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Estimating the Parameters of a Fatigue Model Using Benders Decomposition

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Abstract This paper shows how Benders decomposition can be used for estimating the parameters of a fatigue model. The two alternative objective functions to be optimized are the likelihood and the sum of squares error functions, which relate to the maximum likelihood and the minimum error principles, respectively. These functions depend on five parameters of different nature. This makes the parameter estimation problem of the fatigue model suitable for the Benders decomposition, which allows using well-behaved and robust estimation parameter methods for the different subproblems. To build the Benders cuts, explicit formulas for the sensitivities (partial derivatives) are obtained. This permits building the classical iterative method, in which upper and lower bounds of the optimal value of the objective function are obtained until convergence. The method is illustrated by its application to a real-world problem reported by Holmes.

Keywords Linear optimization · Least-squares · Maximum likelihood · Sensitivity analysis · Benders' decomposition · Fatigue

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1 Introduction

The fatigue problem consists of analyzing the strength of a given piece of material when subjected to cycles of deterministic or random loads. It is well known that the static strength of a piece, that is, the static stress resisted by the piece without failure is much higher than the stress resisted when this stress is repeated many times. This repetition of small stresses frequently causes the failure of many real-world structures and it occurs unexpectedly because of the low value of the repeating stresses involved. Thus, determination of the fatigue strength is of crucial importance in real life.

Many researchers have confronted the fatigue problem in the past. The existing literature contains a very large list of models that have been built to deal with the problem of fatigue. They try to predict the lifetime N (in cycles or a multiple of cycles) in terms of the stress range or amplitude $\Delta\sigma$, though some of them include other parameters or material properties, such as the endurance limit $\Delta\sigma_0$ or the ultimate strength $\Delta\sigma_{\rm st}$.

The learning process of fatigue models has been traditionally done by many different methods, and the existing literature has taken care of many variants of well known methods (see, for example, Castillo et al (1999), Castillo and Fernández-Canteli (2001), etc.).

However, since the learning is normally done by maximizing the likelihood function or minimizing a sum of squares of residuals, general optimization methods (see Castillo et al (2001)) can also be used.

The Benders decomposition technique, via the well known Benders cuts, is closely related to sensitivity analysis (see Choi and Choi (1992), Castillo et al (2004), Castillo et al (2005a) or Castillo et al (2007b)). In fact, we can obtain closed formulas for the partial derivatives (sensitivities) of the likelihood function or the sum of squares of residuals with respect to each particular parameter, which are the sensitivities of the objective function with respect to the parameter values.

Benders decomposition is particularly appropriate to address this problem because if fixing the complicating variables to specific values the resulting problem (subproblem) is significantly less complex, and well-behaved and robust estimation parameter methods can be applied.

The paper is structured as follows. In Section 2 we provide some background on the fatigue problem, we list some of the existing models and show how to derive a physically valid fatigue model. In Section 3 we propose two estimation methods based on Benders decomposition, one based on the maximum likelihood principle, and another based on a least squares technique. In Section 4 we illustrate the proposed method by its application to an actual data set given by Holmen (1979). Finally, in Section 5 we provide some conclusions.

2 Some background on fatigue models

In this section, we introduce the reader to fatigue models.

Different intuitive models (parabolic, hyperbolic, exponential, linear, etc.) have been proposed in the literature to determine the fatigue strength (see Wøhler (1870), Basquin (1910), Palmgren (1924), Coleman (1958), Bastenaire (1972), ASTM (1981), Spindel and Haibach (1981), Lawless (1982), Castillo et al (1985), Castillo and Galambos (1987), Castillo and Hadi (1994, 1995), Kohout (1999), Pascual and Meeker (1999),

Model	Functional Form	Dimensional Parameters	Dimensionless Parameters
Wöhler (1870)	$\log N = A - B\Delta\sigma;\ \Delta\sigma \geq \Delta\sigma_0$	$B, \Delta\sigma_0$	A
Basquin (1910)	$\log N = A - B\log\Delta\sigma;\ \Delta\sigma \geq \Delta\sigma_0$	$B, \Delta\sigma_0$	A
Strohmayer (1914)	$\log N = A - B\log(\Delta\sigma - \Delta\sigma_0)$	$B, \Delta\sigma_0$	A
Palmgren (1924a)	$\log(N + D) = A - B\log(\Delta\sigma - \Delta\sigma_0)$	$B, \Delta\sigma_0$	A, D
Palmgren (1924b)	$\log N = A - B\log(\Delta\sigma - \Delta\sigma_0)$	$B, \Delta\sigma_0$	A
Weibull (1949)	$\log(N + D) = A - B\log((\Delta\sigma - \Delta\sigma_0)/(\Delta\sigma_{st} - \Delta\sigma_0))$	$\Delta\sigma_0, \Delta\sigma_{st}$	A, B, D
Stüssi (1955)	$\log N = A - B\log((\Delta\sigma - \Delta\sigma_0)/(\Delta\sigma_{st} - \Delta\sigma))$	$\Delta\sigma_0, \Delta\sigma_{st}$	A, B
Bastenaire (1972)	$(\log N - B)(\Delta\sigma - \Delta\sigma_0) = A\exp[-C(\Delta\sigma - \Delta\sigma_0)]$	$A, C, \Delta\sigma_0$	B
Spindel−Haibach (1981)	$\log(N/N_0) = A\log(\Delta\sigma/\Delta\sigma_0) - B\log(\Delta\sigma/\Delta\sigma_0) + B\left\{(1/\alpha)\log\left[1 + (\Delta\sigma/\Delta\sigma_0)^{-2\alpha}\right]\right\}$	$\Delta\sigma_0$	N_0, A, B, α
Castillo et al. (1985)	$\log(N/N_0) = \dfrac{\lambda + \delta(-\log(1-p))^{1/\beta}}{\log(\Delta\sigma/\Delta\sigma_0)}$	$\Delta\sigma_0$	$N_0, A, \lambda, \delta, \beta$
Kohout-Vechet	$\log\dfrac{\Delta\sigma}{\Delta\sigma_\infty} = \log\left(\dfrac{N + N_1}{N + N_2}\right)^b$	$\Delta\sigma_\infty$	N_1, N_2, b
Pascual−Meeker (1999)	$\log N = A - B\log(\Delta\sigma - \Delta\sigma_0)$	$B, \Delta\sigma_0$	A

