 28^oC;
- **step 6**: store the values calculated in step 5;
- **step 7**: generate more three random samples as in step 2 and repeat steps 3 to 6;
- **step 8**: steps 2 to 7 should be repeated until 1000 samples have been generated (for each test stress condition);
- **step 9**: at the end of the simulation, calculate for each percentile and fraction of defectives of interest, estimated **for the storage condition** 28^oC:
  - the average of the 1000 estimated values;
  - the standard deviation (SD) based on the 1000 values;

– the absolute bias (B), the relative bias (RB) and the MSE (mean square error).

These steps were implemented for each one of the sample plans listed in Table 10.

4.2 Simulation Results: model with one covariate only

Tables 11 to 13 present the results of the simulation study for percentiles for the "use" storage condition 28^oC, with β_0=-4,4 and β_1=0,03, 0,05 and 0,07 respectively (N=378).There is no clear pattern when we compare 1:1:1 and 4:2:1 plans, taking into account bias, relative bias or standard deviations. There are few exceptions, for instance, for $\delta = 1,2$ and β_1=0,03 plan 1:1:1 is better than 4:2:1 when we compare their relative bias. The same result was found for β_1= 0,05 and 0,07. For $\delta = 1,4$ and β_1=0,05 and 0,07 the RB of plan 1:1:1 is smaller than the value calculated for plan 4:2:1. On the other hand, for β_1=0,03 the situation reverses.

Table 11: Simulation results(1000 samples) for percentiles of the condition 28^oC with $\beta_0 = -4,4$, $\beta_1 = 0,03$ (N=378 specimens)

	δ									
	1,2		1,4		1,6		1,8		2	
p	alocação		alocação		alocação		alocação		alocação	
	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1
10^{-6}	$0,0009^{(1)}$	0,0009	0,0029	0,0027	0,0064	0,0060	0,0130	0,0153	0,0222	0,0239
	$240^{(2)}$	246	153	146	103	95	78	92	64	69
	$0,0027^{(3)}$	0,0026	0,0079	0,0081	0,0186	0,0165	0,0359	0,0417	0,0597	0,0648
10^{-5}	0,0035	0,0036	0,0088	0,0084	0,0167	0,0151	0,0287	0,0337	0,0452	0,0470
	135	141	91	87	63	57	48	57	41	43
	0,0125	0,0095	0,0241	0,0237	0,0493	0,0446	0,0854	0,0952	0,1311	0,1392
10^{-4}	0,0125	0,0132	0,0255	0,0244	0,0412	0,0353	0,0591	0,0691	0,0870	0,0856
	72	76	51	49	37	32	28	32	25	25
	0,0357	0,0355	0,0748	0,0718	0,1325	0,1216	0,2027	0,2190	0,2853	0,2974
10^{-3}	0,0415	0,0439	0,0669	0,0643	0,0947	0,0721	0,1094	0,1273	0,1550	0,1368
	36	38	26	25	20	15	14	17	14	12
	0,1341	0,1361	0,2347	0,2225	0,3578	0,3295	0,4741	0,4996	0,6115	0,6219
10^{-2}	0,1250	0,1263	0,1543	0,1520	0,2154	0,1238	0,1873	0,2063	0,2624	0,1865
	16	16	12	11	11	6	7	8	7	5
	0,5107	0,5224	0,7324	0,6906	0,9637	0,8804	1,0984	1,1245	1,3195	1,2566

(1) bias=estimate-real; (2) relative bias= (abs.value(bias)/real)×100%; (3) SD

Table 14 presents the results of the simulation study for fraction of defectives ("use" condition 28^oC), for β_0=-4,4 e β_1=0,03. Once again, there is no indication that one allocation plan is better than the other. The results obtained for other parameter values are similar and will not be shown here.

