

Adjustment of complex probabilistic models and estimation of confidence intervals in a discrete manner

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Abstract: This article shows that complex probabilistic models can be properly adjusted from feedback data, if an efficient optimization method is used to overcome the multiple optima of the likelihood function. It proposes a generic method to estimate confidence intervals by inverting the Fisher matrix calculated in a discrete manner in order to avoid the derivation of analytical expressions which are specific to each model used.

Keywords: Adjustment, global optimization, genetic algorithms, confidence interval, Fisher matrix, discrete calculation

1. INTRODUCTION

Developed by Ronald Aylmer Fisher, the maximum likelihood estimation is a common statistical method used to estimate the parameters of a probabilistic model from a given sample. It consists in choosing parameter values that maximize the likelihood of the observations, i.e., the probability of observing them. In the case of uncensored data, the expression of the likelihood is:

$$L(X, \theta) = \prod_{i=1}^n f(x_i, \theta) \quad (1)$$

With $f(x_i, \theta)$ = Probability density of the model if X is a continuous variable.

It is equivalent and simpler to maximize the log-likelihood for which the product becomes a sum.

This optimization problem is usually solved by cancelling the first derivative (if the likelihood function is differentiable), verifying that the second derivative is negative. It also deals with local optimization techniques such as pseudo gradient or non-linear simplex (Nelder Mead algorithm).

But the adjustment can not be achieved by a simple optimization technique when there are many local optima. That's why most of the existing tools are limited to the usual laws of probability and sometimes give erroneous results when the models become more complex.

Stochastic methods like heuristic or Meta heuristics have largely proved their effectiveness in finding global optima, although the optimality of the solutions can not be guaranteed or demonstrated. Also, it appears interesting to use them to make adjustments, especially because they require no a priori knowledge on the functions to be optimized, except for the result obtained for each configuration of parameters.

Therefore, an adjustment function for complex probabilistic models was developed from a global optimization tool (GENCAB of CAB INNOVATION) based on genetic algorithms, differential evolution and non-linear simplex [2]. This hybridization of global and local techniques allows the convergence to be accelerated and the tool to become robust to the variety of problems.

The purpose of this communication is to show that complex probabilistic models can be properly adjusted from feedback data, if an efficient optimization method is used to overcome the multiple optima of the likelihood function.

This article also proposes a generic method to estimate confidence intervals, for parameters or functions of these parameters (quantile, distribution function ...), by inverting the Fisher matrix. The latter is calculated in a discrete manner in order to avoid the derivation of analytical expressions which are specific to each model used.

2. ADJUSTMENT OF COMPLEX PROBABILISTIC MODELS

Using a global optimization tool allows complex models – that were difficult or impossible to treat – to be adjusted as illustrated by the examples below.

This ability to fit complex models can be easily demonstrated by using a set of simulated data from a model with a known configuration of parameters and by obtaining the same parameters configuration when fitting this simulated data set with the tool.

2.1. Reliability models

In a feedback analysis, it is not always easy to separate the early failure, occasional failures and breakdowns of wear. Thus we can adjust them globally using a Multi-phases reliability model.

