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Metropolis-Hastings method for Wohler curve parameter identification

Keywords

Wohler curve, Metropolis-Hastings, probabilistic fatigue

Abstract

In this work, the Metropolis-Hastings sampling technique has been used for the parameter identification of Wohler curve of aluminium alloy 2024-T4. The Metropolis-Hasting algorithm is one of the most widespread Markov chain Monte Carlo methods for posterior distribution estimation, and it is presented with an adaptive formulation to estimate the probability density functions of Wohler parameters. Results are presented in terms of distribution shape and parameter correlations. The information about parameter distributions of Wohler equation is useful to prepare risk analyses based on statistical safe life approach.

1. Introduction

The aim of this work is to apply the consolidated theory of Markov chain Monte Carlo (MCMC) methods to identify the parameters of fatigue curves, commonly defined as $S-N$ ¹ curves or Wohler curves. In this context, data coming from specimen of aluminium alloy 2024-T4 are considered. MCMC methods, differently from other system identification methods that are based on maximum likelihood, allow describing the probability density function (pdf) of the inferred parameters, without any assumption on their shapes. The objective of the work is the investigation of parameter pdf with the Metropolis-Hastings (MH) algorithm, also called Random Walk Metropolis (RWM), with a critical analysis of the obtained results. The paper is organised as follows: section 2 provides a brief

description of the Wohler curve and the mathematical equation used to represent fatigue data. Section 3 describes the fundamentals of Markov chain models and a brief explanation of the Metropolis-Hastings algorithm. The application of the MH algorithm to fatigue data is presented in section 4, describing also the adaptive proposal distribution to avoid the problem of proposal variance selection. Section 5 shows the results with a critical analysis on the estimated parameters, the correctness of the achieved pdf and the comparison with consolidated nonlinear fitting methods. A conclusive section summarizes the work and further developments of this analysis.

2. Wohler curve

In contrast to the static strength, a large scatter characterizes the fatigue limit. As a result, the curves usually employed in fatigue analyses should be described in statistical terms in order to produce reliable results. The most used fatigue curve is the $S-N$ curve or Wohler curve that is able to describe the

¹ The name “ $S-N$ ” comes from the output-input variables describing the mathematical model: S is the applied stress (output of the model) and N is the number of load cycles (input of the model).

three different zones of the diagram load versus number of load cycles: the static or quasi-static loading zone, the finite-life zone and the infinite life zone. The mathematical equation able to describe these three zones is presented in (1) [5], [9]. Obviously, other formulations that are able to describe only one region (zone II) or two regions (zones II and III) of the curve could be implemented in fatigue analyses.

$$S = S_0(1 + A/(N + G))^m \quad (1)$$

where A , G and m are numerical constants depending on the material, S represents stress [MPa], N is the number of load cycles, S_0 represents stress at infinite life [MPa]. *Figure 1* shows the schematic diagram of a typical Wohler curve highlighting the three different regions of quasi-static loading (I), finite life (II) and infinite life (III) of materials.

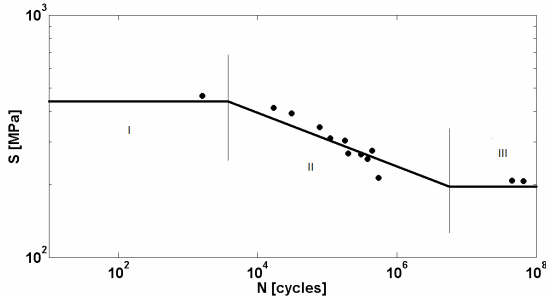


Figure 1. Example of Wohler curve in the ($\log N$, S) plane.

