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Maximum likelihood estimation techniques for concurrent flaw subpopulations

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Failure of structural materials is often caused by the presence of two or more types of defect subpopulations. The maximum likelihood estimation technique for evaluating the Weibull parameters of these underlying subpopulations in the case of known fracture origin is presented. The maximum likelihood estimation equations are derived, and solved by means of nonlinear programming. The estimators obtained therefrom are tested for both accuracy and consistency against a series of simulation runs. For data sets containing a relatively small sample size, the advantage of the method of maximum likelihood over two established nonparametric techniques is demonstrated.

1. Introduction

The strength of structural materials is often determined by two or more types of inherent subpopulations of defects. Each type of defect is assumed to possess its own intrinsic distributional properties, and the ultimate breaking strength is determined not only from these individual distributions, but also from their interaction with one another. For purposes of discussion let us assume there are only two types of defect subpopulations, types A and B. In the *concurrent* case, defects of both types are assumed present in each test specimen, with the same definition extending to the general setting of more than two subpopulations.

The Weibull distribution, cf. Weibull [1], Mann *et al.* [2], Jayatilaka and Trustrum [3], Trustrum and Jayatilaka [4], and Jeryan [5], has found great favour in describing the individual defect subpopulations, primarily because of its flexibility and simplicity. Versions with both two and three parameters are commonly used. Recent literature has focused on the need for a rigorous technique of estimating the parameters of the underlying Weibull subpopulations in the concurrent case. The purpose of this paper is to investigate the maximum likelihood technique for estimating Weibull parameters of the concurrent case.

Our model then depends on the following three assumptions:

1. two (and only two) types of defect subpopulations, types A and B, are present in each test specimen;
2. each defect subpopulation possesses a two-parameter Weibull distribution;
3. the type of defect that causes failure in a test specimen can always be determined by a post-mortem analysis.

It is important to note that the technique discussed in this paper considers the censored information present in each sample. That is, if a specimen fails by a defect of type A, it obviously did not fail by a defect of type B at the breaking strength. This information must be observed in estimating the Weibull parameters for both type A and B defects.

We begin with a brief review of the existing literature on the problem. Graphical techniques for determining the underlying Weibull parameters are discussed in Johnson [6] and Easler *et al.* [7]. These techniques plot the strength data using a linear transformation of coordinates. In most concurrent cases this will generate a curve with a distinct "knee" in it that enables one to generate estimates of both the scale and shape parameters of both subpopulations. While the method illustrates the concept of competing

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Weibull subpopulations quite well, properties of the estimators such as accuracy and consistency are difficult to verify.

In Nelson [8], the technique of hazard plotting is introduced. The technique depends on the fact that the composite hazard rate for two concurrent subpopulations is simply the sum of the individual hazard rates. To estimate values for the Weibull parameters from a given set of data, one ranks the data and works with hazard sums. Linear regression is employed, as outlined in Nelson [8], with failure strengths transformed to be used as the dependent variable.

In Jakus *et al.* [9], an approach known as mean order ranking is used to estimate the Weibull parameters in the concurrent case. The procedure is adapted from Johnson [10]. The method attempts to take into account all of the censored information available in the sample by reranking the separated data. For each censored data point, a new increment in the ranking function is calculated based on the previous ranking and the number of data points beyond the present censored set. These new increments are, in turn, used to determine a new ranking function for each subpopulation. The Weibull parameters are estimated for each subpopulation by linear regression after an appropriate transformation of coordinates.

In this paper we propose the maximum likelihood estimation (MLE) technique to estimate the Weibull parameters for a bimodal, concurrent strength distribution. MLE is a wholly parametric technique, depending explicitly on the form of the Weibull model to generate its estimates. This is not true of hazard plotting and mean order ranking, where nonparametric ranking and regression techniques are used to generate estimates. Divorcing a portion of the estimation procedure from the model whose parameters are being estimated fails to use all of the relevant information. This can be particularly critical when there is little information available. In the final section we compare the performance of MLE, hazard plotting, and mean order ranking for small sample sizes.

