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Calculation of Weibull life expectancy parameters from fracture data using the maximum likelihood criterion and a Nelder-Mead simplex minimisation algorithm

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This paper describes a mathematical technique to calculate the model parameters for a classical Weibull statistic. This type of statistic can be applied in a number of life time expectancy problems. A typical example is the brittle behaviour of components produced from technical ceramics. A Nelder-Mead simplex algorithm is introduced to obtain the Weibull parameters using the maximum likelihood criterion. Program code for a Matlab for Windows environment is presented.

1. Introduction

The prediction of the life expectancy of structural components is important, especially in the specific case of a component produced from a technical ceramic. It is well known that ceramic materials behave in a brittle way and, in general, show no ability to deform plastically as metals do. As a result of the occurrence of defects such as residual porosity or sintering flaws induced by e.g. contaminants, the nominal stress will be amplified in the vicinity of these defects by crack tip stress intensification mechanisms. These defects, being distributed at random throughout the volume of the component, will cause a series of test specimens to break at different nominal stress values: the failure stress thus shows a probability distribution.

The problem of life expectancy prediction for a ceramic component can be solved by first measuring the properties of the material on a large series of normalised specimens under normalised testing conditions. The measured values can be treated further in a statistical way to be able to extrapolate these data to the geometry of the actual component. In general a failure probability distribution can be described successfully following a model introduced by Weibull, involving a two parameter probability function. The estimation of these Weibull parameters from the data of mechanical tests on a large number of specimens can be obtained through several mathematical calculation techniques. In this paper it is explained how to calculate these two parameters by a Nelder-Mead simplex algorithm for function minimisation and using the maximum likelihood criterion.

2. Life prediction and the Weibull approach

Weibull (cf. [1, 4]) derived the following two parameter probability equation of fracture

$$P = 1 - \exp\left[-\frac{1}{V_0}\int_V \left(\frac{\sigma}{\sigma_\beta}\right)^m \mathrm{d}V\right] \tag{1}$$

with

P : probability of failure of the component,

V : volume of the component,

V_0 : arbitrary scaling volume (mostly taken as $1\,\mathrm{mm}^3$),

σ : tensile stress at a given position in the volume,

σ_β : first Weibull distribution parameter, associated with the material and indicated as the Weibull scale parameter, corresponding to the stress level where 63.2% of specimens with unit volume would fail,

m : second Weibull distribution parameter, also associated with the material and indicated as the volume Weibull modulus.

The Weibull parameter m is related to the homogeneity of the distribution of flaws: a low m modulus corresponds to a material in which the flaws are distributed nonuniformly giving rise to a broad failure stress distribution. A series of test specimens from a low m material statistically will show specimens failing at a high stress but also specimens failing at a low stress, depending on the statistical occurrence of a critical flaw in a critical stress zone. High m materials show a very homogeneous distribution of flaws giving rise to a reproducible failure stress corresponding to a sharp steplike failure stress distribution curve. Steel at room temperature typically has a Weibull modulus of $m = 60$. It should be noted that low- density porous materials may also show high m-values since the pores are distributed very homogeneously throughout the volume.

For a component the risk of failure can be calculated according to Eq. (1) by an integration over the entire volume of the component. De Salvo presented this for geometries such as tension specimens or bending specimens of rectangular or circular cross section (centre point loading, third point loading, fourth point loading, ...) in [1].

3. Weibull parameters from destructive mechanical bending tests

For a specific material the values of m and σ_β can be determined by measuring the bending failure stress of each specimen in a large series of standardised bending specimens. For such simple geometry test specimens, the integration over the volume in the failure probability equation (1) is straightforward resulting in simple equations (cf. [1]). To illustrate this we consider a rectangular beam-like sample (height H parallel to the y-axis, width W, length L parallel to the x-axis) being subjected to a constant bending moment over its length. Along the x-axis a neutral fibre exists, giving rise to tensile stresses at one side of this neutral fibre and compressive stresses at the other side. Since tensile stresses cause the brittle material to fail as a result of crack propagation from defect sites, it is sufficient to integrate Eq. (1) over the tensile stress region within half of the volume of the bending specimen. In this case the tensile stress varies linearly with the distance from the neutral fibre (at the specimen centre $y = 0$)

$$\sigma = 0 \qquad \text{at} \quad y = 0$$

and

$$\sigma = MOR \qquad \text{at} \quad y = \frac{H}{2},$$

MOR : the extreme fibre fracture stress or Modulus Of Rupture.