3. Markov Chain model

According to [10], a First-order Markov Chain is a sequence of random variables \square_k (with k belonging to the set of natural numbers) such that the conditional distribution of \square_k (knowing all the discrete values \square_{k-m} with $m \geq 1$) is the same as the conditional distribution of \square_k given only \square_{k-1} (2).

$$P(\vartheta_k | \vartheta_{k-1}, \vartheta_{k-2}, \dots, \vartheta_1) \equiv P(\vartheta_k | \vartheta_{k-1}) \quad (2)$$

The transition kernel K drives the link between two subsequent random variables; it is a conditional probability satisfying the detailed-balance condition or reversibility condition of the chain (3):

$$K(\vartheta_{k-1} | \vartheta_k) f(\vartheta_k) = K(\vartheta_k | \vartheta_{k-1}) f(\vartheta_{k-1}) \quad (3)$$

where $f(\square_k)$ is the stationary probability of the realization \square_k . However, finding the solution of $K(\square_k/\square_{k-1})$ is complicated. The following subsection

presents the MH algorithm accounting for the kernel K satisfying eq. (3).

3.1. Metropolis-Hastings sampling technique for parameter identifications

The Metropolis–Hasting algorithm is historically the first and remains the most important MCMC algorithm. It is usually implemented to estimate parameter pdfs in presence of highly nonlinear functions and non-Gaussian distributions. Additionally, it estimates the noise associated to the observations given as input of the algorithm. It draws a series of dependent samples of the parameters according to the transition kernel K by the decomposition of the transition kernel itself. According to the MH theory, the transition kernel $K(\square_k/\square_{k-1})$ can be split into a proposal distribution q and an acceptance probability α that continue to satisfy (3). The splitting of the transition kernel becomes $K(\square_k/\square_{k-1}) = q(\square_k/\square_{k-1})\alpha(\square_k/\square_{k-1})$. In this way, the detailed balance condition change from (3) to (4), but the stationary distribution $f(\square)$ is still unknown.

$$\begin{aligned} q(\vartheta_{k-1} | \vartheta_k) \cdot \alpha(\vartheta_{k-1} | \vartheta_k) \cdot f(\vartheta_k) \\ = q(\vartheta_k | \vartheta_{k-1}) \cdot \alpha(\vartheta_k | \vartheta_{k-1}) \cdot f(\vartheta_{k-1}) \end{aligned} \quad (4)$$

Let assume a series of independent identically distributed observations y depending on the value of \square through a whatever nonlinear relationship $y = h(\square)$. If the relation $h(\cdot)$ is known, the conditioned probability of \square given the observations y can be evaluated. According to Bayes' rule [1], the conditioned probability $f(\square/y)$ follows the relation (5), where $g(\square)$ is the prior probability of \square . The conditioned pdf can be evaluated by the substitution of $f(\square/y)$ with the likelihood of \square given the observations $\pi(\square/y)$.

$$f(\vartheta | y) \propto f(y | \vartheta) g(\vartheta) \propto \pi(\vartheta | y) g(\vartheta) \quad (5)$$

Starting from equation (4), the acceptance probability $\alpha(\square_k/\square_{k-1})$ is extracted.

$$\begin{aligned} \alpha(\vartheta_k | \vartheta_{k-1}) = \\ \min \left(\frac{\pi(\vartheta_k | y) \cdot g(\vartheta_k) \cdot q(\vartheta_{k-1} | \vartheta_k)}{\pi(\vartheta_{k-1} | y) \cdot g(\vartheta_{k-1}) \cdot q(\vartheta_k | \vartheta_{k-1})}, 1 \right) \end{aligned} \quad (6)$$

It represents the probability to accept the k -th sample of \square given the previous sample \square_{k-1} . For a normally-distributed random noise affecting the observations y , the likelihood of the k -th sample $\pi(\square_k/y)$ reads:

$$\pi(\vartheta_k | y) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-\varphi_y(\vartheta_k)}{2\sigma^2}\right), \quad (7)$$

where $\varphi_y(\square_k)$ is the cost function representing the error between the observation y and the simulation of the system based on the parameter sample \square_k [12], that is $\varphi_y(\square_k)=[y-h(\square_k)]^2$, while σ is the standard deviation of the uncertainty or noise affecting the observations. It is important to consider that σ belongs to the vector of parameter \square_k , thus a sample of σ is generated at each step k . The new state \square_k is accepted with probability $\alpha(\square_k/\square_{k-1})$. This means the sample \square_k is accepted if r (random number sampled from a uniform distribution $U(0,1)$) is less than $\alpha(\square_k/\square_{k-1})$; otherwise it is refused and the current sample remains equal to the previous one \square_{k-1} . At the end of the algorithm, the conditional mean and variance of \square can be evaluated with (8) and (9), respectively.