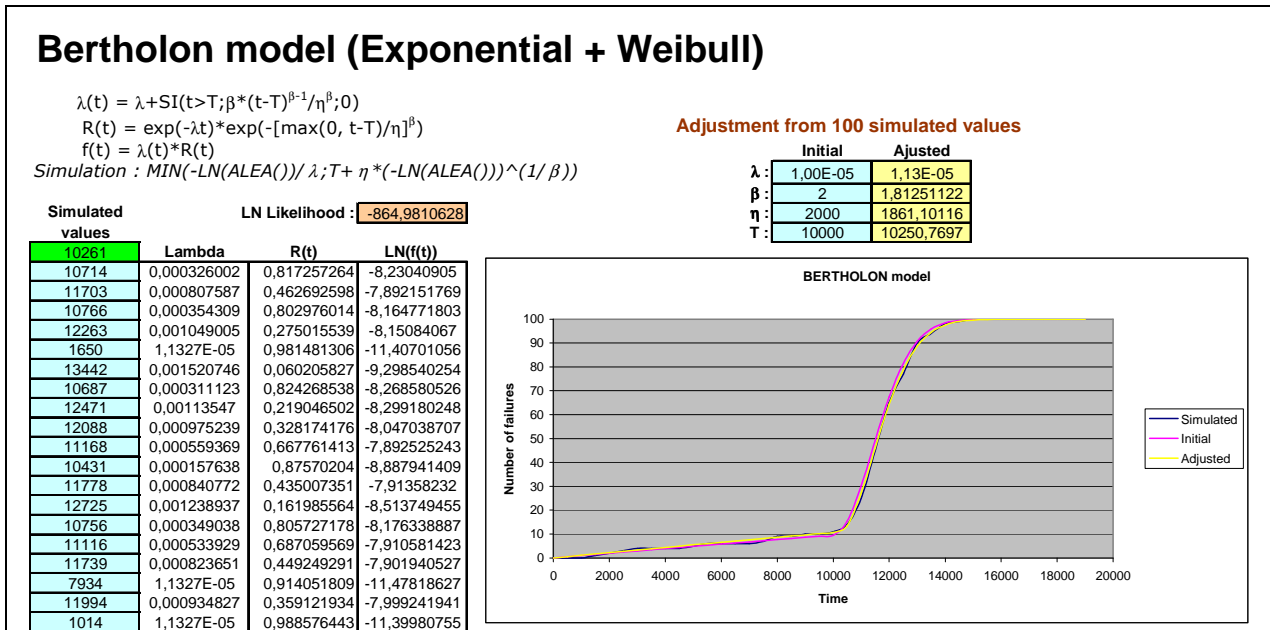


Figure 1. Bertholon model fit from simulated data

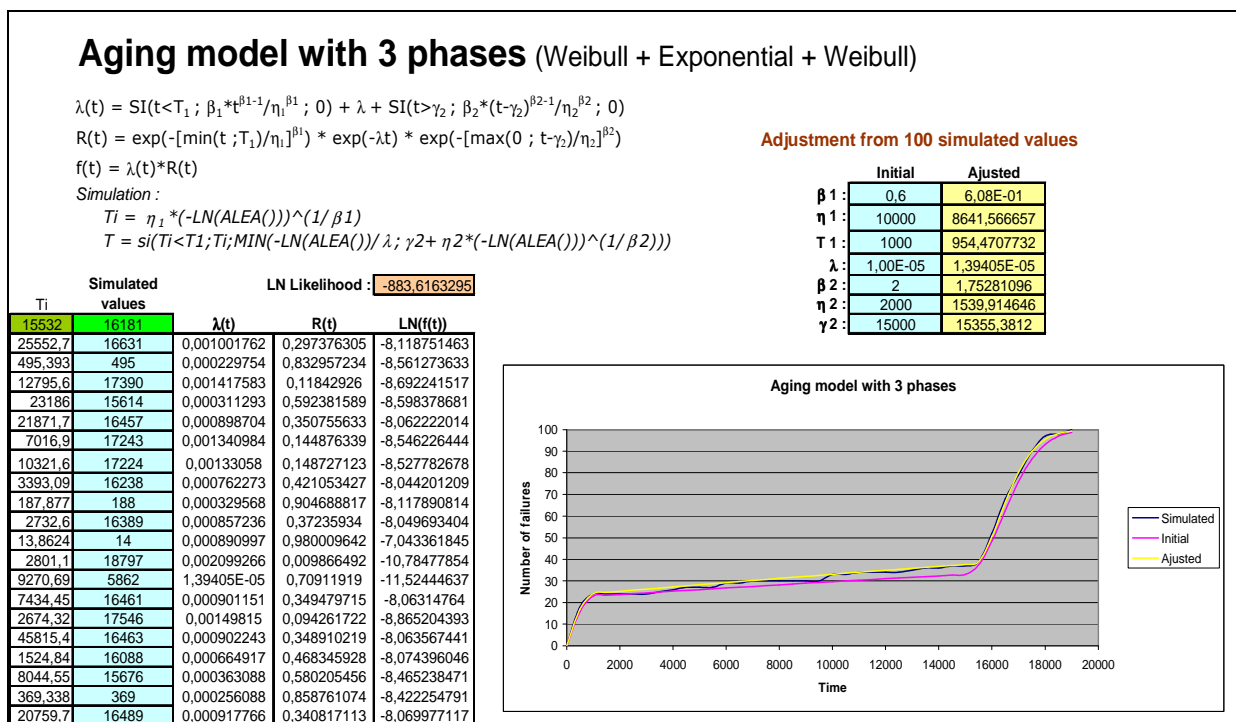


Figure 2. Fit of the full bathtub curve from simulated data

The Bertholon [1] model combines an exponential law and a Weibull law to imitate the second and third part of the bathtub curve (occasional failures and wear). Figure 1 shows the good fit of such a model computed from 100 previously simulated values. This returns approximately the same values than the four initial model parameters used for simulation.

By combining an exponential and 2 Weibull laws, this model can be generalized in a model with seven parameters characterizing the three phases of the bathtub curve as shown in Figure 2.

The expressions of the probability densities used to calculate the log likelihood functions and the functions used to simulate data are given in the figures above, in the same way as the curves representing the distribution functions of the theoretical model, the experimental model from simulated data and the fitted model.

Similarly, it is often difficult to separate data for multiple concurrent failures phenomena. Thus we can adjust them globally using a Multi-modes reliability model as multi-Weibull laws. Figure 3 shows the fit of a bi-Weibull model computed from simulated values.