Thus,

$$\sigma = \left(MOR \cdot \frac{2}{H}\right) \cdot y\,. \tag{2}$$

For an infinitesimal volume $\mathrm{d}V$ one can also write the following equation

$$\mathrm{d}V = W \cdot L \cdot \mathrm{d}y\,. \tag{3}$$

Substituting Eqs. (2) and (3) in (1), one obtains

$$P = 1 - \exp\left[-\frac{1}{V_0}\int_0^{\frac{H}{2}}\left(\frac{MOR \cdot 2 \cdot y}{\sigma_\beta \cdot H}\right)^m \cdot W \cdot L \cdot dy\right]. \tag{4}$$

After integration, Eq. (4) results in

$$P = 1 - \exp\left[-\frac{V}{2 \cdot (m+1) \cdot V_0}\left(\frac{MOR}{\sigma_\beta}\right)^m\right] \tag{5}$$

or, by simplification to the classic Weibull equation, introducing σ_0,

$$P = 1 - \exp\left[-\left(\frac{MOR}{\sigma_0}\right)^m\right], \tag{6}$$

σ_0 : volume specimen characteristic strength or the *characteristic* modulus of rupture.

For bending test conditions (centre-point loading, third-point loading, ...) on simple specimen geometries, equations analogous to (5) and (6) can be derived (cf. [1]). As seen from Eqs. (5) and (6) in these cases it is straightforward to recalculate the Weibull scale parameter σ_β from σ_0 , m and the specimen geometry (volume). It has to be noticed that there is a specific relation $\sigma_\beta = f(\sigma_0, m, V)$ for each loading configuration and specimen type (cf. [2]).

4. Determination of M and σ_0 using the maximum likelihood criterion and a Nelder-Mead optimisation algorithm

Using Eq. (6) one can obtain the Weibull modulus m and the characteristic modulus of rupture σ_0 of a specific material from the population of fracture data, resulting from destructive bending tests on a large number of test specimens.

In the case of N specimens the specimens are first ranked in increasing order of fracture stress. In this way each specimen obtains a ranking number i with $i = 1, \ldots, N$. It is common practice that the probability of failure P_i for each specimen with rank i is calculated from a specific equation including the specimen ranking number and the total number of specimens. As an example for median rank regression analysis the probability of failure of the specimen with rank i is given by Nemeth (cf. [2]) by

$$P_i = 1 - \frac{i - 0.3}{N + 0.4}. \tag{7}$$

The probability of failure P_i for each specimen is then related to MOR_i as obtained from the bending test on that specific specimen and a set of N pairs of (MOR_i, P_i) values are obtained. It should be remarked that in practice a number of equations, slightly different from Eq. (7), are used to calculate P_i.

A Weibull probability graph is obtained by plotting the (MOR_i, P_i) values as $\mathrm{Ln\,Ln}\,[1/(1-P_i)]$ versus $\mathrm{Ln}\,(MOR_i)$. Such a graph should show a linear relation since it is in fact possible to transform Eq. (6) into a linear one by taking twice the natural logarithm:

$$\mathrm{Ln\,Ln}\left(\frac{1}{1-P}\right) = m \cdot \mathrm{Ln}\,(MOR) - m \cdot \mathrm{Ln}\,(\sigma_0). \tag{8}$$

When using Eq. (8) it seems straightforward to apply an ordinary linear regression technique based on the Gauss least-squares criterion to obtain estimates for σ_0 and m. This technique however supposes a normal distribution of errors. Since this assumption is not valid, the maximum likelihood method has to be applied [2]. An estimate of the parameters σ_0 and m is obtained by the maximisation of the likelihood function L for the two "variables" σ_0 and m using the MOR_i values from the N specimens

$$L = \prod_{i=1}^{N} \frac{m}{\sigma_0} \left(\frac{MOR_i}{\sigma_0}\right)^{m-1} \exp\left[-\left(\frac{MOR_i}{\sigma_0}\right)^{m}\right]. \tag{9}$$

One observes that the P_i values, calculated from an equation such as (7) based on a ranking, do not appear in Eq. (9). Only the MOR_i values are relevant to the maximum likelihood approach.