$$E(\vartheta | y) \approx \frac{1}{N_S - k_0} \sum_{k=k_0+1}^{N_S} \vartheta_k \quad (8)$$

$$V(\vartheta | y) \approx \frac{1}{N_S - k_0} \sum_{k=k_0+1}^{N_S} [\vartheta_k - E(\vartheta | y)]^2 \quad (9)$$

where \square_k are the samples selected from the Markov chain, k_0 is the transient or burn-in period and N_S is the number of selected steps of the Markov chain. Equation (10) represents the posterior distribution of \square estimated from the prior knowledge and the observations y .

$$f(\vartheta | y) \approx p(\mu_{\vartheta|y} = E(\vartheta | y), \sigma_{\vartheta|y}^2 = V(\vartheta | y)) \quad (10)$$

4. Application of MH to fatigue data

4.1. Input: experimental data

Samples of 2024-T4 aluminium alloy for various wrought products at longitudinal direction were obtained from [6] and presented in *Table 1*. The data of stress S with respect to load cycles N represent the input of the MCMC algorithm that is the observations y defined in section 3. *Figure 2* shows the data in the $(\log N, S)$ plane after the conversion² of stress from ksi to the international measure unit MPa.

Table 1. Data for Wohler curve.

² 1 ksi = 6.8948 MPa

sample ID #	# of cycles	Maximum stress [MPa]	sample ID #	# of cycles	Maximum stress [MPa]
1	4637	441	24	305936	265
2	5454	462	25	359308	317
3	7940	510	26	377259	255
4	9928	456	27	412619	328
5	11347	464	28	441700	276
6	15393	447	29	541853	213
7	16890	414	30	1407627	330
8	18943	463	31	1409601	345
9	21926	414	32	2518789	290
10	25836	407	33	6057754	276
11	26880	483	34	7064963	303
12	30703	393	35	9217544	262
13	34775	448	36	10087410	248
14	45705	389	37	11128156	269
15	77741	345	38	13094778	248
16	79503	385	39	16134403	276
17	109715	310	40	22701832	303
18	180577	303	41	40452002	220
19	199939	269	42	45293174	206
20	209976	393	43	56040321	276
21	225370	414	44	56751803	310
22	225771	56	45	65624234	265
23	250953	50	46	95785653	317

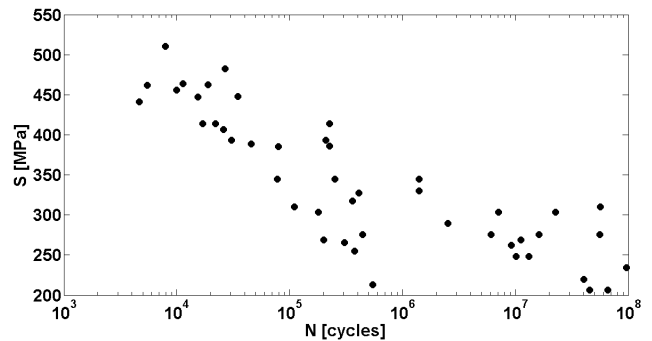


Figure 2. Experimental data in $(\log N, S)$ plane

4.2. Initialization of MH algorithm

As described in section 3, the Metropolis-Hastings algorithm requires the initialization of the objective parameters, a proposal distribution from which samples are drawn, and a prior probability density function. The starting values of the parameters should not influence the algorithm performance. In fact, the MCMC assures the convergence of the chain in a finite number of samples. The advice here is to use reasonable values in order to avoid too many useless samples. Obviously, the prior distribution is connected with the values used to start the algorithm. Since a prior knowledge on the parameter distributions is not available (no expected values nor shape of the pdfs), uniform distributions are selected as prior pdfs of the interested parameters.

