New prediction interval and band in the nonlinear regression model: Application to predictive modelling in food science

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Title:

New prediction interval and band in the nonlinear regression model:

Application to predictive modelling in foods

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Abstract:

This paper is concerned with the proposal of a new **prediction interval** and band for the nonlinear regression model. The construction principle of this interval and band is based on an exact (the meaning of the term "exact" will be given later) confidence region for parameters of the nonlinear regression model. This region, fully described in Vila & Gauchi (2007), provides a rigorous justification for the new **prediction interval** and band that we propose. This new band is then compared to the classical bands (which are asymptotic and thus approximate for small n), and also to the band based on the bootstrap resampling method. The comparison of these bands is undertaken with simulated and real data from predictive modelling in food science.

Keywords: Prediction interval; Prediction band; Nonlinear regression; Parametric confidence region; Predictive modelling; **Food Science**.

1 Introduction

The question of the construction of **prediction intervals** (PI) for a single value or a mean and for **prediction bands** (PB) was extensively studied and solved in the case of linear regression models. The most frequently used solution was developed by Working and Hotelling (1929) and is detailed in Draper and Smith (1981). It leads to the familiar hyperbolic curves surrounding the regression model

curve. However, several methods are always in competition for nonlinear regression models, and there is no rule for making a definitive choice for a given model. Our aim is therefore to compare four well-known PI and PB on simulated and real data to the new PI and PB we propose, using familiar predictive microbiology models in foods. The first two PI and PB are based on a first-order Taylor approximation of the model analytic form and are called asymptotic PI and PB (see Bates and Watts, 1988). The third PI and PB are based on the bootstrap resampling method (Efron and Tibshirani, 1993). The new PI and PB we propose are based on an exact (see Section 4 for the meaning of the term "exact") confidence parametric region (the X -region fully described in Vila & Gauchi, 2007). The new PI will be referred to as PI_X and the new PB as PB_X .

It is necessary to draw the reader's attention to a crucial point here. We are not actually dealing with genuine prediction regions (note the difference between the words "regions" and "bands") of the model curve. A true prediction region for the model curve is a region where there is a fixed probability of finding this whole model curve completely inside this region. In fact, this question has not yet been totally solved because a genuine region can be too large and of no use to the practitioner. Thus, an approach based on a genuine prediction region is not always a relevant approach. Instead, we prefer to propose a PB made of joint adjacent prediction intervals. The global predictive capability will therefore be

quantified by the band area. The rest of the article is organized as follows. Section 2 presents some useful notations for the reader. Section 3 provides information on asymptotic and bootstrap bands. Section 4 gives details on the new PI_X and PB_X we propose. Section 5 is devoted to the comparison of the four bands in the food science predictive modelling field; and Section 6 is the conclusion.

2 Notations

Let us consider the standard parametric nonlinear regression model

$$y_i = \eta(x_i, \theta^*) + \varepsilon_i \quad ; \quad i = 1, \dots, n \quad (1)$$

with the following notations: (a) y_i is the i^{th} observation of the response (the corresponding $n \times 1$ vector of the y_i is referred to as y); (b) x_i is an $m \times 1$ vector – a support point – with component x_{il} , $l = 1, \dots, m$, and $x_i \in \Xi \subset \mathbb{R}^m$, where Ξ , a compact subset of $\mathbb{R}^m$, is the experimental domain. For the sake of briefness, we will refer to the $n \times m$ matrix X as the whole set of the m explanatory variables set at n levels; (c) We assume that the errors ε_i , components of the $n \times 1$ vector ε , are independent and normally distributed; they have the same variance σ^2 (generally unknown). Then, $\varepsilon \sim \mathcal{N}(0, \Sigma)$, where $\Sigma = \sigma^2 I_n$ (I_n is the $n \times n$ identity matrix); (d) θ^* is the $p \times 1$ vector of the unknown p parameters to be estimated, $\theta^* \in \Theta \subset \mathbb{R}^p$, where Θ is the parametric domain, a compact subset of $\mathbb{R}^p$; (e) $\eta(\cdot)$ is a continuous

real-valued scalar function of x defined on $\Xi \times \Theta$, twice differentiable with respect to the parameters and the variables; we will simply refer to the corresponding $n \times 1$ vector as η or η_θ (function of the θ variable); (f) n is the total number of observations y_i .

We used the ordinary nonlinear least squares estimate $\hat{\theta}$ as an estimate of θ^*

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{Argmin}} \left\{ (y - \eta_\theta)^T \Sigma^{-1} (y - \eta_\theta) \right\} = \underset{\theta \in \Theta}{\operatorname{Argmin}} \|y - \eta_\theta\|_\Sigma^2 \quad (2)$$

We also considered the Fisher information matrix $M_F(X, \theta^*)$

$$M_F(X, \theta^*) = \sigma^{-2} J_{X, \theta^*}^T J_{X, \theta^*} \quad (3)$$

where J_{X, θ^*} is the $n \times p$ Jacobian matrix, with the j^{th} column consisting of the n components of $\partial \eta(X, \theta^*) / \partial \theta_j^*$, $j = 1, \dots, p$.