Model	Dimensionless Functional Form	Dimensional Parameters	Dimensionless Parameters
Wöhler (1870)	$\log(N/N_0) = A - C\dfrac{\Delta\sigma}{\Delta\sigma_0};\ \Delta\sigma \geq \Delta\sigma_0$	$\Delta\sigma_0$	A,C, N_0
Basquin (1910)	$\log(N/N_0) = A - B\log\dfrac{\Delta\sigma}{\Delta\sigma_0};\ \Delta\sigma \geq \Delta\sigma_0$	$\Delta\sigma_0$	N_0, A, B
Strohmayer (1914)	$\log(N/N_0) = A - B\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right)$	$\Delta\sigma_0$	N_0, A, B
Palmgren (1924a)	$\log(N/N_0 + D) = A - B\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right)$	$\Delta\sigma_0$	N_0, A, B, D
Palmgren (1924b)	$\log(N/N_0) = A - B\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right)$	$\Delta\sigma_0$	N_0, A, B
Weibull (1949)	$\log(N/N_0 + D) = A + B\left[\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right) - \log\left(\dfrac{\Delta\sigma_{st}}{\Delta\sigma_0} - 1\right)\right]$	$\Delta\sigma_0, \Delta\sigma_{st}$	N_0, A, B, D
Stüssi (1955)	$\log N/N_0 = A - B\left[\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right) - \log\left(\dfrac{\Delta\sigma_{st}}{\Delta\sigma_0} - \dfrac{\Delta\sigma}{\Delta\sigma_0}\right)\right]$	$\Delta\sigma_0, \Delta\sigma_{st}$	N_0, A, B
Bastenaire (1972)	$\log(N/N_0) = \dfrac{A\exp\left[-C\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right)\right]}{\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1}$	$\Delta\sigma_0$	N_0, A, C
Spindel−Haibach (1981)	$\log(N/N_0) = A\log(\Delta\sigma/\Delta\sigma_0) - B\log(\Delta\sigma/\Delta\sigma_0) + B\left\{(1/\alpha)\log\left[1 + (\Delta\sigma/\Delta\sigma_0)^{-2\alpha}\right]\right\}$	$\Delta\sigma_0$	N_0, A, B, α
Castillo et al. (1985)	$\log(N/N_0) = A/\log(\Delta\sigma/\Delta\sigma_0)$	$\Delta\sigma_0$	N_0, A
Kohout-Vechet	$\log(\Delta\sigma/\Delta\sigma_\infty) = b\log\left(\dfrac{1 + N_1/N}{1 + N_2/N}\right)$	$\Delta\sigma_\infty$	N_1, N_2, b
Pascual−Meeker (1999)	$\log N/N_0 = A - B\log\left(\dfrac{\Delta\sigma}{\Delta\sigma_0} - 1\right)$	$\Delta\sigma_0$	N_0, A, B

Table 1 Models proposed in the literature for the Lifetime-Stress level curves. Dimensional (upper table) and dimensionless (lower table) forms.

Castillo and Fernández-Canteli (2001)). The upper part of Table 1 contains some of these models in their original forms. Note that some of the curves in Table 1 are linear relationships between stress range $\Delta\sigma$ and number of cycles N in arithmetic or logarithmic scales, while others adopt non-linear relationships. Note also that all authors agree on using a logarithmic scale for the lifetime, but there are some discrepancies in the scale to be used for the stress range, because some use arithmetic scale, and others, logarithmic scale.

Unfortunately, some of the above expressions do not lead to physically valid models. For a model to be physically valid it has to be valid irrespective of the units of measure of the different variables involved (see Aczél (1966, 1984) and Castillo and Ruiz Cobo (1992)). For example the model

$$\log N = A - B\varDelta\sigma$$

requires all summands to have the same units of measurement. Since N is lifetime and $\varDelta\sigma$ is stress, the constants A and B must have dimensions, and hence, if data units are changed, the values of the constants A and B must be changed accordingly. Thus, this model is not a physically valid model.

The lower part of Table 1 shows the same models in its upper part but transformed to exhibit dimensionless variables and the dimensionless magnitudes provided by the Buckingham theorem (see Buckingham (1915)).

2.1 Derivation of a fatigue model

In this section we give one example of how to derive a physically valid fatigue model.

Our starting assumption is that we consider the following 5 variables as the only ones relevant to the fatigue problem: P, N, N_0, $\varDelta\sigma$ and $\varDelta\sigma_0$, where P is the probability of fatigue failure of an element if subject to N cycles at a stress range $\varDelta\sigma$, N_0 is the threshold value for N, the minimum lifetime for any $\varDelta\sigma$, and $\varDelta\sigma_0$ is the endurance limit below which fatigue failure does not occur.

Using the $\varPi$-Theorem (see Castillo and Fernández-Canteli (2001)) this initial number of variables can be reduced to a set of 3 non-dimensional variables: $N^* = \log(N/N_0)$, $\varDelta\sigma^* = \log(\varDelta\sigma/\varDelta\sigma_0)$ and P, so that the initial relation among the 5 variables

$$r(N, N_0, \varDelta\sigma, \varDelta\sigma_0, P) = 0$$

can be reduced without loss of generality to a relation

$$P = q\left(\frac{N}{N_0}, \frac{\varDelta\sigma}{\varDelta\sigma_0}\right) \tag{1}$$

involving only three variables, where $q(\cdot)$ is a function to be determined.

In this paper, and for historical reasons, we replace (1) by

$$P = q\left(\log\frac{N}{N_0}, \log\frac{\varDelta\sigma}{\varDelta\sigma_0}\right), \tag{2}$$

because logarithmic scales are used for N and $\varDelta\sigma$.

Castillo et al (1985) derive the following model, which can also be justified based on microestructural properties of the material (see Bolotin (1998)):

$$\begin{array}{c} F[\log N; \log\varDelta\sigma] = 1 - \exp\left\{-\left[\dfrac{(\log N - B)(\log\varDelta\sigma - C) - \lambda}{\delta}\right]^{\beta}\right\} \\ \log N \geq B + \dfrac{\lambda}{\log\varDelta\sigma - C}, \end{array} \tag{3}$$

where F is the cumulative distribution function (cdf) of N^* given $\varDelta\sigma$, $B = \log N_0, C = \log\varDelta\sigma_0$, and λ, δ and β are the non-dimensional model parameters.

The following considerations uniquely identify model (3):

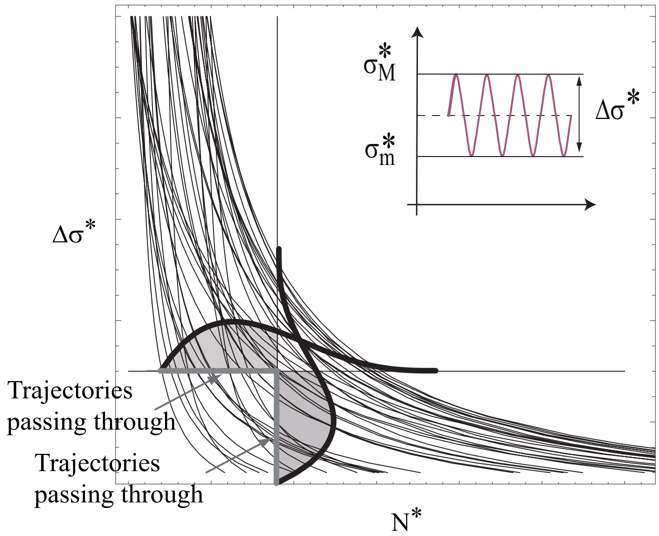

Fig. 1 Random S-N curves associated with different random pieces and illustration of the compatibility condition.