Table 2 shows the interested parameters and the

corresponding distributions; the subscripts *low* and *up* means *lower limit* and *upper limit*, respectively. The uncertainty associated to the data (σ) is expressed in logarithmic form because it has to be greater than zero.

A multivariate Gaussian pdf drives the sample drawing (proposal distribution). Since there is no initial correlation between the different parameters, the proposal distribution corresponds to a series of independent normal distributions (11). Heuristic considerations according to the mean values and the limits of the quantities drive the selection of the initial proposal variances.

Table 2. Parameter distributions

\square	prior pdf
A	$U([A_{low}, A_{up}])=U([140, 220])$
G	$U([G_{low}, G_{up}])=U([22000, 40000])$
m	$U([m_{low}, m_{up}])=U([0, 1])$
S_0	$U([S_{0low}, S_{0up}])=U([150, 300])$
$\log \sigma$	$U([\log \sigma_{low}, \log \sigma_{up}])=U([\log(10), \log(100)])$

$$q(\vartheta) = MVN \left(\mu = \begin{bmatrix} \mu_A \\ \mu_G \\ \mu_m \\ \mu_{S_0} \\ \mu_{\log \sigma} \end{bmatrix}, \Sigma = \begin{bmatrix} \sigma_A^2 & 0 & 0 & 0 & 0 \\ 0 & \sigma_G^2 & 0 & 0 & 0 \\ 0 & 0 & \sigma_m^2 & 0 & 0 \\ 0 & 0 & 0 & \sigma_{S_0}^2 & 0 \\ 0 & 0 & 0 & 0 & \sigma_{\log \sigma}^2 \end{bmatrix} \right) \quad (11)$$

where MVN is multivariate normal distribution. The probability density function of the n -dimensional multivariate normal distribution is given by:

$$f(x, \mu, \Sigma) = \frac{1}{\sqrt{\det \Sigma} \cdot (2\pi)^n} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

Although the selection of the starting mean values is not difficult, the proposal variance remains an open issue. Too large a variance produces a high ratio of refused samples over accepted samples, while too small a variance slows down the convergence of the chain.

Consequently, a MH algorithm with adaptive proposal distribution is employed to overcome the problem. The selected adaptive algorithm was initially proposed in [8] used in [2]-[4] for fatigue crack growth analyses. The employment of adaptive proposal distribution avoids the problem reported above on the acceptance ratio of the samples and enhances the convergence properties. The algorithm is able to recursively update the variance of proposal pdf based on the last residuals of the chain.

Nonetheless, the adaptation depends on two parameters, namely the *memory* H and *frequency* U

parameters. The first one defines the number of samples used to calculate the residuals, while the second one governs the frequency of the proposal variance updating procedure. Table 3 shows the pseudo-code of the MH algorithm with adaptive proposal distribution.

Table 3. MH algorithm with adaptive proposal pdf [2]

1. Initialize the parameter vector ϑ_0 according to the proposal PDF.
2. Initialize the likelihood of vector ϑ_0 given the measures y , taking into account the prior pdf.
3. Initialize the matrix of the chain $\theta = [\vartheta_0]$.
4. Set the memory of the proposal H and the frequency parameter U .
5. For $i = 1$ to N_S
- Draw sample $\square_i \sim q(\square) = MVN(\square_{i-1}, \Sigma)$
- Calculate a fictitious stress $S = S(\square_i)$.
- Evaluate the likelihood of the sample given the measure $\pi(\square_i/y)$ according to (7) and the prior probability $g(\square_i)$
- Accept the sample \square_i with probability $\alpha(\square_i/\square_{i-1})$ defined in (6).
- If the remainder of $i/U = 0$
Store the last H residuals of the chain:
$R = res(\theta_H)$
Generate covariance matrix of the proposal:
$\Sigma = cd^2/(H-1) RR^T$
Endif
Endfor
6. Erase the burn-in period and select far-between samples to avoid the possibility of correlated samples from the chain