A number of iterative mathematical techniques exist to determine the values for σ_0 and m giving the maximum value for L. In this paper it is shown that the maximisation of L can be done by a Nelder-Mead simplex method (cf. [3]) for the minimisation of a function. It is trivial that in this case $-L$ will be minimised which of course equals to the maximisation of $+L$. The simplex method is readily available as a subroutine in standard software packages. In this way, programming the problem on a personal computer is very straightforward and σ_0 and m are calculated fast as a result of the simplex algorithm. The reader is referred to the article by Nelder and Mead [3] stressing the specific development purpose of the simplex technique for statistical problems and involving the maximisation of a likelihood function, in which the unknown parameters enter non-linearly.

5. IMPLEMENTATION OF THE SIMPLEX ALGORITHM

5.1. Program

To demonstrate the simplex algorithm Matlab for Windows was used. Matlab is considered as a standard in the scientific environment since most of the software routines evolved from the scientific users themselves. In this software, specific m-files are readily available as subroutines. The file `fmins.m` contains the simplex algorithm calculating the parameter values to minimise a function F with j parameters a_j. According to the Weibull parameters $a_1 = m$ and $a_2 = \sigma_0$ the number j of parameters a_j equals 2 in this case; $F(a_1, a_2) = -L$. To be able to use `fmins.m` to calculate the optimum values for σ_0 and m an additional function file `maxlhfun.m` was created representing the maximum likelihood function L from Eq. (9). An additional m-file `weibull2.m` was created as the main routine. The main routine `weibull2.m` and function file `maxlhfun.m` are shown in the next page. These files can readily be added to the Matlab m-file environment for general use.

When activating the main module `weibull2.m`, the program requests the name of the ASCII-file holding the data from the series of test specimens. This file should have N lines, each line showing the MOR_i and P_i value for the i-th specimen. After specifying the name of the data-file, the program will load the fracture data and start the simplex. The progress of the simplex can be controlled on the computer screen since each iteration is plotted. After reaching the specified accuracy for the parameter values the numerical results for σ_0 and m will be added to the plot (see Section 5.2 for an example).

5.2. Numerical examples and tests

Two sets of data from the literature were used to test the program.

Table 1 shows the extreme fibre fracture stresses MOR_i as taken from Table IX in [2] and the probability of failure values P_i calculated from Eq. (7) for a series of 80 bending test specimens. Based on the maximum likelihood criterion Nemeth [2] obtained $\sigma_0 = 556$ MPa and $m = 6.48$.

To control the simplex algorithm and the Matlab program as described in Section 5.1 the data from Table 1 were used. Figure 1 shows the results as produced by the simplex algorithm. The maximum likelihood estimates of σ_0 and m are identical to those obtained in [2].

The second test was made using the extreme fibre fracture stresses (MOR_i) and probability of failure values P_i extracted from Table G.2 in [5] and shown in Table 2. These MOR_i and P_i values

Main routine file weibull2.m:

```
% WEIBULL: calculation of Weibull parameters using a simplex algorithm and
% the maximum likelihood criterion for N specimens
% Datafile with N rows is in ASCII-format and has obligatory the extension .dat
% First number in a row holds MOR_i and second number holds prob. of failure P_i
echo off
global data MOR P Plothandle
% Input of (MOR, Failure Probability) data set
disp(' Input file (filename.dat) is in ASCII-format')
fname    = input(' Name of data-file ? (without extension .dat !) ','s');
filein = [fname '.dat'];
% Control of the existence of the filename
if ~exist(filein) , disp(' Filename does not exist ! Try again '),break,end ;
% Transfer of data from the input file into the variables
eval(['load ' filein]);
data = eval(fname);
n = length(data);
MOR = data(:,1);
P = data(:,2);
% Start of calculations
LnM = log(MOR); LnLnP=log(-log(1-P));
xlmin = floor(min(LnM)) ; xlmax = ceil(max(LnM));
ylmin = floor(min(LnLnP)) ; ylmax = ceil(max(LnLnP));
tekstx = xlmin + 0.02 ; teksty = ylmax - 0.2 ;
% Plotting of test results - drawing characteristics
hold on
axis([xlmin xlmax ylmin ylmax]);
xlabel('Ln(MOR)'), ylabel('LnLn[1/(1-P)]');
set(gca,'Xgrid','on','Ygrid','on');
plot(LnM,LnLnP,'ow','Erasemode','none');
% Start of Nelder-Mead curvefitting (function : maxlhfun.m)
% Vector [a(1) a(2)] holds the Weibull parameters.
% a(1) holds the Weibull modulus m and (2) holds the characteristic modulus of
% rupture sigmao.  One should put starting values in vector [a(1) a(2)]
a = [10 600]';
Plothandle = plot(LnM,LnLnP,'EraseMode','xor');
% Define accuracy :
accuracy=1.0e-3
a = fmins('maxlhfun',a,0,accuracy);
% Displaying the results on the plot
text(tekstx,teksty ,['  m        = ' num2str(a(1))]);
text(tekstx,teksty-0.5 ,['sigmao = ' num2str(a(2))]);
title(['Datafile : ' fname],'FontSize',16);
hold off;
```