1. **Weakest link principle**: The fatigue lifetime of a longitudinal element is the minimum fatigue life of its constituent pieces.
2. **Stability**: The selected family of distributions must be valid for all possible specimen lengths.
3. **Limit behavior**: To include the extreme case of subdividing a piece in infinitely many small size pieces, the family of distribution functions must be an asymptotic family (see Galambos (1987) and Castillo (1988)).
4. **Limited range**: The involved non-dimensional variables, N^* and $\Delta\sigma^*$, have a finite lower end, which must coincide with the theoretical lower end of the selected cdf.
5. **Compatibility**: In the $S-N$ field, the cumulative distribution function of the lifetime given stress range, $E(N^*;\Delta\sigma^*)$, should be compatible with the cumulative distribution function of the stress range given lifetime, $F(\Delta\sigma^*;N^*)$, that is,

$$E(N^*;\Delta\sigma^*) = F(\Delta\sigma^*;N^*). \tag{4}$$

   Figure 1, where the curves represent the $S-N$ behavior of different specimens, shows that any curve passing through the left part of the horizontal gray segment must also pass trough the lower part of the vertical gray segment in the figure. This implies that the shadowed areas, which represent probabilities, must be equal, that is, Equation (4) must hold.

The physical meaning of the different parameters (see Figure 2) are the following:

B: threshold value of log-lifetime.
C: endurance limit (logarithm of $\Delta\sigma$).
λ: parameter defining the position of the corresponding zero-percentile hyperbola.
δ: Weibull scale factor.

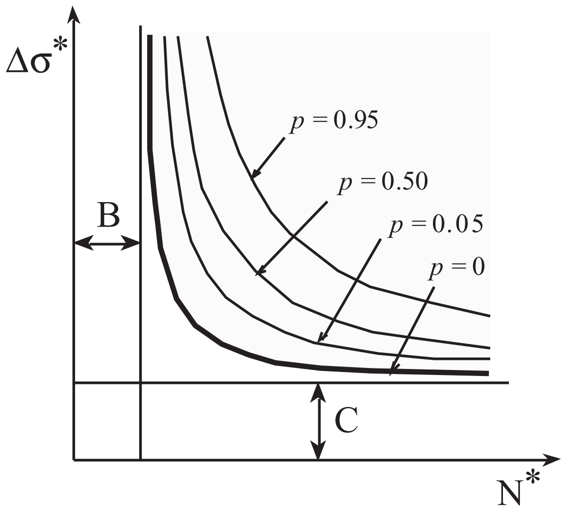

Fig. 2 Percentiles curves representing the relationship between lifetime, N^*, and stress range, $\Delta\sigma^*$, in the $S-N$ field for the fatigue model (3).

β: Weibull shape parameter of the cdf in the $S-N$ field.

Note that parameter C defines the vertical variation of data, parameters B, δ and β define the horizontal variation of data, and λ defines both horizontal and vertical variations.

Note also that parameters B, C and λ are parameters constrained by the data values.

As it is shown above, the five parameters of the model (B, C, λ, δ, β) are of different nature, are can be treated differently in a natural way using the Benders decomposition algorithm.

2.2 Parameter estimation

In this section we assume that we have a sample $\{(\Delta\sigma_i, N_i)|i = 1, 2, \cdots, n\}$ of independent values obtained from a set of experimental tests.

Due to the difficulty of estimating the five parameters in a single process and to the fact that parameters (a) B and C, (b) λ, and (c) δ and β, can be considered as three different types of parameters, several authors have suggested estimating model (3) based on two steps. First the threshold parameters B and C are estimated. Then, the non-dimensional values N^* and $\Delta\sigma^*$ can be calculated and the parameters of the Weibull model λ, β, and δ are estimated. This two-step procedure is explained below.

2.2.1 Estimation of the threshold values

Since the mean of a Weibull $W(\lambda, \delta, \beta)$ distribution in (3) is $\mu = \lambda + \delta\Gamma(1 + 1/\beta)$, we have:

$$E[\log N|(\log \Delta\sigma - C)] = B + \frac{K}{(\log \Delta\sigma - C)}, \tag{5}$$

where

$$K = \lambda + \delta\Gamma[1 + 1/\beta].$$

Equation (5) suggests estimating B and C by:

$$\underset{B,C}{\text{Minimizing}} \sum_{i=1}^{n} \left(\log N_i - B - \frac{K}{(\log \Delta\sigma_i - C)} \right)^2 \tag{6}$$

subject to

$$C \leq \min_i (\log \Delta\sigma_i) \tag{7}$$

$$B \leq \min_i (\log N_i). \tag{8}$$

Constraints (7) and (8) are included to guarantee that the values B and C are valid threshold values for all data points.

2.2.2 Estimation of the Weibull parameters

Once B and C have been estimated, all the data points can be pooled together by calculating the values of

$$V_i = (\log N_i - B)(\log \Delta\sigma_i - C) = N_i^* \Delta\sigma_i^*,$$

to estimate δ, β and λ, since they all follow a Weibull distribution $W(\lambda, \delta, \beta)$.

Several methods have been proposed for estimating the parameters of the Weibull distribution (see references in Castillo and Hadi (1994)). Jenkinson (1969) uses the method of sextiles. The maximum likelihood method (ML) has been considered by Jenkinson (1969) and Prescott and Walden (1980, 1983). Smith (1985) considers the applicability of ML and discusses non-regular cases. The maximum likelihood estimates (MLE) require numerical solutions, and for some samples the likelihood may not have a local maximum. Furthermore, for $\beta < 1$, the likelihood can be made infinite and hence the MLE does not exist. Hosking et al (1985) suggest estimating the parameters and quantiles by probability-weighted moments (PWM), introduced by Greenwood et al (1979). They find that PWM outperform the ML method in many cases. Hosking et al (1985), however, consider only cases where the shape parameter β lies within the range $\beta < 2$ because it has been observed in practice that β usually lies in this range. While the PWM method performs quite admirably within the above restricted range of β, it presents problems outside this range.

The variances of these estimates and confidence intervals for the corresponding parameter or quantile values can be obtained using methods such as the jackknife and the bootstrap methods (Efron (1979), Diaconis and Efron (1983), Efron and Tibshirami (1993), Davison and Hinkley (1997), and Chernick (1999)).

It is important to emphasize that the above two-step procedure does not necessarily identify the optimal solution of the original problem. This is a consequence of splitting the solution procedure in two independent steps. To achieve the optimal solution, a process that iteratively repeats the two-step procedure is necessary. However, such an iterative process is essentially heuristic and its convergence is by no means guaranteed.