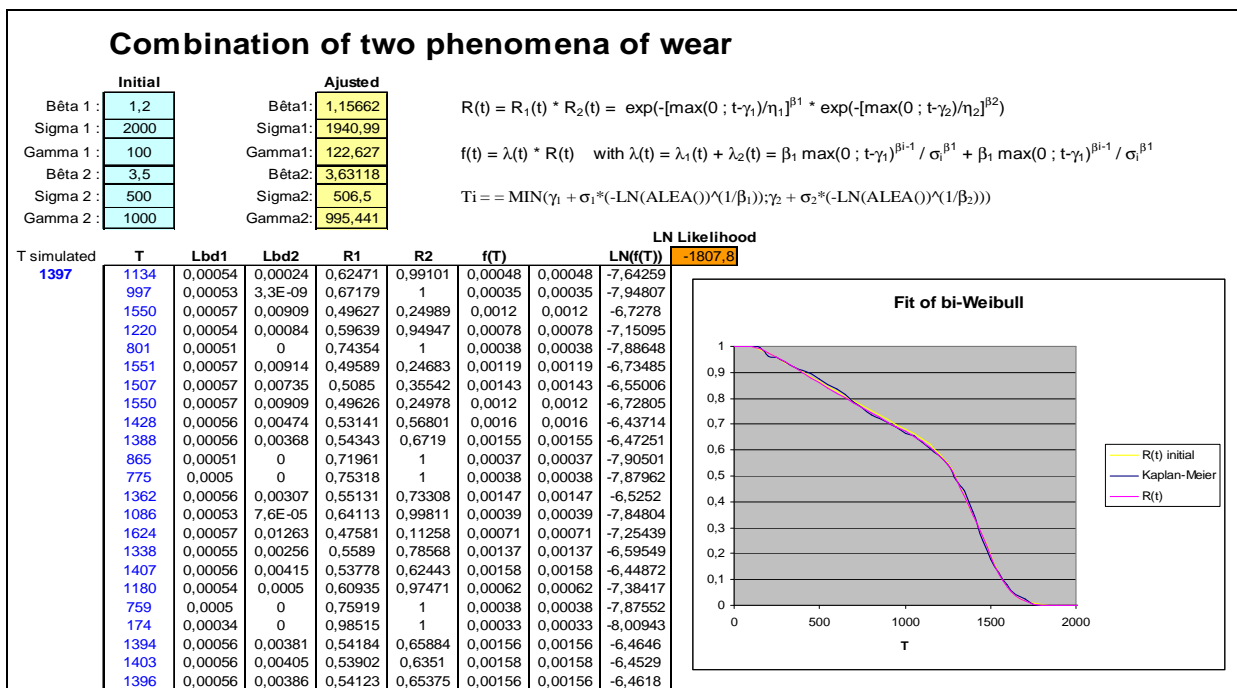


Figure 3. Fit of bi-Weibull from simulated data

2.2. Acceleration Models

Models of accelerated aging are used to reduce the duration of reliability tests by increasing the level of stress. But they can also be used to adjust models of reliability from data obtained under various operational conditions, as shown by the following examples.

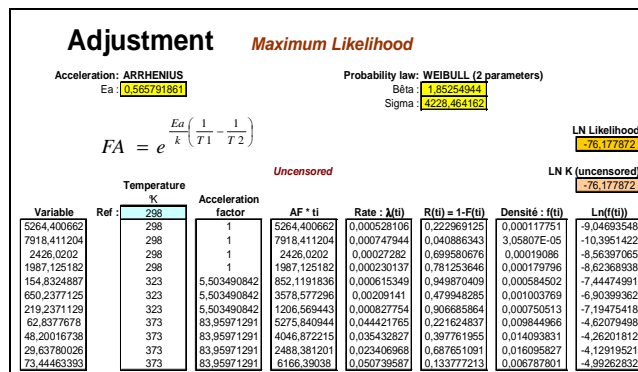


Figure 4. Fit of Weibull distribution coupled with the Arrhenius model (temperature)

Thus, it is possible to adjust various probability distributions (exponential, Weibull, lognormal ...) associated with different acceleration models (Arrhenius, Eyring, Basquin, Cox ...) to operate globally feedback data from equipments subjected to various conditions of use and environment.

It is also possible to enrich reliability databases, such as MIL-HDBK-217 or FIDES guide [4], considering only operational data, both as regards the basic failure rates as the value of parameters used in the expression of acceleration factors.

Thus, figure 5 shows the fit of the integrated circuit model of FIDES Guide, from data previously simulated.