2. Maximum likelihood estimation techniques

To develop our MLE model, we must first introduce some notation. Each Weibull subpopulation has a probability density function

$$f_i(x) = \frac{m_i}{s_i}\left(\frac{x}{s_i}\right)^{m_i-1} \exp\left[-\left(\frac{x}{s_i}\right)^{m_i}\right] \qquad x \geqslant 0,\ i = A, B \tag{1}$$

and survival probability function

$$\bar{F}_i(x) = 1 - F_i(x) = \exp\left[-\left(\frac{x}{s_i}\right)^{m_i}\right] \qquad x \geqslant 0,\ i = A, B \tag{2}$$

where $F_i(x)$ is the cumulative failure probability associated with type i defect. The combined survival probability function is

$$\bar{F}(x) = \bar{F}_A(x)\bar{F}_B(x) = \exp\left[-\left(\frac{x}{s_A}\right)^{m_A} - \left(\frac{x}{s_B}\right)^{m_B}\right] \qquad x \geqslant 0 \tag{3}$$

It is assumed that a sample of n items is analysed, with n_i of the samples falling from a type i defect, i = A, B; and $n_A + n_B = n$. Let $x_j^i = j$th ordered observation of a failure caused by a type i defect, $j = 1, \ldots, n_i$, i = A, B, and $x_j = j$th ordered observation of the combined failure data, $j = 1, \ldots, n$.

The maximum likelihood technique is based on the following reasoning: the likelihood function for a specified model is a function of the parameters of the model and the values of the sample. When the likelihood function is evaluated at the values in the sample, it represents the joint probability of that particular outcome being realized as a function of the model parameters. Naturally we want to maximize this joint probability with respect to these parameters, which obtains the maximum likelihood estimators for these parameters. In general maximum likelihood estimators possess many desirable statistical properties. For example, the maximum likelihood estimators are often a function of the minimum variance unbiased estimators. For further details, see Mann *et al.* [2] or Mendenhall *et al.* [11]. Depending on the form of the model, MLE poses a problem of variable mathematical tractability. The details of the technique for the case of concurrent Weibull subpopulation follow.

The likelihood function, L, for this model is

$$L \equiv L(m_i, s_i; x_1^i, \ldots, x_n^i) = \prod_{j=1}^{n_A} f_A(x_j^A)\bar{F}_B(x_j^A) \prod_{j=1}^{n_B} f_B(x_j^B)\bar{F}_A(x_j^B)$$

Consider those terms treating an x_j^A. Their contribution to the likelihood function, $f_A(x_j^A)\bar{F}_B(x_j^A)$, is the joint probability of $X_A \in (x_j^A, x_j^A + \Delta x_j^A)$, $X_B \geqslant x_j^A$, where X_i is a generic random variable from subpopulation i, i = A, B. The sample values x_j^B are treated in the same fashion. Multiplying the two products together we obtain the likelihood function.

It is easier to work with the natural logarithm of the likelihood function, which of course takes on its maximum value at the same point. Taking the natural logarithm and substituting into Equations 1 and 2, we obtain

$$\begin{aligned}\ln L = {} & n_A \ln\left(\frac{m_A}{s_A}\right) + (m_A - 1)\sum_{j=1}^{n_A} \ln\left(\frac{x_j^A}{s_A}\right) \\ & - \sum_{j=1}^{n_A}\left[\left(\frac{x_j^A}{s_A}\right)^{m_A} + \left(\frac{x_j^A}{s_B}\right)^{m_B}\right] \\ & + n_B \ln\left(\frac{m_B}{s_B}\right) + (m_B - 1)\sum_{j=1}^{n_B} \ln\left(\frac{x_j^B}{s_B}\right) \\ & - \sum_{j=1}^{n_B} \left(\frac{x_j^B}{s_B}\right)^{m_B} + \left(\frac{x_j^B}{s_A}\right)^{m_A} \end{aligned} \tag{4}$$