3 The proposed estimation methods and Benders decomposition schemes

In this section, we propose two different five-parameter estimation methods based on Benders decomposition.

3.1 Parameter estimation based on maximum likelihood

In model (3) five parameters B, C, λ, δ and β need to be estimated. To this end, we will use firstly a maximum likelihood method, for which the best parameter estimates maximize the likelihood

$$\begin{aligned}\ell(B,C,\lambda,\delta,\beta) = &-\sum_{i=1}^{n}\left[\frac{(\log N_i - B)(\log \Delta\sigma_i - C) - \lambda}{\delta}\right]^{\beta} \\ &+(\beta-1)\sum_{i=1}^{n}\log\left[\frac{(\log N_i - B)(\log \Delta\sigma_i - C) - \lambda}{\delta}\right] \\ &+n\log\beta - n\log\delta + \sum_{i=1}^{n}\log(\log \Delta\sigma_i - C), \end{aligned} \tag{9}$$

where $(N_i, \Delta\sigma_i); i = 1, 2, \ldots, n$ is the set of data points resulting from laboratory tests.

Thus, to estimate the model parameters we need to solve the following optimization problem

$$\underset{B,C,\lambda,\delta,\beta}{\text{Maximize}} \quad \ell(B,C,\lambda,\delta,\beta) \tag{10}$$

subject to

$$\lambda \le \min_{i=1,n} (\log N_{(i)} - B)(\log \Delta\sigma_{(i)} - C) \tag{11}$$

$$B \le \min_{i=1,n} \log N_i \tag{12}$$

$$C \le \min_{i=1,n} \log \Delta\sigma_i, \tag{13}$$

which is a nonlinear optimization problem with a nonlinear constraint (11) and upper bounds for the threshold values B and C.

To estimate the Weibull parameters λ, δ and β, a wide range of methods is available. However, it is well known that estimation of λ might lead to unbounded problems, which have been referred to in the existing literature (see Castillo et al (1985)). On the other hand, we have very reliable and robust methods for estimating δ and β. Consequently, we divide the five optimization variables in three sets:

1. Threshold variables B and C, which can be considered as complicating variables, i.e. if fixed they lead to simpler problems.
2. Variable λ which, for fixed values of the complicating variables and using a two parameter Weibull estimation method, can be easily solved using a bisection method.
3. Weibull variables δ and β which, for fixed values of B, C and λ, well-behaved and robust estimation methods exist.

Thus, we use a standard maximum likelihood estimation method for a two-parameter Weibull distribution, that solves the subproblem

$$\underset{\delta,\beta}{\text{Maximize}}\ \ell(B_0, C_0, \lambda_0, \delta, \beta) \tag{14}$$

where B_0, C_0 and λ_0 are fixed.

We can easily evaluate the sensitivities of the optimal value of Problem (14) with respect to B, C and λ using the following theorem (see Castillo et al (2006) or Castillo et al (2007a)).

Theorem 1 (Objective function sensitivities with respect to parameter $\boldsymbol{a}$) *If the optimization problem*

$$\underset{\boldsymbol{x}}{\textit{Minimize}}\ z_P = f(\boldsymbol{x}, \boldsymbol{a}) \tag{15}$$

subject to

$$\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{a}) = \boldsymbol{b} : \boldsymbol{\lambda} \tag{16}$$

$$\boldsymbol{g}(\boldsymbol{x}, \boldsymbol{a}) \leq \boldsymbol{c} : \boldsymbol{\mu}, \tag{17}$$

has an regular optimum at $\boldsymbol{x}^*$, no degenerate inequality constraints exist, and f, $\boldsymbol{h}$ and $\boldsymbol{g}$ are regular enough, then, the sensitivity of the objective function with respect to the components of the parameter $\boldsymbol{a}$ is given by

$$\frac{\partial z_P^*}{\partial \boldsymbol{a}} = \nabla_{\boldsymbol{a}} \ell(\boldsymbol{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}), \tag{18}$$

which is the gradient vector of the Lagrangian function

$$\ell(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = f(\boldsymbol{x}, \boldsymbol{a}) + \boldsymbol{\lambda}^T(\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{a}) - \boldsymbol{b}) + \boldsymbol{\mu}^T(\boldsymbol{g}(\boldsymbol{x}, \boldsymbol{a}) - \boldsymbol{c}) \tag{19}$$

with respect to $\boldsymbol{a}$ evaluated at the optimal solution $\boldsymbol{x}^*, \boldsymbol{\lambda}^*$, and $\boldsymbol{\mu}^*$.

Using this theorem, we obtain

$$\begin{aligned}
\left.\frac{\partial \ell^*}{\partial B}\right|_{B=B_0;C=C_0} &= \sum_{i=1}^{n} \frac{\beta}{\delta}\left[\frac{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda}{\delta}\right]^{\beta-1} (\log \varDelta\sigma_i - C) \\
&\quad - \sum_{i=1}^{n} \frac{(\beta-1)(\log \varDelta\sigma_i - C)}{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda} \qquad (20)\\
\left.\frac{\partial \ell^*}{\partial C}\right|_{B=B_0;C=C_0} &= \sum_{i=1}^{n} \frac{\beta}{\delta}\left[\frac{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda}{\delta}\right]^{\beta-1} (\log N_i - B) \\
&\quad - \sum_{i=1}^{n} \frac{(\beta-1)(\log N_i - B)}{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda} - \sum_{i=1}^{n} \frac{1}{\log \varDelta\sigma_i - C} \qquad (21)\\
\left.\frac{\partial \ell^*}{\partial \lambda}\right|_{B=B_0;C=C_0} &= \sum_{i=1}^{n} \frac{\beta}{\delta}\left[\frac{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda}{\delta}\right]^{\beta-1} \\
&\quad - \sum_{i=1}^{n} \frac{\beta-1}{(\log N_i - B)(\log \varDelta\sigma_i - C) - \lambda} \qquad (22)
\end{aligned}$$

where ℓ^* refers to the optimal objective function of subproblem (14).

Note that for fixed values of the threshold variables $B = B_0$ and $C = C_0$ (complicating variables), the optimal values of variable λ, δ, and β can be easily obtained using problem (14), which hereinafter is denominated "subproblem", and the bisection method. The aim is to calculate the value of $\lambda = \lambda_0$ that makes the derivative (22) to be zero, i.e.:

$$\begin{aligned}\frac{\partial \ell^*}{\partial \lambda} &= \sum_{i=1}^{n} \frac{\beta}{\delta}\left[\frac{(\log N_i - B_0)(\log \Delta\sigma_i - C_0) - \lambda_0}{\delta}\right]^{\beta-1} \\ &\quad - \sum_{i=1}^{n} \frac{\beta - 1}{(\log N_i - B_0)(\log \Delta\sigma_i - C_0) - \lambda_0} = 0, \qquad (23)\end{aligned}$$

and considering the constraint:

$$\lambda \leq \min_{i=1,n} (\log N_{(i)} - B_0)(\log \Delta\sigma_{(i)} - C_0). \qquad (24)$$

Since for fixed values of the complicating variables B and C, a robust estimation method for λ, δ, and β (non complicating variables) is proposed, problem (10)-(13) has the appropriate structure to apply the Benders decomposition advantageously. The aim is to reproduce the objective function as a function solely of the complicating variables.