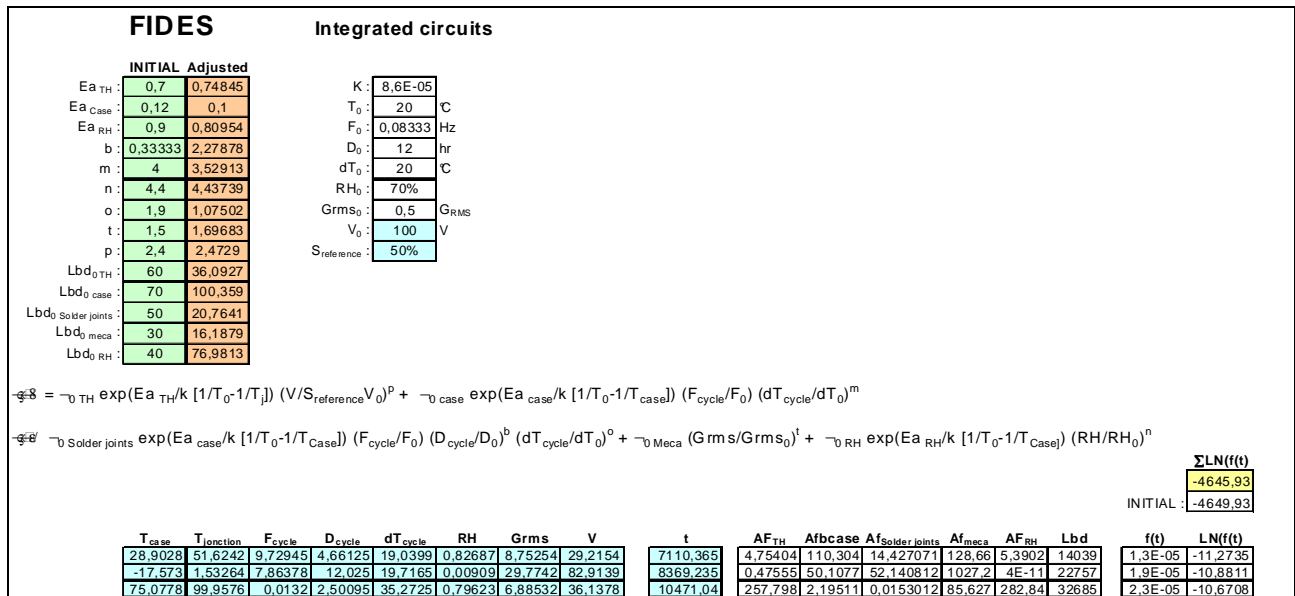


Figure 5. Fit of FIDES model from simulated values

Although this model is particularly complex, it is again possible to find the approximate values of 14 different parameters used to simulate the data.

2.3. Models of maintenance

Models of preventive and corrective maintenance considering the phenomena of rejuvenation can also be adjusted in this way.

In the Generalized Renewal Process, corrective maintenance has a rejuvenating effect proportional to the time elapsed since the previous maintenance (GRP 1) or to the virtual age (GRP 2).

$$\text{GRP1: } A_r = A_{r-1} + q*(t_r - t_{r-1}) \quad \text{GRP2: } A_r = q*(A_{r-1} + t_r - t_{r-1}) \quad (2)$$

Figure 6 shows the fit of GRP2 model from simulated data.

Jack [3] considered that the rejuvenation effect of equipment is more important in the case of preventive maintenance (change of several wear parts) than corrective action (change only the part down). In his model of type 2, the virtual age of equipment at the end of maintenance is equal to the one he had just before, multiplied by a proportion ρ_p in the case of a preventive maintenance or ρ_c in the case of corrective maintenance.

Figure 7 shows the fit of Jack 2 model from simulated data.

GRP 2 process (Generalized Renewal Process)

Density of probability (Weibull): $f(t) = \beta(A_r + t - t_r)^{\beta-1} / \sigma^\beta \exp[(A_r/\eta)^\beta - ([A_r + t - t_r]/\sigma)^\beta]$

	Initial	Ajusted
β :	2,00	1,87
σ :	500,00	493,69
q :	0,85	0,86

Adjustment

LN Likelihood: -936,708803

Simulation $t = tr + \sigma[-\ln(ALEA()) + (A_r/\sigma)^\beta]^{1/\beta} - A_r$

Failure (hours)	Operating time	Virtual age	LN(f(t))
532	532	459	-6,66360369
882	349	697	-6,78769657
972	90	678	-5,65854973
1051	80	653	-5,62264552
1094	43	600	-5,493481
1117	23	537	-5,47981259
1145	28	488	-5,57853328
1193	48	462	-5,69438692
1432	239	604	-6,31469755
1856	423	886	-7,41323781
1873	17	779	-5,16351285
1888	15	684	-5,25015991
2420	532	1048	-8,33797539
2448	28	928	-5,11118329
2531	83	872	-5,519183
2562	31	778	-5,24769942

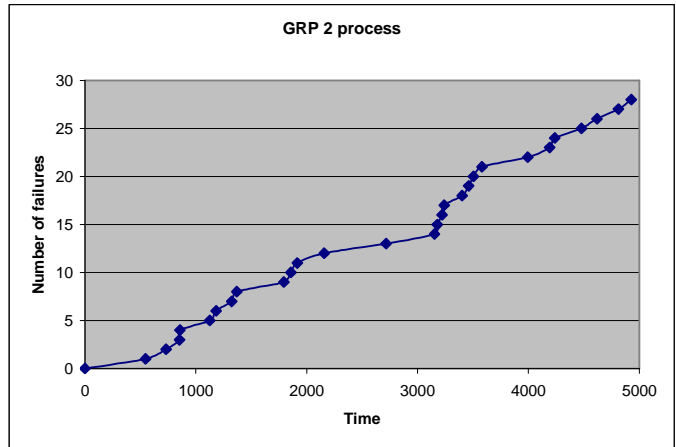


Figure 6. Fit of GRP2 model from simulated values

Aging model Jack 2

Density of probability (Weibull): $f(t) = \beta(A_r + t - t_r)^{\beta-1} / \eta^\beta \exp[(A_r/\eta)^\beta - ([A_r + t - t_r]/\eta)^\beta]$