The four partial derivatives, one with respect to each parameter to be estimated, are

$$\frac{\partial \ln L}{\partial s_i} = \frac{-n_i m_i}{s_i} + \frac{m_i}{s_i}\sum_{j=1}^{n}\left(\frac{x_j}{s_i}\right)^{m_i} \qquad i = A, B \tag{5}$$

$$\begin{aligned}\frac{\partial \ln L}{\partial m_i} = {} & \frac{n_i}{m_i} + \sum_{j=1}^{n_i} \ln\left(\frac{x_j^i}{s_i}\right) \\ & - \sum_{j=1}^{n}\left(\frac{x_j}{s_i}\right)^{m_i} \ln\left(\frac{x_j}{s_i}\right) \qquad i = A, B\end{aligned} \tag{6}$$

The standard solution procedure is to set each of the four partial derivatives (Equatons 5, 6) equal to zero. Finding this solution by traditional methods such as iterative search is not feasible, so a nonlinear programming technique was employed. Before we discuss the details of this solution procedure, we review the role of the sample. No ranking functions or linear regression are employed. Rather the data from each subpopulation is simply put into Equations 5 and 6 which are, in turn, solved to yield estimators of the Weibull parameters.

3. Solution procedure

The nonlinear programming approach reformulates the problem with a nonlinear objective function and a set of linear constraints. Formally stated, the problem becomes:

Find m_A, s_A, m_B, s_B to:
minimize

$$\begin{aligned}\phi & \equiv \phi(m_i, s_i; x_1^i, \ldots, x_n^i) \\ & = \sum_{i=A,B}\left[\left(\frac{\partial \ln L}{\partial m_i}\right)^2 + \left(\frac{\partial \ln L}{\partial s_i}\right)^2\right]\end{aligned} \tag{7}$$

subject to

$$m_A \geqslant 0, s_A \geqslant 0, m_B \geqslant 0, s_B \geqslant 0 \tag{8}$$

The objective function (Equation 7) is the sum of the squares of the four partial derivatives of the natural logarithm of the likelihood function. By minimizing this function we are deriving the individual derivatives to a value of zero. It should be pointed out that with the application of this technique to the problem, the solutions generated values of the objective function on the order of 10^{-10}, ensuring in fact that for all practical purposes we were actually solving Equations 5 and 6. The constraints of Equation 8 are needed to ensure that the maximum likelihood estimators found by the technique are, in fact, non-negative as they indeed must be.

The nonlinear programming algorithm used was Marquardt's algorithm, cf. Kuester and Mize [12]. The algorithm is a gradient search technique which involves a compromise between the methods of steepest descent and the traditional Gauss–Newton in selecting the next step size in the search. The interested user need not be familiar with the details of the nonlinear programming technique, since a prepared code written in Fortran IV is available from the authors. For most data sets from relatively low shape parameters the algorithm will converge in a reasonable number of iterations, yielding accurate estimators with excellent consistency. In a relatively few test cases the algorithm did not converge within the time limits of the existing computing facilities. This problem is frequently encountered in search-method algorithms when the size of the convex (concave) neighbourhood surrounding the optimum is relatively small, as in the case here.

To circumvent this problem, a transformation of the data was utilized. This transformation depends on the fact that a non-negative power

TABLE I Summary of simulation parameters and maximum likelihood estimators. Total sample size = 50, ten simulation runs

Simulation parameters	Subpopulation sizes estimates	Maximum likelihood estimates: mean	Standard deviation of estimators	
			Simulated	Theoretical
$s_A = 400$	Theoretical	422.26	19.146	19.566
$s_B = 600$	$n_A = 42.64, n_B = 7.36$	633.89	107.35	72.27
$m_A = 3$	Simulated	3.3554	0.2963	0.40706
$m_B = 5$	$n_A = 41.30, n_B = 8.70$	4.7426	0.6931	1.286
$s_A = 600$	Theoretical	596.62	61.258	58.757
$s_B = 600$	$n_A = 26.93, n_B = 23.07$	582.00	44.250	28.72
$m_A = 2$	Simulated	2.1099	0.2649	0.3843
$m_B = 4$	$n_A = 26.50, n_B = 23.50$	4.1646	0.7815	0.628
$s_A = 300$	Theoretical	295.28	11.998	8.495
$s_B = 300$	$n_A = 27.64, n_B = 22.36$	301.28	5.0205	4.950
$m_A = 6$	Simulated	6.4464	1.0504	1.0205
$m_B = 13.5$	$n_A = 29.50, n_B = 20.50$	13.713	2.9787	2.1408
$s_A = 350$	Theoretical	346.75	26.642	21.586
$s_B = 300$	$n_A = 12.58, n_B = 37.42$	300.41	3.4532	3.118
$m_A = 7$	Simulated	8.6033	2.7304	2.5619
$m_B = 14.5$	$n_A = 13.00, n_B = 37.00$	15.811	1.2468	1.9647