4.3. Estimation of Wohler curve parameters

The algorithm receives as input the data (N_i, S_i) representing the failure load cycle and the stress applied to the i -th specimen, respectively. The length of the chain is heuristically selected on 50000 samples. The memory and frequency parameters are set equal to 1200, because of the nonlinearity of the Wohler curve, as suggested in [8]. The limits of the prior pdf are selected according to reasonable range of the quantities of interest as well as the first values of the chain (see Table 2). The pdfs of the parameters can be estimated from the resulting samples of the chain, as well as the standard deviation associated to the observations. Figures 3-4 show the posterior distribution of the parameters and noise standard deviation, respectively.

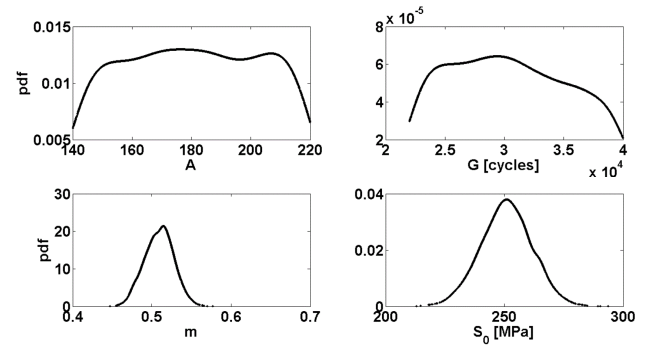


Figure 3. Posterior distributions of parameters.

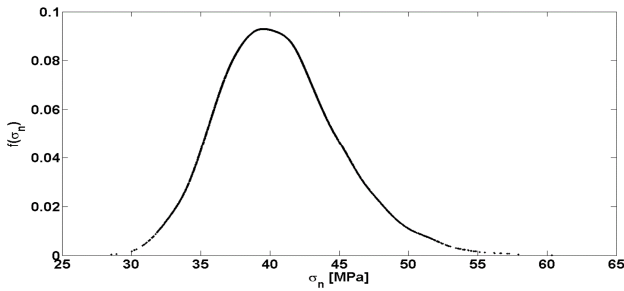


Figure 4. Distribution of noise standard deviation.

4.4. Critical analysis of results

As is clearly visible from *Figure 3*, the two posterior distributions for A and G are close to uniform distributions in the whole range covered by the prior pdf. The result does not change by performing several simulations with different reasonable limits of the prior distributions. This preliminary result shows that the Wohler curve is only slightly affected by the averages of these two parameters.

The exaggerated enlarging of the uniform prior pdf produces unreasonable values for the two parameters, and then the bounds proposed in *Table 4* can be considered reasonable limits for the quantities under investigation. It is clear that MH algorithm can be used as a valid tool for Sensitivity Analysis (SA): the main outcome here is that the used model is more sensitive to m and S_0 parameters than to A and G [7]. Nevertheless, further analyses should be made in order to understand the effects of A and G on the Wohler equation; for instance local & global SA, correlation coefficient methods, ANOVA or Fourier Amplitude Sensitivity Test (FAST) [7].

Table 4. Estimated statistical features of parameters

\square	A	G	m	S_0	σ
μ_{\square}	185	29560	0.51	251.1	40
σ_2^{\square}	415	2.5E+7	3E-4	114.1	18.8

$\rho_{\square_i, \square_j}$	A	G	m	S_0
A	1	0.04	0.62	0.03
G	0.04	1	-0.38	-0.25
m	0.62	-0.38	1	0.72
S_0	0.03	-0.25	0.72	1