Now, if the two allocation plans are analysed separately, we observe that the bias (absolute value) and the SD both increase along with increasing percentile values. This pattern can be verified for both allocation plans. The relative bias (RB) on the

Table 12: Simulation results(1000 samples) for percentiles of the condition 28^oC with $\beta_0 = -4,4$, $\beta_1 = 0,05$ (N=378 specimens)

	δ									
	1,2		1,4		1,6		1,8		2	
p	alocação		alocação		alocação		alocação		alocação	
	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1
10^{-6}	$0,0002^{(1)}$	0,0003	0,0007	0,0009	0,0016	0,0018	0,0039	0,0047	0,0076	0,0060
	$105^{(2)}$	126	68	84	46	50	41	49	39	30
	$0,0006^{(3)}$	0,0008	0,0020	0,0024	0,0054	0,0052	0,0110	0,0131	0,0197	0,0183
10^{-5}	0,0010	0,0011	0,0025	0,0030	0,0045	0,0051	0,0096	0,0115	0,0173	0,0134
	67	78	45	55	30	34	28	34	28	21
	0,0026	0,0033	0,0072	0,0084	0,0161	0,0158	0,0294	0,0340	0,0473	0,0445
10^{-4}	0,0040	0,0045	0,0082	0,0097	0,0118	0,0136	0,0224	0,0268	0,0380	0,0287
	40	45	29	34	19	21	18	22	19	14
	0,0116	0,0139	0,0256	0,0290	0,0479	0,0479	0,0778	0,0874	0,1118	0,1061
10^{-3}	0,0146	0,0161	0,0246	0,0283	0,0281	0,0333	0,0485	0,0578	0,0792	0,0585
	22	24	17	19	10	12	11	13	13	9
	0,0513	0,0586	0,0903	0,0992	0,1408	0,1416	0,2015	0,2190	0,2564	0,2461
10^{-2}	0,0474	0,0512	0,0671	0,0745	0,0587	0,0737	0,0940	0,1114	0,1554	0,1148
	11	11	9	10	5	7	6	7	8	5
	0,2211	0,2416	0,3095	0,3256	0,4033	0,4035	0,5055	0,5262	0,5682	0,5516

(1) bias=estimate-real; (2) relative bias= (abs.value(bias)/real)×100%; (3) SD

Table 13: Simulation results(1000 samples) for percentiles of the condition 28^oC with $\beta_0 = -4,4$, $\beta_1 = 0,07$ (N=378 specimens)

	δ									
	1,2		1,4		1,6		1,8		2	
p	alocação		alocação		alocação		alocação		alocação	
	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1	1:1:1	4:2:1
10^{-6}	$0,0002^{(1)}$	0,0002	0,0006	0,0007	0,0016	0,0015	0,0035	0,0035	0,0069	0,0072
	$143^{(2)}$	147	97	107	80	75	65	66	61	64
	$0,0005^{(3)}$	0,0006	0,0015	0,0017	0,0044	0,0044	0,0093	0,0093	0,0180	0,0162
10^{-5}	0,0008	0,0008	0,0021	0,0023	0,0047	0,0044	0,0089	0,0091	0,0153	0,0165
	91	93	66	73	55	51	46	47	43	46
	0,0020	0,0023	0,0054	0,0058	0,0129	0,0127	0,0237	0,0240	0,0409	0,0379
10^{-4}	0,0032	0,0032	0,0070	0,0078	0,0129	0,0121	0,0217	0,0223	0,0326	0,0365
	56	57	43	48	36	33	31	32	29	32
	0,0084	0,0093	0,0192	0,0203	0,0377	0,0371	0,0608	0,0619	0,0928	0,0882
10^{-3}	0,0124	0,0123	0,0222	0,0254	0,0332	0,0313	0,0501	0,0522	0,0654	0,0771
	33	32	26	30	22	20	20	21	18	21
	0,0362	0,0385	0,0684	0,0703	0,1091	0,1073	0,1543	0,1580	0,2086	0,2020
10^{-2}	0,0432	0,0424	0,0638	0,0779	0,0766	0,0737	0,1070	0,1148	0,1185	0,1513
	17	17	14	18	12	11	12	13	10	13
	0,1535	0,1601	0,2393	0,2379	0,3112	0,3070	0,3848	0,3967	0,4625	0,4540