Reliability: $\exp[(A_r/\eta)^\beta - ([A_r + t - t_r]/\eta)^\beta]$

	Initial	ajusted
β :	2	2,21
η :	600	623,14
pc :	0,7	0,70
pp :	0,3	0,26

Adjustment

LN Likelihood: -489,7434593

Simulation $t_i = tr + \eta[-\ln(ALEA()) + (A_r/\eta)^\beta]^{1/\beta} - A_r$

Preventive (hr)	Corrective (hr)	Virtual age	Operating time	Density of probability (logarithm)	Reliability (logarithm)	LN Likelihood
300	152	45	152	-7,391030033	-0,044427389	-7,391030033
		143	148	-7,133316036	-0,071782509	-0,071782509
600	303	43	3	-7,397104212	-0,001766909	-7,397104212
		253	297	-6,633710255	-0,259924753	-0,259924753
900	1198	411	300	-6,417985913	-0,631766755	-0,631766755
		210	298	-6,417998097	-0,933283993	-6,417998097
1200	1945	157	2	-6,951898998	-0,001630553	-0,001630553
		340	300	-6,473365922	-0,456695325	-0,456695325
1500	2498	476	300	-6,408214813	-0,798549453	-0,798549453
		183	145	-6,08651462	-0,439687221	-6,08651462
1800	2498	252	155	-6,572563567	-0,192952001	-0,192952001
		410	300	-6,41836628	-0,629484725	-0,629484725
2100	2498	150	98	-6,128653362	-0,241653983	-6,128653362
		98	98	-6,128653362	-0,241653983	-6,128653362
2400	2498	262	202	-6,572974171	-0,239658559	-0,239658559
		418	300	-6,415501097	-0,647968249	-0,647968249

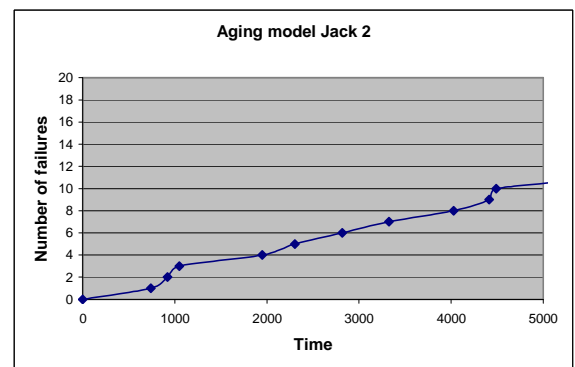


Figure 7. Fit of Jack 2 model from simulated values

2.4. Degradation model and predictive reliability model

A degradation phenomenon can be modelled by a gamma process (with increasing degradation) or a Wiener process (with possible improvements). Between two consecutive observations, the degradation rate is a random variable modelled by a gamma law in the first case and a normal law in the second one [5].

The degradation process can be stationary, if the degradation rate is independent of time, or evolutionary. In this case, the parameter α of the gamma law or the average of the normal distribution can be replaced by a parametric function of time (linear, polynomial, etc.).

An acceleration factor, such as the one of Arrhenius, can be applied to this function (or to the scale parameter of the gamma law) to account for the influence of operating conditions.

The degradation model can be transformed into predictive reliability model, by adding a threshold of acceptability of the degradation level, possibly random (e.g. Gaussian), as shown in Figure 8.

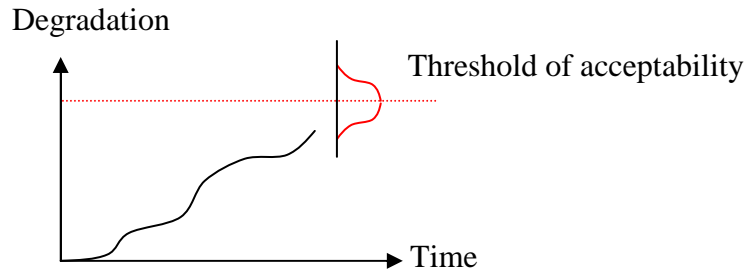


Figure 8. Degradation process

Figure 9 shows a degradation phenomenon simulated by a non-stationary gamma process performed after adjusting data feedback.