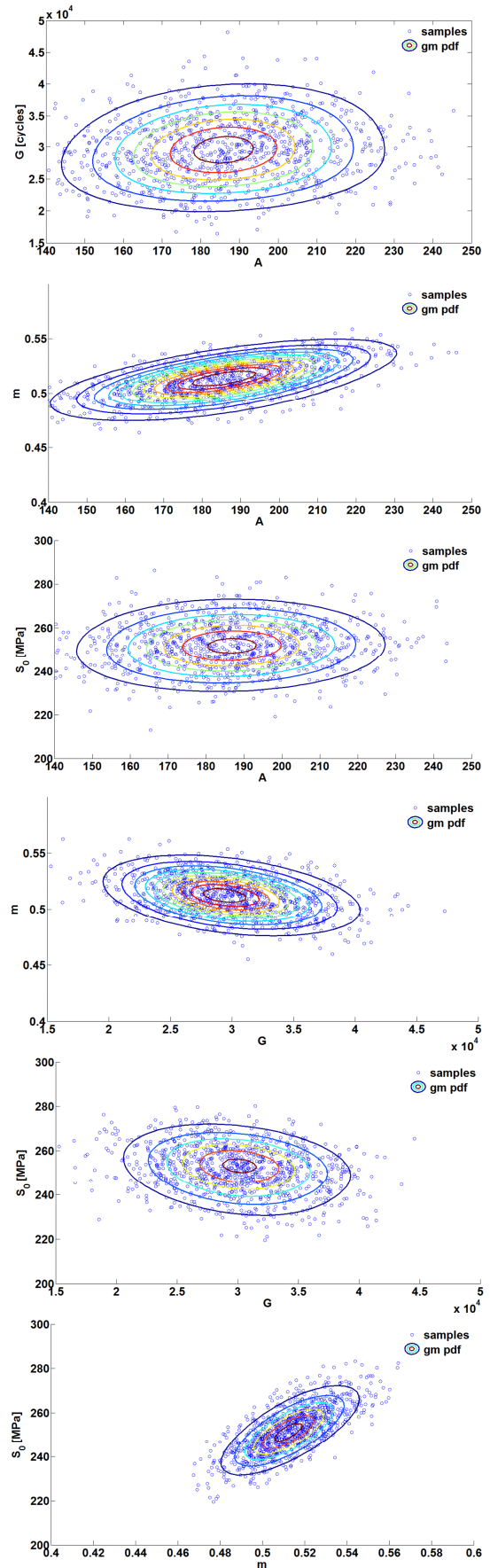


Figure 5. Gaussian-mixture fit of estimated parameters

Figure 3 does not show the correlation between the parameters of the curve, available from the MH algorithm. In order to appreciate the correlation between the parameters obtained by the algorithm, a Monte Carlo Sampling (MCS) is performed and the results are shown using the Gaussian Mixture Distribution (GMD) function. The GMD method allows estimating multivariate distributions as a summation of several Gaussian pdf. The commercial routine implemented in Matlab© is used to show the multivariate distributions of the Wohler parameters. A series of samples is extracted from the estimated pdf of the parameters, and the probability of these samples is superimposed to the graph. Since the parameters A and G are not normally-distributed, multivariate Gaussian functions are of course a rough approximation of the real distributions. However, it is enough to underline the presence of correlations between the parameters. Table 4 reports mean values μ_{\square} , variances σ_{\square}^2 and correlations $\rho_{\square_i, \square_j}$ assuming normally-distributed parameters.

As visible in Tables 4 and Figure 5, a clear correlation exists between the infinite life stress S_0 and the exponent of the Wohler curve m . Since both of them are normally distributed, the graph can be considered a correct representation of these two parameter distributions. Looking at the other graphs, a slight correlation may exist between m and A , and other slight correlations affect the couples (S_0, G) and (m, G) . However, the parameters G and A are not normally distributed and the actual mean values and dispersion indexes should be addressed before evaluating the correlation with other parameters. Even though the previous subsection assesses the averages, variances and correlations among the parameters, the correctness of the results are not proved. So, the estimated pdf will be used to produce approximated average and confidence boundaries for the output of the Wohler equation that is the stress S as a function of load cycles N .