of a Weibull random variable is also a Weibull random variable. To see this, let X have a Weibull density with parameters (m, s). Let $Y = X^2$. Then

$$\begin{aligned} f_Y(y) &= f_X(y^{1/2}) \left|\frac{\partial x}{\partial y}\right| \\ &= \left(\frac{m}{s}\right)\left(\frac{y^{1/2}}{s}\right)^{m-1} \\ &\quad \times \exp\left[-\left(\frac{y^{1/2}}{s}\right)^m\right]\left(\frac{1}{2y^{1/2}}\right) \\ &= \left(\frac{m'}{s'}\right)\left(\frac{y}{s'}\right)^{m'-1} \exp\left[-\left(\frac{y}{s'}\right)^{m'}\right] \qquad (9) \end{aligned}$$

where $m' = m/2$, $s' = s^2$. A similar result holds for $Y = X^r$, for any $r \geqslant 1.0$.

To utilize this development, consider a data set for which the algorithm did not converge. Square all data values, retaining the same fracture origins, and find estimators m', s' for this transformed data. Then re-invert these estimators using $m = 2m'$, $s = (s')^{1/2}$. This yields the correct estimators for the original data set. This squaring transformation works for almost all cases; if not, a cubing transformation is employed. By means of several logical-if statements, this transformation of data was incorporated into the authors' Fortran IV code. These transformations enabled us to achieve convergence in all of the simulation runs used to examine the performance of the maximum likelihood technique.

4. Performance of technique

To test the accuracy and consistency of the MLE technique discussed in this paper, a number of Monte Carlo simulation runs were performed using samples of size $n = 50$. The fracture strength for each of the 50 specimens in a given sample population was calculated by choosing a pair of random fracture strengths, one from distribution A and one from B. If the fracture strength from A was less than that from B, the specimen was designated as failing from flaw type A at that fracture strength. Conversely, if fracture strength B was less than A, the specimen was designated as failing at a flaw of type B. For each set of Weibull parameters, ten runs were executed using the same random number seed across techniques. This enabled us to measure both the accuracy and consistency of each technique. Accuracy was measured by the proximity of the estimated parameter values to the true values used to generate the simulation data, and consistency was measured by the size of the standard deviations of the ten runs. A summary of the actual and estimated parameter values for four combinations of shape and scale parameters is listed in Table I. Good agreement in all cases is evident.

The simulated and theoretical subpopulation

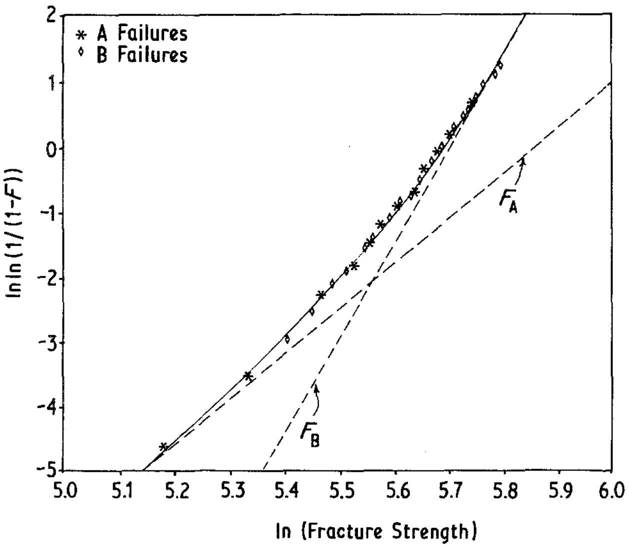

Figure 1 Predicted concurrent strength distribution.

sample sizes n_A and n_B are also listed in Table I. The simulated sample sizes are obtained by averaging the values obtained from the ten runs for each set of Weibull parameters. The theoretical sample sizes are obtained by calculating the probability that the random variable X_A is less than X_B.