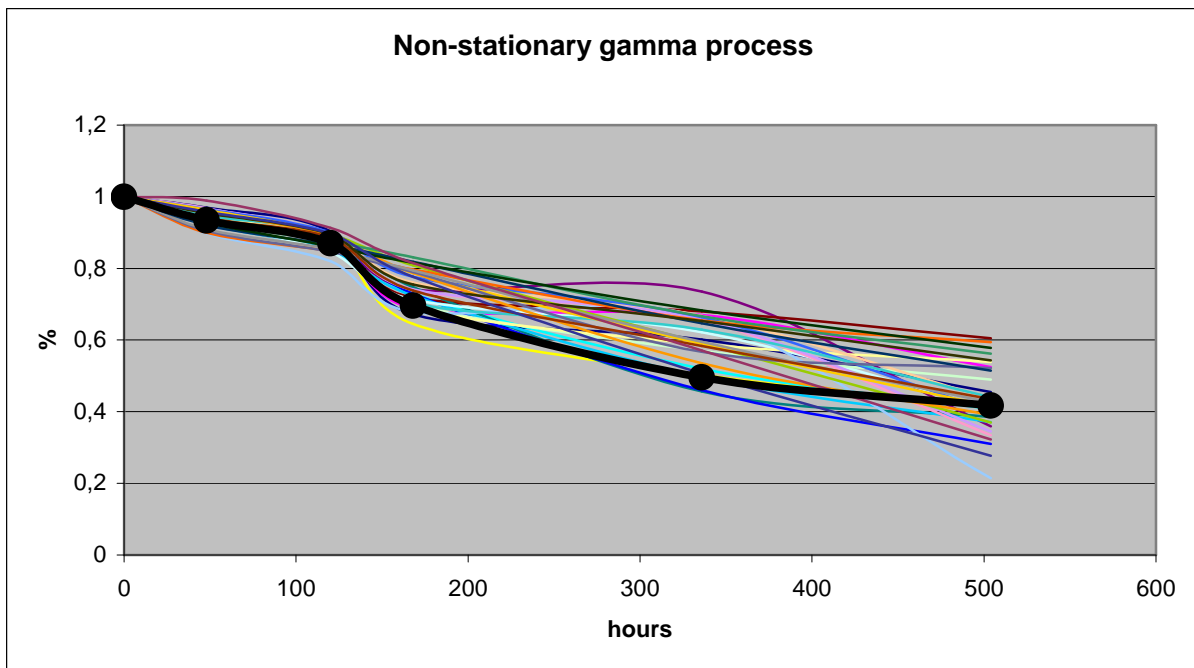


Figure 9. Simulation and data feedback of a degradation process

3. ESTIMATION OF CONFIDENCE INTERVALS IN A DISCRETE MANNER

The estimation theory allows the development of asymptotic confidence intervals from the Fisher information. These intervals can be used only above a minimum sample size for which thirty elements is a commonly accepted value. Indeed, the number of elements has to tend to infinity so that we reach the required level of confidence without control of the speed of convergence.

3.1. Asymptotic confidence intervals

The Fisher information is the variance of the score function, which is the gradient (partial derivative) of the logarithm of the likelihood function.

$$I_n(\theta) = E \left(\left[\frac{\partial \ln L(X, \theta)}{\partial \theta} \right]^2 \right) = -E \left(\frac{\partial^2 \ln L(X, \theta)}{\partial \theta^2} \right) \quad (3)$$

As a first approximation, the maximum likelihood estimator of θ is distributed according to a Gaussian whose variance is equal to the inverse of the Fisher information.

The asymptotic confidence interval of Θ , with confidence level equal to $\beta = 1 - \alpha$, is then:

$$\left[\hat{\theta}_n - \frac{1}{\sqrt{n I(\theta)}} z_{1-\alpha/2}; \hat{\theta}_n + \frac{1}{\sqrt{n I(\theta)}} z_{1-\alpha/2} \right] \quad (4)$$

with $Z_{1-\alpha/2}$ the distribution function of standard normal distribution function.

In the case of a probabilistic model with more parameters, the Fisher information matrix is defined as follows:

$$F_{ij} = I_n(\theta)_{ij} = E \left(\left[\frac{\partial \ln L(X, \theta)}{\partial \theta_i} \right] \left[\frac{\partial \ln L(X, \theta)}{\partial \theta_j} \right] \right) = -E \left(\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_i \partial \theta_j} \right) \quad (5)$$

Or in the case of three parameters:

$$F = I_n(\theta) = \begin{pmatrix} -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_1^2} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_1 \partial \theta_2} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_1 \partial \theta_3} \\ -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_2 \partial \theta_1} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_2^2} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_2 \partial \theta_3} \\ -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_3 \partial \theta_1} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_3 \partial \theta_2} & -\frac{\partial^2 \ln L(X, \theta)}{\partial \theta_3^2} \end{pmatrix} \quad (6)$$

The inverse of the Fisher information matrix is an approximation of the covariance matrix of maximum likelihood estimators.

An asymptotic confidence interval can then be calculated for each parameter from the diagonal elements of this matrix (variance).