(1) bias=estimate-real; (2) relative bias= (abs.value(bis)/real)×100%; (3) SD

Table 14: Simulation results (1000 samples)- fraction defectives at t_0 weeks - condition: 28^oC, $\beta_0 = -4,4$, $\beta_1 = 0,03$ (N=378 specimens)

t_0	δ = 1,2 alocation 1:1:1	1,2 4:2:1	1,4 1:1:1	1,4 4:2:1	1,6 1:1:1	1,6 4:2:1	1,8 1:1:1	1,8 4:2:1	2 1:1:1	2 4:2:1
1	$0,0019^{(1)}$	0,0023	0,0013	0,0013	0,0009	0,0011	0,0006	0,0006	0,0003	0,0004
	$15^{(2)}$	17	20	19	27	31	36	40	37	49
	$0,0104^{(3)}$	0,0116	0,0062	0,0063	0,0037	0,0038	0,0022	0,0026	0,0013	0,0014
2	0,0028	0,0031	0,0022	0,0020	0,0016	0,0020	0,0012	0,0013	0,0008	0,0009
	9	10	13	12	16	20	22	23	23	28
	0,0189	0,0203	0,0125	0,0125	0,0084	0,0083	0,0056	0,0060	0,0036	0,0038
4	0,0040	0,0040	0,0038	0,0032	0,0024	0,0037	0,0026	0,0025	0,0019	0,0021
	6	6	8	7	8	12	13	13	15	16
	0,0347	0,0354	0,0257	0,0252	0,0189	0,0186	0,0142	0,0147	0,0106	0,0104
8	0,0062	0,0052	0,0072	0,0055	0,0033	0,0078	0,0063	0,0058	0,0060	0,0053
	4	3	6	5	4	9	9	9	12	10
	0,0636	0,0616	0,0536	0,0522	0,0438	0,0435	0,0375	0,0372	0,0329	0,0302
12	0,0081	0,0063	0,0110	0,0083	0,0040	0,0127	0,0114	0,0109	0,0127	0,0106
	3	3	6	4	2	8	9	8	12	10
	0,0898	0,0851	0,0822	0,0801	0,0719	0,0727	0,0671	0,0655	0,0650	0,0581
16	0,0093	0,0069	0,0142	0,0105	0,0042	0,0174	0,0172	0,0172	0,0210	0,0176
	3	2	5	4	2	7	8	8	11	9
	0,1124	0,1056	0,1092	0,1064	0,1007	0,1030	0,1000	0,0978	0,1030	0,0919
20	0,0092	0,0067	0,0158	0,0114	0,0034	0,0204	0,0218	0,0227	0,0282	0,0245
	2	2	4	3	1	6	7	7	10	9
	0,1309	0,1226	0,1322	0,1288	0,1273	0,1305	0,1319	0,1299	0,1410	0,1267
24	0,0077	0,0053	0,0153	0,0105	0,0007	0,0206	0,0234	0,0252	0,0314	0,0282
	2	1	3	2	0,2	5	6	6	8	8
	0,1449	0,1358	0,1499	0,1462	0,1492	0,1524	0,1585	0,1569	0,1723	0,1570
32	0,0012	-0,0004	0,0080	0,0032	-0,0103	0,0115	0,0141	0,0172	0,0202	0,0200
	0,2	0,06	1	0,6	2	2	2	3	4	4
	0,1608	0,1508	0,1689	0,1654	0,1746	0,1755	0,1878	0,1845	0,2031	0,1896

(1)bias=estimate-real value; (2) relative bias= (abs.value(bias)/real value)×100%; (3) SD other hand, decreases with increasing percentile values. For fraction of defectives no pattern was identified.

The results for N=756 will not be shown here. As one would expect, an increase in the total sample size leads to a reduction of the SD of the estimates.