The resulting objective function $\ell^*(B, C)$ of the subproblem (14) and equation (23) is a lower bound ℓ_{down} of the optimal objective function value because the subproblem (14) is more constrained than the original one (10)-(13). The information obtained solving the subproblems allows us reproducing more and more accurately the original problem. Moreover, if the objective function $\ell(B, C)$ is concave in the feasibility region, the following *master* problem approximates from above the original one:

$$\underset{\alpha, B, C}{\text{Maximize}}\ \alpha \qquad (25)$$

subject to

$$\begin{aligned}\alpha &\leq \ell^{(\nu)} + \frac{\partial \ell^{(\nu)}}{\partial B}\left(B - B^{(\nu)}\right) + \frac{\partial \ell^{(\nu)}}{\partial C}\left(C - C^{(\nu)}\right) && (26)\\ B &\leq \min_{i=1,n} \log N_i && (27)\\ C &\leq \min_{i=1,n} \log \Delta\sigma_i, && (28)\end{aligned}$$

which is a linear problem easily solvable using the simplex algorithm.

The first constraint of the problem above is called a Benders cut and the problem itself is denominated master problem. The optimal objective function value of this problem is an upper bound of the optimal objective function value of the original problem because problem (25)-(28) is a relaxation of the original problem. The solution of this master problem provides new values for the complicating variables B, C that are used for solving the subproblem again. Using the new information provided by those subproblems is possible to generate additional Benders cuts:

$$\alpha \leq \ell^{(l)} + \frac{\partial \ell^{(l)}}{\partial B}\left(B - B^{(l)}\right) + \frac{\partial \ell^{(l)}}{\partial C}\left(C - C^{(l)}\right);\ l = 1, \ldots, \nu, \qquad (29)$$

which, using information from previous ν iterations, allows us formulating a more accurate master problem that provides new values of complicating variables. The procedure continues until upper and lower bounds of the objective function optimal value are close enough.

An additional advantage of considering the Benders decomposition using two complicating variables is that it allows the graphical visualization of the objective function $\ell(B, C)$.

3.2 Computational issues

Although the parameter estimation of the five parameter fatigue model may look a simple problem which can be solved using any non-linear optimization routine, it presents many numerical problems. For this reason, using the method proposed in the previous subsection several computational issues are discussed:

1. Complicating variables B and C are horizontal and vertical asymptotes, respectively, as shown in Figure 2. Since the target of the Benders decomposition is to reproduce the function $\ell(B, C)$, additional and more constrained upper and lower bounds to (27) and (28) are given:
$$\min_{i=1,n} \log N_i - kr_N \leq B \leq \min_{i=1,n} \log N_i - 0.05 r_N \tag{30}$$
$$\min_{i=1,n} \log \Delta\sigma_i - kr_{\Delta\sigma} \leq C \leq \min_{i=1,n} \log \Delta\sigma_i - 0.05 r_{\Delta\sigma} \tag{31}$$
where k is a positive constant, $r_N = \max_{j=1,n} \log N_j - \min_{i=1,n} \log N_i$ is the range of the data lifetime logarithm, and $r_{\Delta\sigma} = \max_{l=1,n} \log \Delta\sigma_l - \min_{i=1,n} \log \Delta\sigma_i$ is the range of the data stress logarithm. This allows reproducing a concave envelope of the objective function over a defined rectangle, which corresponds to the master feasibility region (see Figure 3).
Note that from the practical point of view a possible initial value of constant k is 2, which in case the complicating variable bounds became active, is increased by one unit at a time.
2. For given values of the complicating variables, the remainder parameters λ, δ, and β must be obtained. For obtaining λ, the bisection method is used. This method requires two values λ^{up} and λ^{lo} so that the corresponding derivatives (23) change sign. A good starting value for λ^{up} is given by (24), i.e.
$$\lambda^{\text{up}} = \min_{i=1,n} (\log N_{(i)} - B_0)(\log \Delta\sigma_{(i)} - C_0) - 10^{-6}.$$
The lower bound is
$$\lambda^{\text{lo}} = \min_{i=1,n} (\log N_{(i)} - B_0)(\log \Delta\sigma_{(i)} - C_0) - k_2 \sigma_\lambda,$$
where σ_λ is the standard deviation of the values $(\log N_{(i)} - B_0)(\log \Delta\sigma_{(i)} - C_0);\ \forall i = 1, \ldots, n$. Note that k_2 starts from 1 an increases 1 unit at a time until the derivative changes sign with respect to the derivative associated with the upper bound. If for a large enough k_2-value, there is no change of sign, which means that with the actual values of the complicating variables the λ-value is unbounded, thus alternative values of the complicating variables are selected randomly within the master feasibility region.

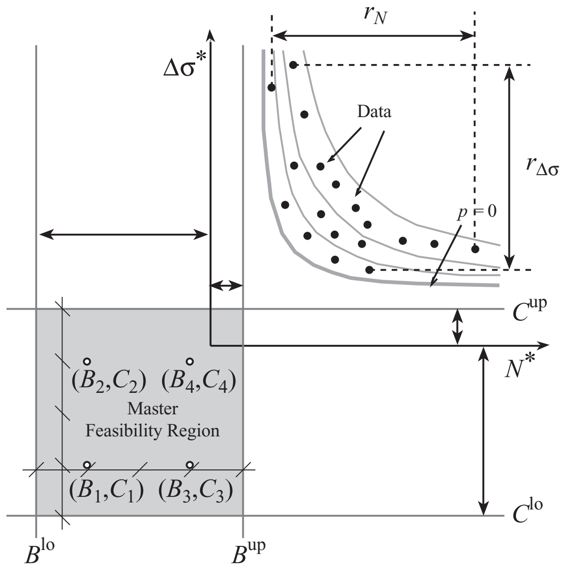

Fig. 3 Initial bounds for the complicating variables corresponding to the master feasibility region.

3. Since the purpose of the Benders decomposition is to create a concave envelope, the optimal values of the non-complicating variables for four points (B_1, C_1), (B_2, C_2), (B_3, C_3), and (B_4, C_4) distributed over the master feasibility region, as shown in Figure 3, are obtained and used to construct four initial Bender cuts.