Similarly, an asymptotic confidence interval can be calculated for any function $g(\theta)$ of the different parameters (quantile, distribution function ...) by calculating the variance of this function as follows:

$$\sigma_{\hat{g}_n}^2(\theta) = \nabla g(\theta)^T I_n^{-1}(\theta) \nabla g(\theta) \quad (7)$$

with $\nabla g(\theta)$ et $\nabla g(\theta)^T$ the gradient of g and its transpose and $I_n^{-1}(\theta)$ the inverse of the Fisher matrix

3.2. Discrete calculation method

To avoid the calculation of second derivatives and partial derivatives in the Fischer matrix, it is possible to make these calculations in a generic manner for any probability models by using a discrete calculation method based on Taylor formulas.

The second derivatives in Θ_i of the log likelihood function can be calculated as follows from a small increment h:

$$\begin{aligned}
 f(\hat{\theta}_i + h) &= f(\hat{\theta}_i) + \frac{\partial f}{\partial \theta_i}(\hat{\theta}_i) \times h + \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i) \times \frac{h^2}{2} + \varepsilon(h) \\
 f(\hat{\theta}_i - h) &= f(\hat{\theta}_i) - \frac{\partial f}{\partial \theta_i}(\hat{\theta}_i) \times h + \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i) \times \frac{h^2}{2} + \varepsilon(h) \\
 f(\hat{\theta}_i + h) + f(\hat{\theta}_i - h) &= 2f(\hat{\theta}_i) + \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i) \times h^2 + 2\varepsilon(h) \\
 \Rightarrow \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i) &= \lim_{h \rightarrow 0} \frac{f(\hat{\theta}_i + h) + f(\hat{\theta}_i - h) - 2f(\hat{\theta}_i)}{h^2}
 \end{aligned} \tag{8}$$

Similarly, the partial derivatives in $\Theta_i \Theta_j$ can be calculated as follows using small increments h and k:

$$\begin{aligned}
 f(\hat{\theta}_i + h, \hat{\theta}_j + k) &= f(\hat{\theta}_i, \hat{\theta}_j) + h \times \frac{\partial f}{\partial \theta_i}(\hat{\theta}_i, \hat{\theta}_j) + k \times \frac{\partial f}{\partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) + \frac{1}{2} [h^2 \times \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i, \hat{\theta}_j) + 2hk \times \frac{\partial^2 f}{\partial \theta_i \partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) + k^2 \times \frac{\partial^2 f}{\partial \theta_j^2}(\hat{\theta}_i, \hat{\theta}_j)] + (h^2 + k^2) \varepsilon(h, k) \\
 f(\hat{\theta}_i - h, \hat{\theta}_j - k) &= f(\hat{\theta}_i, \hat{\theta}_j) - h \times \frac{\partial f}{\partial \theta_i}(\hat{\theta}_i, \hat{\theta}_j) - k \times \frac{\partial f}{\partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) + \frac{1}{2} [h^2 \times \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i, \hat{\theta}_j) + 2hk \times \frac{\partial^2 f}{\partial \theta_i \partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) + k^2 \times \frac{\partial^2 f}{\partial \theta_j^2}(\hat{\theta}_i, \hat{\theta}_j)] + (h^2 + k^2) \varepsilon(h, k) \\
 f(\hat{\theta}_i + h, \hat{\theta}_j + k) + f(\hat{\theta}_i - h, \hat{\theta}_j - k) &= 2f(\hat{\theta}_i, \hat{\theta}_j) + h^2 \times \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i, \hat{\theta}_j) + 2hk \times \frac{\partial^2 f}{\partial \theta_i \partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) + k^2 \times \frac{\partial^2 f}{\partial \theta_j^2}(\hat{\theta}_i, \hat{\theta}_j) + 2(h^2 + k^2) \varepsilon(h, k) \\
 \Rightarrow \frac{\partial^2 f}{\partial \theta_i \partial \theta_j}(\hat{\theta}_i, \hat{\theta}_j) &= \lim_{(h,k) \rightarrow (0,0)} \frac{f(\hat{\theta}_i + h, \hat{\theta}_j + k) + f(\hat{\theta}_i - h, \hat{\theta}_j - k) - 2f(\hat{\theta}_i, \hat{\theta}_j) - h^2 \times \frac{\partial^2 f}{\partial \theta_i^2}(\hat{\theta}_i, \hat{\theta}_j) - k^2 \times \frac{\partial^2 f}{\partial \theta_j^2}(\hat{\theta}_i, \hat{\theta}_j)}{2hk}
 \end{aligned} \tag{9}$$