4.3 Simulation Study with the Weibull model with two covariates.

The model presented in Section 2 (equation [2]), considering only two covariates has the form given below:

$$\begin{aligned} \boldsymbol{X_j} &= (X_j^0, ..., X_j^q) = (X_j^0, X_j^1, X_j^2) = (1, X_j^1, X_j^2) \text{ and} \\ \boldsymbol{\beta} &= (\beta_0, \beta_1, \beta_2)' \end{aligned}$$

Therefore,

$$\begin{aligned} \alpha_j &= \exp(\beta_0 + \beta_1 X_j^1 + \beta_2 X_j^2) \\ \text{e } \delta &= \exp(\gamma) \text{ for all } j = 1, 2, ..., n_i \text{ and } i = 1, 2, ..., k \end{aligned}$$

Then, $\boldsymbol{\theta} = (\beta_0, \beta_1, \beta_1, \gamma)'$ is the parameter to be estimated by maximum likelihood.

Here we have considered the scenario of an overstress testing, with two stress variables (for instance, temperature and humidity). As it was discussed in the previous section, the purpose is to evaluate through a simulation study, the performance of estimates for fraction of defectives and percentiles of the failure time distribution in the **"use" condition**, assumed to be [$28^o C$; 40% RU].

The overstress conditions, parameter values and sample plans used, were chosen through an analysis of the stress levels present in the real data set.

Table 15 presents the overstress conditions and parameter values used in the simulations and Table 16 presents the sample plans considered.

4.4 Simulation Results: model with two covariates

Tables 17 and 18 present the simulation results for the percentiles of the failure time distribution for condition [$28^o C$, 40%].

The pattern is the same for the two situations ilustrated. The bias and standard deviation both increase with the increase of the percentiles. The relative bias, on the contrary, decreases with the increase of the percentile.

Now, if one fixes a percent value (p value), the analysis across that line shows that the bias and standard deviation both increase with increasing values of δ. The relative bias decreases.

For the fraction defectives (Tables 19 and 20) the results are very similar to the ones decribed above.As the reference time increases (t_0), the bias and SD of fraction defectives increase. The relative bias though decreases.

Table 15: Overstress conditions and parameter values used in the simulation study

	parameters				
conditions	β_0	β_1	β_2	δ^*	(γ)
(1) $37^oC, 60\%$	-6,5	0,08	0,0112	1,2	(0,19)
(2) $37^oC, 80\%$	-6,5	0,08	0,0112	1,2	(0,19)
(3) $45^oC, 60\%$	-6,5	0,08	0,0112	1,2	(0,19)
(4) $45^oC, 80\%$	-6,5	0,08	0,0112	1,2	(0,19)
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
(17) $37^oC, 60\%$	-6,5	0,08	0,0112	2,0	(0,69)
(18) $37^oC, 80\%$	-6,5	0,08	0,0112	2,0	(0,69)
(19) $45^oC, 60\%$	-6,5	0,08	0,0112	2,0	(0,69)
(20) $45^oC, 80\%$	-6,5	0,08	0,0112	2,0	(0,69)
(21) $37^oC, 60\%$	-7,2	0,112	0,005	1,2	(0,19)
(22) $37^oC, 80\%$	-7,2	0,112	0,005	1,2	(0,19)
(23) $45^oC, 60\%$	-7,2	0,112	0,005	1,2	(0,19)
(24) $45^oC, 80\%$	-7,2	0,112	0,005	1,2	(0,19)
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
(37) $37^oC, 60\%$	-7,2	0,112	0,005	2,0	(0,69)
(38) $37^oC, 80\%$	-7,2	0,112	0,005	2,0	(0,69)
(39) $45^oC, 60\%$	-7,2	0,112	0,005	2,0	(0,69)
(40) $45^oC, 80\%$	-7,2	0,112	0,005	2,0	(0,69)

(*) range: 1,2 a 2 (in steps of size 0,2).