3.3 Maximum Likelihood Algorithm

Benders decomposition to estimate the parameters of a fatigue model corresponding to the $S - N$ field, i.e. for solving problem (10)-(13), works as follows.

Input. The data set $\{(\Delta\sigma_i, N_i);\ i = 1, 2, \dots, n\}$, a small tolerance value ε to control convergence and initial value of constant $k = 2$.
Output. The solution of problem (10)-(13).

- **Step 0: Initialization.** Set $\nu = 1$, $B^{(\nu)} = B_1$, $C^{(\nu)} = C_1$, $\ell^{(\nu)}_{\text{up}} = \infty$.
  Step 1: Subproblem solution. Get the non-complicating variables λ, δ and β using the bisection method and subproblem (14).
  Update the objective function lower bound, $\ell^{(\nu)}_{\text{down}} = \ell^{(\nu)}(B^{(\nu)}, C^{(\nu)})$.
- **Step 2: Convergence check.** If $\nu \leq 4$ or $||\ell^{(\nu)}_{\text{up}} - \ell^{(\nu)}_{\text{down}}|| \leq \varepsilon$, go to Step 3, otherwise the solution with a level of accuracy ε of the objective function is the current one, then check if the optimal complicating variables $B^{(\nu)}$ or $C^{(\nu)}$ belong to the boundary of the master feasibility region, if they do update the k-value $k \leftarrow k + 1$ and go to Step 0 restarting the process again, otherwise stop.
- **Step 3: Master problem solution.** Calculate the derivatives with respect to the complicating variables using equations (20) to (21). Update the iteration counter,

$\nu \leftarrow \nu + 1$ and if $\nu > 4$ solve the master problem (25)-(28), otherwise use the next initial point within the feasibility region $B^{(\nu)} = B_{\nu-1}$, $C^{(\nu)} = C_{\nu-1}$, and set $\alpha^{(\nu)} = \infty$.
Note that at every iteration a new constraint is added. In case $\nu > 4$, the solution of the master problem provides $B^{(\nu)}, C^{(\nu)}$, and $\alpha^{(\nu)}$.
Update objective function upper bound, $\ell_{\text{up}}^{(\nu)} = \alpha^{(\nu)}$. The algorithm continues in Step 1.

3.4 Benders Decomposition Convergence Analysis

The proposed algorithm provides the solution of the problem in a finite number of iterations whenever the objective function is concave, otherwise, the procedure fails to converge (Geoffrion (1972)).

By definition, a function $F(\boldsymbol{x})$ is concave if and only if $F(\boldsymbol{y}) \leq F(\boldsymbol{x}) + \nabla F(\boldsymbol{x})^T(\boldsymbol{y} - \boldsymbol{x})$ holds for all $\boldsymbol{x}$, $\boldsymbol{y} \in \text{domain}F(\boldsymbol{x})$. This condition is equivalent to constraint (29), then if $l \to \infty$ this constraint reproduces exactly the original objective function in the optimal solution neighborhood, which means that both problems are equivalent if and only if function $F(\boldsymbol{x})$ is concave. In that case the original problem (10)-(13) and the master problem (25)-(28) are equivalent and converge to the same solution.

3.5 Parameter estimation based on least squares and the Benders decomposition

Alternatively, to estimate the model parameters in model (3) we can minimize the sum of squares of the differences between the actual and the predicted values of $\log N_i$, that is, we can solve the following optimization problem

$$\underset{\delta,\beta,\lambda,B,C}{\text{Minimize}} \quad Q = \sum_{i=1}^{n} \left(\log N_i - B - \frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{\log \Delta\sigma_i - C} \right)^2 \tag{32}$$

subject to

$$\lambda \leq \min_{i=1,n} (\log N_i - B)(\log \Delta\sigma_i - C) \tag{33}$$

$$B \leq \min_{i=1,n} \log N_i \tag{34}$$

$$C \leq \min_{i=1,n} \log \Delta\sigma_i, \tag{35}$$

where $p_i = i/(m+1)$ is a plotting position (see Castillo (1988) or Castillo et al (2005b)) and m is the number of specimens at a given level of $\Delta\sigma$. Note that problem (32)-(35) is a nonlinear optimization problem with a nonlinear constraint and upper bounds for the threshold values B and C.

Analogously as with the maximum likelihood estimation method, if B and C are considered as complicating variables and fixed to given values ($B = B_0$; $C = C_0$), we can easily estimate λ, δ and β, by solving the problem:

$$\underset{\lambda,\delta,\beta}{\text{Minimize}} \ Q = \sum_{i=1}^{n} \left(\log N_i - B_0 - \frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{\log \Delta\sigma_i - C_0} \right)^2 \tag{36}$$

subject to

$$\lambda \leq \min_{i=1,n} (\log N_i - B)(\log \Delta\sigma_i - C), \tag{37}$$

which is also a nonlinear problem with an upper bound for one of the variables. This problem can be easily solved using any nonlinear optimization routine or using the Newton method. For this particular case we have used a trust region reflective algorithm under Matlab with upper and lower bounds through the function `fmincon`. For details about the method see Coleman and Li (1994) and Coleman and Li (1996).

Using the sensitivity analytical expression in Castillo et al (2005a) or Conejo et al (2006), we can easily evaluate the sensitivities of the optimal value of Problem (36)-(37) with respect to B and C, resulting

$$\frac{\partial Q^*}{\partial B} = -2\sum_{i=1}^{n}\left(\log N_i - B - \frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{\log \Delta\sigma_i - C}\right) \tag{38}$$

$$\frac{\partial Q^*}{\partial C} = -2\sum_{i=1}^{n}\left(\log N_i - B - \frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{\log \Delta\sigma_i - C}\right)\frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{(\log \Delta\sigma_i - C)^2}, \tag{39}$$

where Q^* refers to the optimal objective function value in (36).

Alternatively, the derivative of the objective function in (36)-(37) with respect to the complicating variables can be obtained if we rewrite the problem as

$$\underset{\lambda,\delta,\beta,B,C,}{\text{Minimize}} \sum_{i=1}^{n}\left(\log N_i - B - \frac{\lambda + \delta(-\log(1-p_i))^{1/\beta}}{\log \Delta\sigma_i - C}\right)^2 \tag{40}$$

subject to

$$\lambda \leq \min_{i=1,n} (\log N_i - B)(\log \Delta\sigma_i - C), \tag{41}$$

$$B = B_0 \ : \ \mu_1 \tag{42}$$

$$C = C_0 \ : \ \mu_2 \tag{43}$$

$$\lambda = \lambda_0 \ : \ \mu_3, \tag{44}$$

where B and C are used as artificial variables, which are fixed by constraints (42)-(44) to their corresponding values in order to obtain the associated sensitivities $\frac{\partial Q^*}{\partial B}$, $\frac{\partial Q^*}{\partial C}$ and $\frac{\partial Q^*}{\partial \lambda}$, as the values of the dual variables μ_1, μ_2 and μ_3, respectively. Thus, this trick allows us obtaining the sensitivities (38)-(39) directly.