Function file maxlhfun.m :

```
function MAXLHF = MAXLHFUN(a)
global data MOR P Plothandle
for i = 1:size(MOR)
z(i) = exp(-(MOR(i)/a(2))^a(1));
end
z=z';
LnLnz = log(-log(z));
MAXLHF=1;
for i = 1:size(MOR)
MAXLHF = MAXLHF*(a(1)/a(2))*((MOR(i)/a(2))^(a(1)-1))*exp(-(MOR(i)/a(2))^a(1));
end
MAXLHF = -MAXLHF;
set(Plothandle,'ydata',LnLnz);
drawnow
```

Table 1

i	*MOR*	*P*	*i*	*MOR*	*P*	*i*	*MOR*	*P*	*i*	*MOR*	*P*
1	281.2	0.0087	21	446.2	0.2575	41	516.2	0.5062	61	588.6	0.7550
2	291	0.0211	22	451.5	0.2699	42	519.8	0.5187	62	591	0.7674
3	358.2	0.0336	23	452.1	0.2823	43	527.6	0.5311	63	591	0.7799
4	385.4	0.0460	24	452.7	0.2948	44	530.7	0.5435	64	593.3	0.7923
5	389	0.0585	25	470.4	0.3072	45	530.7	0.5560	65	598.7	0.8047
6	390.8	0.0709	26	474.1	0.3197	46	545.7	0.5684	66	599.6	0.8172
7	391.8	0.0833	27	475.5	0.3321	47	548.8	0.5808	67	610	0.8296
8	402.8	0.0958	28	475.5	0.3445	48	552.7	0.5933	68	612.7	0.8420
9	412.5	0.1082	29	479.2	0.3570	49	559.6	0.6057	69	619.9	0.8545
10	413.3	0.1206	30	483.5	0.3694	50	562.4	0.6182	70	619.9	0.8669
11	413.9	0.1331	31	484.8	0.3818	51	563.3	0.6306	71	622.2	0.8794
12	417.8	0.1455	32	486.2	0.3943	52	566.1	0.6430	72	622.3	0.8918
13	418.2	0.1580	33	488.6	0.4067	53	566.5	0.6555	73	640.5	0.9042
14	426.9	0.1704	34	492.5	0.4192	54	570.1	0.6679	74	649	0.9167
15	437.6	0.1828	35	493.2	0.4316	55	572.8	0.6803	75	657.2	0.9291
16	440	0.1953	36	496	0.4440	56	575	0.6928	76	660	0.9415
17	441	0.2077	37	505.7	0.4565	57	576.1	0.7052	77	664.3	0.9540
18	442.5	0.2201	38	511.9	0.4689	58	580	0.7177	78	673.5	0.9664
19	443.8	0.2326	39	512.5	0.4813	59	582.6	0.7301	79	673.9	0.9789
20	444.9	0.2450	40	513.8	0.4938	60	588	0.7425	80	725.3	0.9913