Table 16: Sample plans used in the simulations for each scenario listed in Table 15

characteristics		overstress conditions			
		$[37^oC, 60\%]$	$[37^oC, 80\%]$	$[45^oC, 60\%]$	$[45^oC, 80\%]$
N^*=504	n^*	126	126	126	126
	nj^*	7	7	7	7
	nw^*	18	18	18	18
N=1008	n	252	252	252	252
	nj	14	14	14	14
	nw	18	18	18	18

(*) N= total number of specimens under test; n=number of specimens allocated; nj=number of judges; nw=number of follow up weeks.

Table 17: Simulation results (1000 samples) for percentiles for the condition [28^oC, 40%], with $\beta_0 = -6,5$, $\beta_1 = 0,08$, $\beta_2 = 0,0112$ (N=504 specimens)

	δ				
p	1,2	1,4	1,6	1,8	2
10^{-6}	$0,0004^{(1)}$	0,0011	0,0039	0,0066	0,0093
	$75^{(2)}$	46	49	31	21
	$0,0010^{(3)}$	0,0033	0,0109	0,0190	0,0313
10^{-5}	0,0016	0,0038	0,0113	0,0164	0,0207
	48	30	33	21	15
	0,0046	0,0122	0,0321	0,0517	0,0774
10^{-4}	0,0065	0,0120	0,0310	0,0391	0,0445
	29	19	22	14	10
	0,0209	0,0452	0,0947	0,1378	0,1881
10^{-3}	0,0239	0,0344	0,0800	0,0882	0,0916
	16	10	13	9	6
	0,0943	0,1636	0,2751	0,3578	0,4460
10^{-2}	0,0816	0,0906	0,1915	0,1914	0,1874
	8	5	8	5	4
	0,4194	0,5831	0,7945	0,9176	1,0526

(1) bias=estimative-real; (2) relative bias= (abs.value(bias)/real)×100%; (3) SD

Table 18: Simulation results (1000 samples) for percentiles for condition [28^oC, 40%], with $\beta_0 = -7,2$, $\beta_1 = 0,112$, $\beta_2 = 0,005$ (N=504 specimens)

	δ				
p	1,2	1,4	1,6	1,8	2
10^{-6}	$0,0004^{(1)}$	0,0014	0,0038	0,0088	0,0153
	$81^{(2)}$	53	44	39	33
	$0,0011^{(3)}$	0,0036	0,0098	0,0225	0,0422
10^{-5}	0,0018	0,0048	0,0110	0,0223	0,0344
	53	36	31	28	23
	0,0051	0,0134	0,0307	0,0602	0,1010
10^{-4}	0,0075	0,0161	0,0309	0,0537	0,0738
	32	24	20	19	16
	0,0232	0,0492	0,0944	0,1585	0,2377
10^{-3}	0,0282	0,0518	0,0814	0,1212	0,1488
	18	15	13	12	10
	0,1036	0,1771	0,2843	0,4071	0,5450
10^{-2}	0,0954	0,1625	0,1998	0,2492	0,2774
	9	9	7	7	6
	0,4514	0,6285	0,8440	1,0271	1,2259

(1) bias=estimative-real; (2) relative bias= (abs. value(vício)/real)×100%; (3) SD

The analysis of Tables 19 and 20 across any chosen line (lets say, $t_0 = 4$), shows that the SD decreases with the increase of the δ values. There is no pattern for the other two measures of performance (bias and relative bias).

The simulation results with N=1008 are not included here since the pattern observed is the same described above. A reduction in the SD of the estimatives was observed.