Problem (32)-(35) has the appropriate structure to apply the Benders decomposition advantageously. The aim is to reproduce the objective function as a function solely of the complicating variables. The problem (36)-(37) above is denominated the subproblem, and its solution provides values for the non complicating variables, λ, δ and β.

The resulting objective function $Q^*(B, C)$ of subproblem (36)-(37) is an upper bound Q_{up} of the optimal objective function value because the subproblem (36)-(37) is more constrained than the original one, (32)-(35). The information obtained solving the subproblems allows us reproducing more and more accurately the original problem.

Moreover, if the objective function in (32) is convex, the following *master* problem approximates from below the original one:

$$\underset{\alpha, B, C}{\text{Minimize}}\ \alpha \tag{45}$$

subject to

$$\alpha \geq Q^{(l)} + \frac{\partial Q^{(l)}}{\partial B}\left(B - B^{(l)}\right) + \frac{\partial Q^{(l)}}{\partial C}\left(C - C^{(l)}\right);\ l = 1, \dots, \nu \tag{46}$$

$$B \leq \min_{i=1,n} \log N_i \tag{47}$$

$$C \leq \min_{i=1,n} \log \varDelta\sigma_i, \tag{48}$$

where ν is an iteration counter. Note the this problem is linear and easily solvable using the simplex method.

It is relevant to note that the Benders iterative procedure is guaranteed to converge to the optimal solution of the original problem under convexity assumptions of the objective function of the original problem projected on the subspace of the complicating variables. In contrast with the heuristic iterative process mentioned in Section 2 and commonly used, Benders decomposition is not heuristic and its convergence is guaranteed under some reasonable assumptions. Nevertheless, an analogously to the maximum likelihood case, the computational issues 1 and 3 are also considered to improve results and ensure convergence.

3.6 Least Square Algorithm

Benders decomposition to estimate the parameters of a fatigue model corresponding to the $S - N$ field, i.e. for solving problem (32)-(35), works as follows.

Input. The data set $\{(\varDelta\sigma_i, N_i);\ i = 1, 2, \dots, n\}$, a small tolerance value ε to control convergence and initial value of constant $k = 2$.
Output. The solution of problem (32)-(35).

- **Step 0: Initialization.** Set $\nu = 1$, $B^{(\nu)} = B_1$, $C^{(\nu)} = C_1$, $Q^{(\nu)}_{\text{down}} = 0$.
  Step 1: Subproblem solution. Obtain the non-complicating variables λ, δ and β solving subproblem (36)-(37).
  Update the objective function upper bound, $Q^{(\nu)}_{\text{up}} = Q^{(\nu)}(B^{(\nu)}, C^{(\nu)})$.
- **Step 2: Convergence check.** If $\nu \leq 4$ and $||Q^{(\nu)}_{\text{up}} - Q^{(\nu)}_{\text{down}}|| \leq \varepsilon$ go to Step 3, otherwise the solution with a level of accuracy ε of the objective function is the current one, then check if the optimal complicating variables $B^{(\nu)}$ or $C^{(\nu)}$ belong to the boundary of the master feasibility region, if they do update the k-value $k \leftarrow k + 1$ and go to Step 0 restarting the process again, otherwise stop.
- **Step 3: Master problem solution.** Calculate the derivatives with respect to the complicating variables using equations (38)-(39). Update the iteration counter, $\nu \leftarrow \nu + 1$ and if $\nu > 4$ solve the master problem (45)-(48), otherwise use the next initial point within the feasibility region $B^{(\nu)} = B_{\nu-1}$, $C^{(\nu)} = C_{\nu-1}$, and set $\alpha^{(\nu)} = \infty$.
  Note that at every iteration a new constraint is added. In case $\nu > 4$, the solution of the master problem provides $B^{(\nu)}, C^{(\nu)}$, and $\alpha^{(\nu)}$.

Table 2 Holmen data.

$\Delta\sigma$	Lifetime (thousands of cycles)							
0.95	0.037	0.072	0.074	0.076	0.083	0.085	0.105	0.109
	0.120	0.123	0.143	0.203	0.206	0.217	0.257	
0.90	0.201	0.216	0.226	0.252	0.257	0.295	0.311	0.342
	0.356	0.451	0.457	0.509	0.540	0.680	1.129	
0.825	1.246	1.258	1.460	1.492	2.400	2.410	2.590	2.903
	3.330	3.590	3.847	4.110	4.820	5.560	5.598	
0.75	6.710	9.930	12.600	15.580	16.190	17.280	18.620	20.300
	24.900	26.260	27.940	36.350	48.420	50.090	67.340	
0.675	103	280	340	367	486	659	896	1242
	1250	1330	1400	1459	3295	12709	14373	

Update objective function lower bound, $Q^{(\nu)}_{\text{down}} = \alpha^{(\nu)}$. The algorithm continues in Step 1.

4 Example

In this section, the Holmen (1979) fatigue data is used to illustrate the methods proposed in previous sections. The Holmen data consists of 75 fatigue tests using specimens of identical length, at 5 different stress levels as shown in Table 2. The estimation of the parameters has been carried out using the algorithms described in Sections 3.3 and 3.6. Note that they involve a maximization and a minimization problem, respectively.

The iterative method converges in seconds and takes 24 iterations in a common portable computer to converge within an admissible tolerance of $\varepsilon = 10^{-6}$, providing the following final maximum likelihood parameter estimates:

$$B^* = -16.4463; \quad C^* = -0.93911; \quad \lambda^* = 11.2133; \quad \delta^* = 1.7754; \quad \beta^* = 3.4677.$$

The optimal likelihood objective function is $\ell^* = -79.0064$.

Similarly, the final least squares solution is:

$$B^* = -17.3587; \quad C^* = -0.97727; \quad \lambda^* = 12.8918; \quad \delta^* = 1.5341; \quad \beta^* = 2.4167.$$

The optimal objective function value is $Q^* = 7.2684$. The method converges in seconds taking 32 iterations to converge within an admissible tolerance of $\varepsilon = 10^{-6}$.

Note that although it takes 24 and 32 iterations to achieve the prescribed tolerance, respectively, in both cases a visual inspection allows to check that a good approximation is attained after 9 and 12 iterations.

To illustrate the quality of both fits, Figure 4 shows the percentile curves (1%, 5%, 50%, 95% and 99%) and the data points, showing a very good fit.

Figure 5 illustrates the convergence of the fitting processes by showing the lower ℓ_{down} and upper ℓ_{up} bounds corresponding to all iterations. Note that for the maximum likelihood case (left subplot), the master problem solution corresponds to the upper bound, which decreases monotically until convergence is achieved, however the lower bound presents an oscillating behavior which is typical for the Benders approach. On the contrary, for the least squares regression case (right subplot), the master problem solution corresponds to the lower bound, which increases monotically until convergence. This case corresponds to a minimization problem.