4.4.1 Statistical definition of Wohler curve

The statistics related to the Wohler curve is mandatory in a fail-safe design framework. The statistics of Wohler parameters should be used to assess the global variability associated to the curve, in order to produce the probability of failure of components subjected to a particular stress S^* , or employed for a particular number of load cycles N^* . However, the nonlinearity of the formulation in (1) makes difficult the closed form solution of the mean and variance associated to the stress S . An approximation indicated in the literature as the delta method is proposed to overcome the problem [11]: It is a simple first order Taylor expansion of the

nonlinear equation in order to approximate the mean and the variance associated to the Wohler curve. Let N and S be the input and the output of a general nonlinear function, while \square is the vector of parameters affecting the nonlinear relationship, that is $S=S(\square, N)$. The mean value of S is simply calculated using the averages of the parameters (12), while the variance follows the form in (13).

$$\mu_S \approx S(\mu_{\square}, N) \quad (12)$$

$$\sigma_S^2 \approx \sum_i \sum_j \left. \frac{\partial S(\vartheta, N)}{\partial \vartheta_i} \right|_{\vartheta=\mu_{\vartheta}} \left. \frac{\partial S(\vartheta, N)}{\partial \vartheta_j} \right|_{\vartheta=\mu_{\vartheta}} \sigma_{\vartheta_i, \vartheta_j} \quad (13)$$

where the symbols μ and σ indicates mean and variance as in the common notation, taking care that $\sigma_{\square_i, \square_j} = \sigma_{\square_i}^2$ when $i=j$. According to the formulation in (1), the explicit form of the statistical Wohler curve becomes (14) and (15) for mean and variance, respectively.

$$\mu_S \approx \mu_{S_0} \left(1 + \frac{\mu_A}{(N + \mu_G)^{\mu_m}} \right) \quad (14)$$

$$\begin{aligned} \sigma_S^2 \approx & \left(\frac{\partial S}{\partial A} \right)^2 \sigma_A^2 + \left(\frac{\partial S}{\partial G} \right)^2 \sigma_G^2 + \left(\frac{\partial S}{\partial S_0} \right)^2 \sigma_{S_0}^2 + \left(\frac{\partial S}{\partial m} \right)^2 \sigma_m^2 \\ & + 2 \left(\frac{\partial S}{\partial A} \right) \left(\frac{\partial S}{\partial G} \right) \sigma_{A,G} + 2 \left(\frac{\partial S}{\partial A} \right) \left(\frac{\partial S}{\partial S_0} \right) \sigma_{A,S_0} + \\ & + 2 \left(\frac{\partial S}{\partial A} \right) \left(\frac{\partial S}{\partial m} \right) \sigma_{A,m} + 2 \left(\frac{\partial S}{\partial G} \right) \left(\frac{\partial S}{\partial S_0} \right) \sigma_{G,S_0} + \\ & + 2 \left(\frac{\partial S}{\partial G} \right) \left(\frac{\partial S}{\partial m} \right) \sigma_{G,m} + 2 \left(\frac{\partial S}{\partial S_0} \right) \left(\frac{\partial S}{\partial m} \right) \sigma_{S_0,m} \quad (15) \end{aligned}$$

The explanation of all the quantities in (15) is avoided for brevity. All the derivatives of the function are evaluated at $\square = \mu_{\square}$. Once the mean and variance for the Wohler curve are available, the confidence boundaries assume the usual form in (16).

$$S_{\text{sup,inf}} = \mu_S \pm \alpha \sigma_S \quad (16)$$

where the subscripts *sup*, *inf* in (16) are the upper and lower boundaries and α is the percentile value driving the width of the confidence band. Figure 6 shows the confidence bands related to 95% probability ($\alpha = 1.96$).