Table 19: Simulation results (1000 samples) for fraction defectives in t_0 weeks (for 28^oC and 40% UR), with $\beta_0 = -6,5$, $\beta_1 = 0,08$, $\beta_2 = 0,0112$ (N=504 specimens)

	δ				
t_0	1,2	1,4	1,6	1,8	2
1	$0,0006^{(1)}$	0,0005	0,0001	0,0001	0,00006
	$6^{(2)}$	10	4	9	13
	$0,0050^{(3)}$	0,0027	0,0013	0,0007	0,0004
2	0,0010	0,0009	0,0002	0,0002	0,0002
	4	7	3	5	8
	0,0095	0,0060	0,0034	0,0020	0,0012
4	0,0016	0,0017	0,0004	0,0004	0,0004
	3	5	2	3	5
	0,0183	0,0131	0,0086	0,0058	0,0039
8	0,0028	0,0035	0,0013	0,0011	0,0011
	2	4	2	3	4
	0,0355	0,0288	0,0222	0,0170	0,0129
12	0,0041	0,0054	0,0030	0,0023	0,0022
	2	4	3	3	3
	0,0520	0,0455	0,0387	0,0319	0,0261
16	0,0052	0,0073	0,0051	0,0039	0,0037
	2	4	3	3	3
	0,0674	0,0620	0,0567	0,0493	0,0427
20	0,0059	0,0088	0,0074	0,0056	0,0053
	2	3	3	3	3
	0,0812	0,0775	0,0747	0,0677	0,0616
24	0,0061	0,0098	0,0092	0,0071	0,0066
	2	3	3	3	3
	0,0931	0,0914	0,0915	0,0858	0,0812
32	0,0051	0,0096	0,0108	0,0079	0,0068
	1	2	2	2	2
	0,1105	0,1125	0,1176	0,1159	0,1153

(1) bias=estimate-real; (2) relative bias= (abs.value(bias)/real)×100%; (3) SD

Table 20: Simulation results (1000 samples) for fraction of defectives in t_0 weeks (for 28^oC and 40% UR), with $\beta_0 = -7,2$, $\beta_1 = 0,112$, $\beta_2 = 0,005$ (N=504 specimens)

	δ				
t_0	1,2	1,4	1,6	1,8	2
1	$0,0006^{(1)}$	0,0002	0,0001	0,00006	0,00005
	$6^{(2)}$	4	5	6	11
	$0,0048^{(3)}$	0,0024	0,0012	0,0007	0,0004
2	0,0096	0,0002	0,0002	0,0001	0,0001
	4	2	3	3	6
	0,0094	0,0052	0,0031	0,0019	0,0012
4	0,0018	0,0001	0,0004	0,0002	0,0003
	4	0,5	2	2	4
	0,0185	0,0116	0,0079	0,0055	0,0038
8	0,0036	0,00008	0,0011	0,0008	0,0007
	3	0,10	2	2	2
	0,0361	0,0259	0,0206	0,0157	0,0122
12	0,0054	0,0002	0,0025	0,0019	0,0015
	3	0,1	2	2	2
	0,0529	0,0413	0,0361	0,0292	0,0242
16	0,0071	0,0003	0,0042	0,0037	0,0028
	3	0,2	3	3	3
	0,0683	0,0567	0,0531	0,0450	0,0390
20	0,0085	0,0004	0,0060	0,0058	0,0045
	3	0,2	3	3	3
	0,0819	0,0714	0,0701	0,0619	0,0556
24	0,0094	0,0003	0,0075	0,0080	0,0063
	3	0,08	3	3	3
	0,0935	0,0848	0,0861	0,0789	0,0731
32	0,0096	-0,0010	0,0089	0,1082	0,0089
	2	0,2	2	2	2
	0,1105	0,1058	0,1119	0,1159	0,1050

(1) bias=estimate-real; (2) relative bias= (abs.value(bias)/real)×100%; (3) SD

5 Conclusions

For the model with no covariates, the simulation results showed that, in general, one can get results much more precise and with smaller bias with a shorter follow-up time, allocating more panelists to each evaluation time.

For the model with one covariate only, the bias and standard deviations for percentiles estimates both increase with the increase of the percentiles to be estimated. The same pattern was observed for fraction defectives.

The allocation of units to each stress level proposed by Meeker and Hahn (4:2:1) was not any better then the usual allocation 1:1:1 for the model proposed.

All the simulations were based in the Weibull distribution. Other distributions must be tried out.

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