This calculation method was implemented in the GENCAB software and its accuracy was verified by comparing its results with those obtained by the Fisher matrices computed "by hand" by deriving analytical expressions as follows in the case of Weibull law:

$$L(X; \beta, \sigma, \gamma) = \prod_{i=1}^n f(X_i; \beta, \sigma, \gamma) \text{ with } f(X_i; \beta, \sigma, \gamma) = \frac{\beta}{\sigma} \left(\frac{X_i - \gamma}{\sigma} \right)^{\beta-1} \exp\left(-\left(\frac{X_i - \gamma}{\sigma}\right)^\beta\right) \tag{10}$$

$$I_n(\beta, \sigma, \gamma) = \begin{pmatrix} \frac{n}{\beta^2} + \sum_{i=1}^n \frac{(X_i - \gamma)^\beta}{\sigma^\beta} [Ln(\frac{X_i - \gamma}{\sigma})]^2 & \frac{n}{\sigma} - \sum_{i=1}^n \left[\frac{(X_i - \gamma)^\beta}{\sigma^{\beta+1}} \times (1 + \beta \times Ln(\frac{X_i - \gamma}{\sigma})) \right] & - \sum_{i=1}^n \frac{(X_i - \gamma)^{\beta-1}}{\sigma^\beta} \left[1 + \beta \times Ln(\frac{X_i - \gamma}{\sigma}) \right] - \frac{1}{(X_i - \gamma)} \\ \frac{n}{\sigma} - \sum_{i=1}^n \left[\frac{(X_i - \gamma)^\beta}{\sigma^{\beta+1}} \times (1 + \beta \times Ln(\frac{X_i - \gamma}{\sigma})) \right] & \frac{-n\beta}{\sigma^2} + \frac{\beta(\beta+1) \sum_{i=1}^n (X_i - \gamma)^\beta}{\sigma^{\beta+2}} & \frac{\beta^2}{\sigma^{\beta+1}} \sum_{i=1}^n (X_i - \gamma)^{\beta-1} \\ - \sum_{i=1}^n \frac{(X_i - \gamma)^{\beta-1}}{\sigma^\beta} \left[1 + \beta \times Ln(\frac{X_i - \gamma}{\sigma}) \right] - \frac{1}{(X_i - \gamma)} & \frac{\beta^2}{\sigma^{\beta+1}} \sum_{i=1}^n (X_i - \gamma)^{\beta-1} & -(1 - \beta) \sum_{i=1}^n \frac{1}{(X_i - \gamma)^2} - \frac{\beta(\beta-1)}{\sigma^\beta} \sum_{i=1}^n (X_i - \gamma)^{\beta-2} \end{pmatrix} \tag{11}$$

The results obtained are very close as shown in Figure 10.

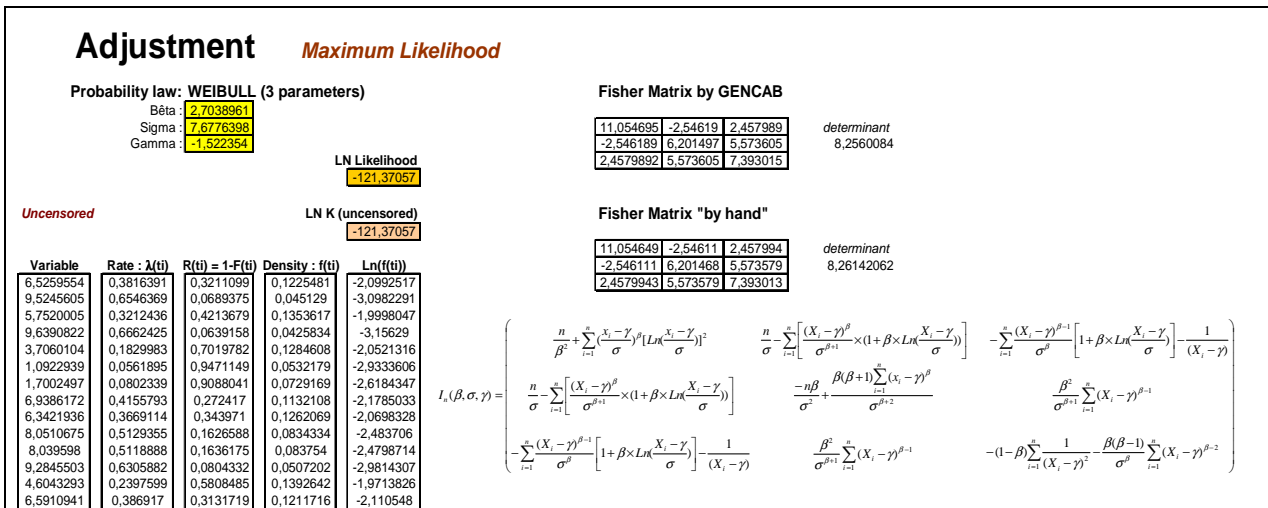


Figure 10. Comparison of results for the Weibull law

4. CONCLUSION

A global optimization tool allows complex probabilistic models to be adjusted and thus facilitates the use of data feedback.

It is particularly valuable for predictive maintenance and health monitoring which are a real “Gaal” for the reliability-community. Indeed, this makes it possible to space out the maintenance actions (on average) while paradoxically reducing the risk of failure.

In addition, asymptotic confidence intervals can be calculated by a generic method, based on the Taylor formula, which gives accurate results.

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