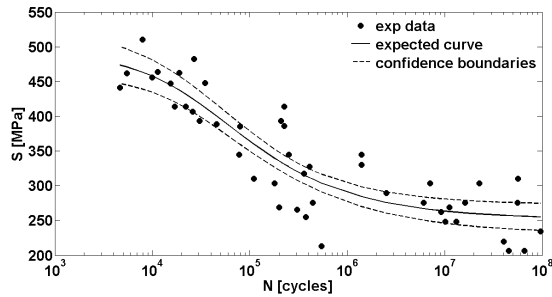


Figure 6. Estimated Wohler curve and confidence bands calculated via the delta method [11].

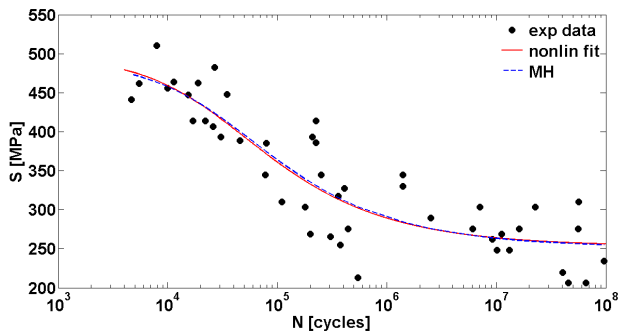


Figure 7. Comparison between nonlinear fitting and Metropolis-Hastings estimation of Wohler curve.

Table 5. Expected values of ϑ using a nonlinear fitting algorithm and MH algorithm

ϑ	μ_{ϑ} Nonlinear fitting	μ_{ϑ} Metropolis-Hastings
A	190.18	185.42
G [cycles]	26364	29560
m	0.519	0.512
S_0 [MPa]	252.86	251.43
σ [MPa]	-	40

As shown in Figure 6, the statistical Wohler curve seems to be in agreement with the experimental data. Although it is obvious for the expected value, the satisfied results reflects also in reasonable confidence boundaries using the variances coming from the MH algorithm. Of course, the achieved results introduced few approximations: the delta method assumes Gaussian pdf for each parameter, while A and G have uniform pdf (at least for the results obtained in this work); moreover, the first order Taylor expansion is representative of the nonlinear function $S(\vartheta, N)$, but is only approximation thereof.

4.4.2 Comparison with nonlinear fitting

The most common fitting technique is the nonlinear regression based on Levenberg-Marquardt algorithm. It has the restricting hypothesis of normally distributed parameters (like the hypothesis made in

the calculation presented above), because it is not able to evaluate the shape of the parameters pdfs. The nonlinear fitting subroutine available in Matlab© is used hereafter to analyze the results of the MH algorithm (Figure 7). Figures 6-7 show quite similar results. The curves are very close to each other, even if the parameters A and G estimated using the Random Walk Metropolis and the nonlinear fitting are slightly different (see Table 5). The infinite life stress S_0 and the m are comparable using the two methods. If two parameters are correctly estimated, probably the fitting procedure made with the MH algorithm is correct, and the values of the two parameters A and G (or the combination of them) have less influence on the Wohler curve than the other two parameters. This is in agreement with the sensitivity considerations made in section 4.4.

5. Conclusion

The possibility to use Metropolis-Hastings sampling technique for parameter identifications has been assessed in this work. MH allows to draw samples from the posterior density function (the probability of model parameters conditioned on the available data), thus representing both a statistical tool for the estimation of parameter uncertainty as well as a valid method for the updating of the prior knowledge on model parameters. As highlighted from the results, the parameters A and G show a very wide range of reasonable values with a uniform (or almost uniform) probability density. The validity of the fitting is proved by the generation of confidence boundaries through delta method and the comparison with the consolidated nonlinear fitting procedure based on the Levenberg-Marquardt algorithm (available as a standard subroutine in Matlab©).

Therefore, further investigation on the Wohler formulation in (1) should be made in order to describe the influence of the two parameters A and G to the curve, their probability density functions and their correlations with the other parameters. One possibility is that the formulation used to describe the curve could be simplified using only three parameters instead of four, which means establishing a dependence of one parameter from the other one, for instance A as a function of G or vice-versa.

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