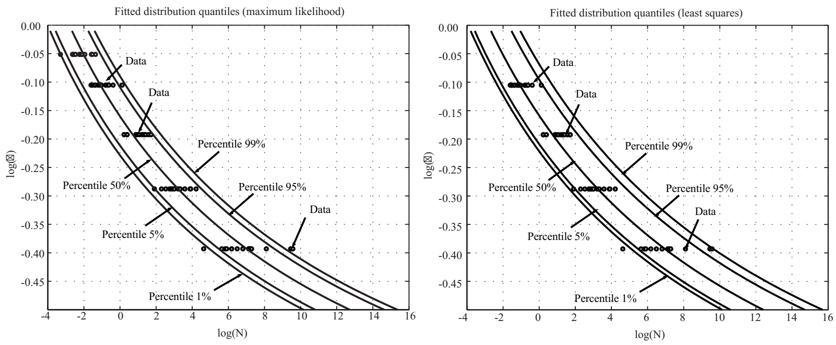

Fig. 4 Percentile (1%, 5%, 50%, 95% 1nd 99%) curves associated with the fitted model together with the data points. The left subplot is the one associated with the maximum likelihood estimates, and the right subplot that corresponding to the least squares estimates.

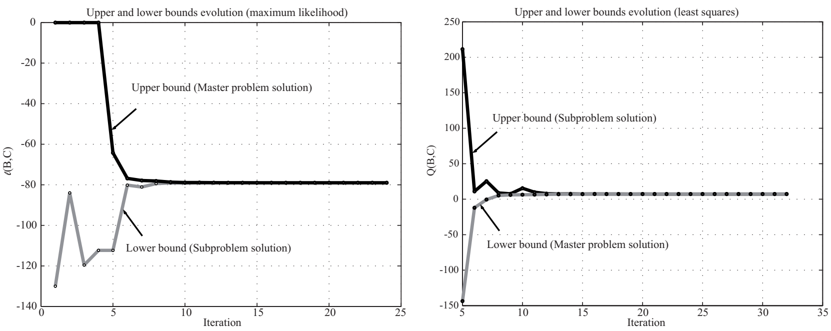

Fig. 5 Illustration of the convergence process showing the upper and lower bounds.The left subplot is the one associated with the maximum likelihood estimates, and the right subplot that corresponding to the least squares estimates.

Finally, Figures 6 and 7 provide two-dimensional plots of the objective functions as a function of the complicating variables B and C, and two vertical cross sections for every case (maximum likelihood and least squares regression) at the optimum, respectively. Note that both functions are locally concave and convex, respectively, over the master feasibility region. This justifies the well functioning of the method.

5 Conclusions

Thus paper uses Benders' decomposition to tackle a fatigue model parameter estimation problem using two different approaches, maximum likelihood and least squares regression. The main conclusions that can be obtained from this paper are:

1. The use of Benders decomposition method arises in a natural way in the case of the fatigue problem because the five parameters of the model considering their physical meaning and their data dependence can be divided in two groups:
   (a) the two parameters B and C which define the regression trend (model location) and are constrained by data values.

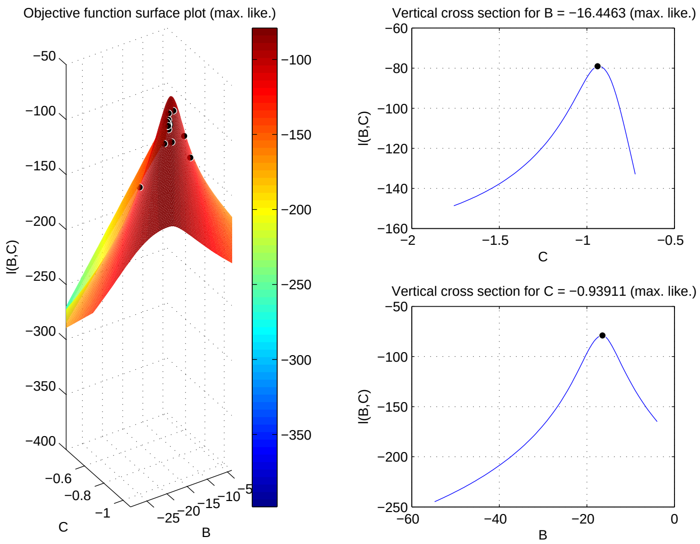

Fig. 6 Objective function (α) surface plot as a function of the complicating variables B and C, and vertical cross sections of α at the optimal solution for the maximum likelihood case.

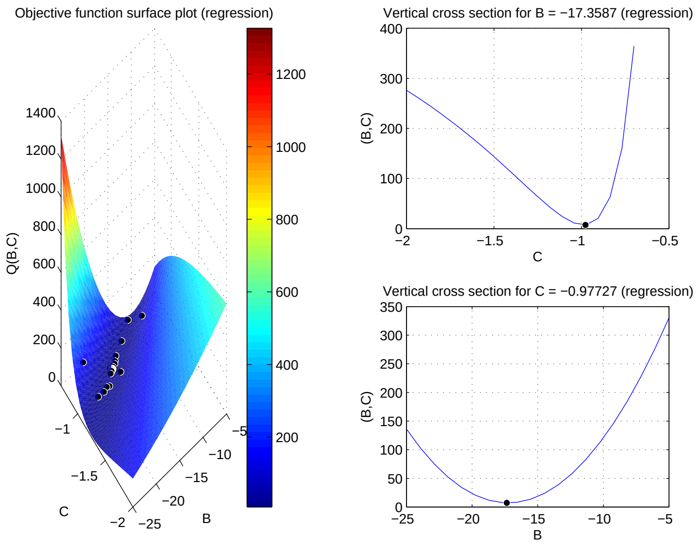

Fig. 7 Objective function (α) surface plot as a function of the complicating variables B and C, and vertical cross sections of α at the optimal solutions for the least squares regression case.

(b) the three Weibull parameters λ, δ and β.

Considering B and C complicating variables renders a simple linear master problem and an easy to solve subproblem. In contrast, solving directly the original problem generally results in numerically ill-conditioning.

2. The proposed two Benders decomposition implementations are both efficient and robust, achieving the optimal solutions in small computational time.
3. The partial derivatives of the objective function with respect to parameters B, C and λ, which are required to build the Benders cuts and the bisection method, can be very easily obtained in closed form.
4. Converting the parameters B, C and λ into artificial variables and adding the corresponding constraints to fix them to their values permits obtaining appropriate derivatives as dual variable values.
5. The proposed methods are illustrated using a real-world data set reported by Holmen (1979), showing the appropriate behavior of the proposed methods.

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