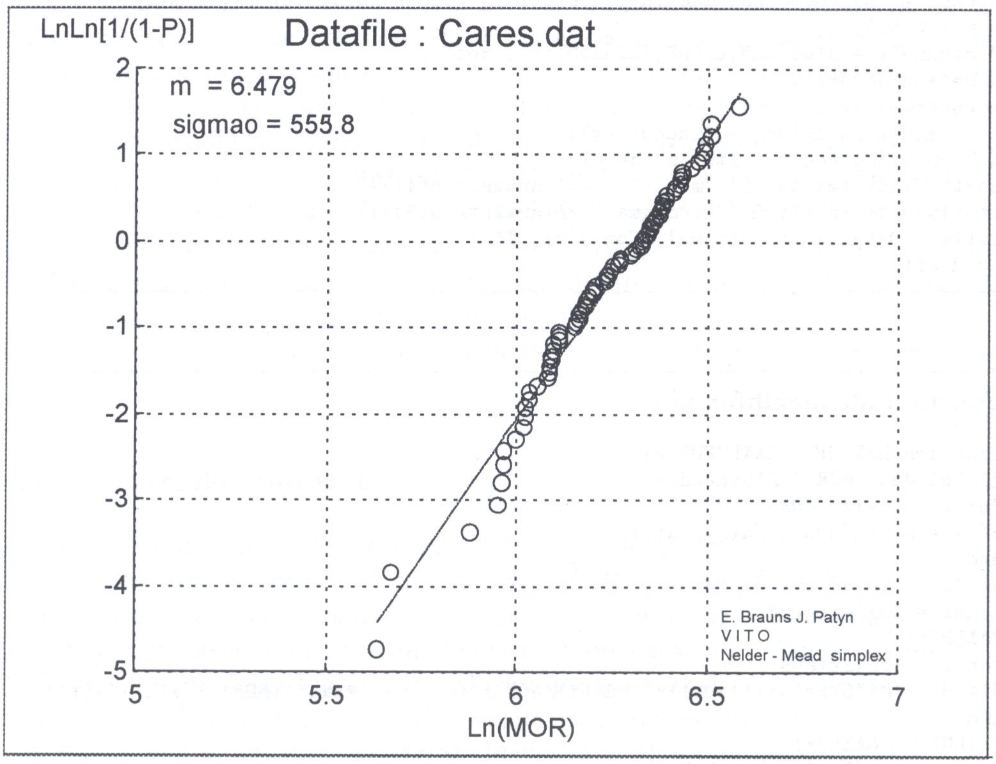

Fig. 1. Regression by Nelder-Mead simplex

Table 2

i	MOR	P	i	MOR	P	i	MOR	P	i	MOR	P
1	190	0.0167	9	246	0.2833	17	267	0.5500	25	287	0.8167
2	210	0.0500	10	247	0.3167	18	274	0.5833	26	288	0.8500
3	227	0.0833	11	252	0.3500	19	277	0.6167	27	296	0.8833
4	232	0.1167	12	257	0.3833	20	279	0.6500	28	297	0.9167
5	237	0.1500	13	258	0.4167	21	280	0.6833	29	310	0.9500
6	239	0.1833	14	262	0.4500	22	280	0.7167	30	322	0.9833
7	242	0.2167	15	264	0.4833	23	281	0.7500			
8	243	0.2500	16	267	0.5167	24	281	0.7833			

Table 3

Number of specimens	20	40	60	80	100
Unbiasing factor	0.931	0.966	0.978	0.984	0.987

for a series of 30 specimens are to be considered as a reference in the near future since [5] will be announced as an European Pre-standard. The simplex algorithm and the Matlab program as described in Section 5.1 resulted in $\sigma_0 = 275.5\,\mathrm{MPa}$ and $m = 10.51$ being identical to the maximum likelihood values $\sigma_0 = 276\,\mathrm{MPa}$ and $m = 10.51$ reported in [5].

It should be stressed that the maximum likelihood estimate of m is a biased estimate, depending on the number of specimens [5]. Its value still has to be multiplied by an unbiasing correction factor (e.g. Table 3).

6. Conclusions

A Nelder-Mead simplex algorithm efficiently calculates the Weibull parameters from the fracture data of a series of test specimens. These parameter values are important with respect to life prediction of components produced from technical ceramics. Weibull probability statistics however can also be applied in other domains of reliability analysis. The proposed Nelder-Mead approach is also useful in these cases.

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