$$P(X_A < X_B) = \int_0^\infty P(X_B > x) P \times [X_A \in (x, x + \mathrm{d}x)]\,\mathrm{d}x = \int_0^\infty \exp\left[-\left(\frac{x}{s_B}\right)^{m_B}\right]\left(\frac{m_A}{s_A}\right) \times \left(\frac{x}{s_A}\right)^{m_A-1} \exp\left[-\left(\frac{x}{s_A}\right)^{m_A}\right]\mathrm{d}x$$

The integration is performed numerically using Simpson's approximation. The theoretical n_A is then calculated by multiplying this probability by $n = 50$, and $n_B = 50 - n_A$. In all cases there was excellent agreement between the simulated and theoretical subpopulation sample sizes.

Fig. 1 compares a predicted concurrent strength distribution based on Equation 3 using the four Weibull parameters found with the MLE technique in one of the computer simulation trials with the 50 fracture strengths generated in that trial. The type of fracture origin for each specimen is identified in the figure by its associated symbol. The dashed lines in the figure describe the individual failure probabilities when the distributions are present one at a time. The two concurrent flaw populations were chosen so that there is a tendency for fracture origins from flaw type A to predominate at lower stresses and for origins of type B to predominate at higher stresses. The agreement between the estimated concurrent strength distribution and the 50 generated data points is good. The differences observed are a result of sampling errors inherent in this moderate number of specimens and the small errors in the estimated Weibull parameters. These differences also emphasize that caution should be used in interpreting minor kinks and knees in real experimental data. It is interesting to note that concurrent distributions result in a single knee in the curve with a positive curvature (knees with a negative curvature cannot occur with concurrent flaw distributions). At high fracture stresses, the concurrent distribution asymptotically approaches the behaviour of the strength distribution with the larger Weibull modulus and at low stresses that of the strength distribution with the smaller Weibull modulus.

The consistency of our estimators is measured by both the simulated and theoretical standard deviations of the estimators (see Table I). The simulated value is obtained by calculating the standard deviation of the ten simulation runs for each parameter for each of the four sets of parameter values. To obtain the approximate theoretical value, we need to calculate the asymptotic variance-covariance matrix, cf. Rao [13], the diagonal elements of which yield the asymptotic variance of the four estimators. To calculate this matrix we need to invert the negative of the expected value of the information matrix. In the

TABLE II Comparison of estimation techniques for small sample sizes. Total sample size = 5, ten simulation runs

Simulation parameters	Mean order ranking estimates		Hazard plotting estimates		Maximum likelihood estimates	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
$s_A = 300$	281.92	14.854	274.11	16.543	294.23	12.010
$s_B = 300$	296.30	10.637	289.20	8.5361	292.67	9.3276
$m_A = 6$	13.892	11.377	10.791	8.3477	9.8296	7.4258
$m_B = 13.5$	3.7088	81.599	30.599	65.618	18.970	6.5643

concurrent case the information matrix takes a block diagonal form

$$I = \left[\begin{array}{c:c} I_A & 0 \\ \hdashline 0 & I_B \end{array}\right]$$

where the elements of I_k, k = A, B, are given by

$$I_k = \begin{bmatrix} \dfrac{\partial^2 \ln L}{\partial s_k^2} & \dfrac{\partial^2 \ln L}{\partial s_k \partial m_k} \\[2ex] \dfrac{\partial^2 \ln L}{\partial m_k \partial s_k} & \dfrac{\partial^2 \ln L}{\partial m_k^2} \end{bmatrix}$$

We note that the block diagonal structure of I allows us to invert each of $-E(I_A)$ and $-E(I_B)$ separately.

In many situations it is impractical to expect a large number of data points on fracture strengths to be available. For this reason we ran small sample ($n = 5$) simulations for the MLE, hazard plotting, and mean order ranking techniques. The results are listed in Table II. Although all three techniques were satisfactory in estimating the scale parameters, only MLE gave reasonable estimates of the shape parameters. The breakdown of the nonparametric techniques in estimating the Weibull parameters of a bimodal concurrent emphasizes the weaknesses inherent in such techniques.

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