A model prediction at any point x_i is defined as

$$\hat{y}_i = \eta(x_i, \hat{\theta}) \quad (4)$$

For further use, we also define the $(1 \times p)$ -vector, a **row** of $J_{X, \theta}$, as:

$$\left[\dot{\eta}(x_i, \hat{\theta}) \right]^T = \left(\frac{\partial \eta(x_i, \theta)}{\partial \theta_1} \Big|_{\theta_1 = \hat{\theta}_1} \cdots \frac{\partial \eta(x_i, \theta)}{\partial \theta_p} \Big|_{\theta_p = \hat{\theta}_p} \right). \quad (5)$$

3 Classical PI and PB

3.1 Principle

As reported by Khorasani & Milliken (1982), the problem of constructing a prediction band around a regression model can be viewed as a problem of simultaneously constructing an infinite set of confidence intervals. Let us assume that $E(y_0) = \eta(x_0, \theta^*)$ is the mean of some y_0 , and that $\hat{y}_0 = \hat{E}(y_0) = \eta(x_0, \hat{\theta})$, the mean prediction, is its estimation. We are interested in determining a PI for y_0 , followed by a PB for the regression model. The objective will be fully satisfied if the confidence level of the PI s and that of the PB s is as close as possible to $1 - \alpha$ where α is a **first-kind error**.

Thus, the first step is to construct a PI for y_0 (located on x_0) defined as:

$$PI(y_0, x_0, \alpha) = [L(\hat{y}_0, x_0, \alpha) ; U(\hat{y}_0, x_0, \alpha)]$$

where $L(\hat{y}_0, x_0, \alpha)$ is the lower bound of the interval, and $U(\hat{y}_0, x_0, \alpha)$ is the upper bound of the interval.

The second step is then to determine a PB over Ξ . It should be observed that if $\Xi \subset R^m$, with $m = 1$, we then consider a band, but if $m \geq 2$, we will refer to it as a **prediction region** (PR), different from a genuine prediction region (see the crucial point in the introduction). The upper curve (or the m -dimensional

upper surface) of the **prediction band** (or a PR) is theoretically made up of an infinite number of upper ends (points) of adjacent PI , and the lower curve is made in a similar way. From a practical point of view, a large number K of adjacent PI at K support points x_i will be built. Typically, K is equal to 200 when $m = 1$, and $K \geq 1000$ when $m > 1$. It should be observed that if m is large – typically larger than 4 – then a Monte Carlo approach would be necessary for randomly (uniformly) choosing the locations x_i in Ξ where $U(\cdot)$ and $L(\cdot)$ could be computed. Alternatively, other methods such as grid methods could be used. For characterizing a band (or a region), we propose to determine an approximation of its area $\mathcal{A}$ (or its volume $\mathcal{V}$) by means of a standard numerical integration (a procedure based on the summation of elementary rectangles that form the band, or a usual Monte Carlo integration procedure in the case of a region).

3.2 Intervals and bands based on an asymptotic approach

Let us consider the random variable

$$\hat{T} = \frac{\hat{y}_0 - y_0}{h_{x_0}^{1/2}(\hat{\theta})} \quad (6)$$

where

$$h_{x_0}(\hat{\theta}) = \hat{\sigma}^2 \left[\dot{\eta}(x_0, \hat{\theta}) \right]^T \left(J_{X, \hat{\theta}}^T J_{X, \hat{\theta}} \right)^{-1} \left[\dot{\eta}(x_0, \hat{\theta}) \right] \quad (7)$$

and where

$$\hat{\sigma}^2 = \frac{1}{n-p} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (8)$$

Classical asymptotic theory (Gallant, 1987) tells us that the limiting distribution (when n tends to infinity) of (6) is a centered normal distribution $\mathcal{N}(0, 1)$ where $h_{x_0}^{1/2}(\hat{\theta})$ is an estimate of the standard error of $\hat{y}_0$. However, for small fixed n , the true distribution of $\hat{T}$ is not a normal one and is not known. Nevertheless, we have somewhat accurate approximations of the true distribution when n is not infinite, which lead to confidence interval approximations. Typically, on the basis of Gallant (1987), we have:

$$PI_t(y_0, x_0, \alpha) = [\hat{y}_0 - t_{n-p;1-\alpha/2} h_{x_0}^{1/2} ; \hat{y}_0 + t_{n-p;1-\alpha/2} h_{x_0}^{1/2}] \quad (9)$$

where $t_{n-p;1-\alpha/2}$ is the $(1 - \alpha/2)$ -percentile for the Student distribution with $n - p$ degrees of freedom. The whole set of the joint PI_t s leads to the PB_t .

On the basis of Bates & Watts (1988), we can use a good alternative defined as:

$$PI_F(y_0, x_0, \alpha) = [\hat{y}_0 - (h_{x_0} p \mathcal{F}_{p,n-p;\alpha})^{1/2} ; \hat{y}_0 + (h_{x_0} p \mathcal{F}_{p,n-p;\alpha})^{1/2}] \quad (10)$$

where $\mathcal{F}_{p,n-p;\alpha}$ is the upper α -percentile for the **Fisher-Snedecor** distribution with p and $n - p$ degrees of freedom. This interval definition leads to a so-called

130 simultaneous **prediction band** PB_F .

131 These methods are called asymptotic in the nonlinear case because it has been
 132 proven (see Gallant, 1987) that PI_t and PI_F tend to an exact PI as $n \rightarrow \infty$. In
 133 this case, the word "exact" means that the coverage probability of y_0 is exactly
 134 equal to $1 - \alpha$. For a fixed n , particularly if n is small, PI_t and PI_F are only
 135 approximate, and their covering probabilities are not equal to $1 - \alpha$, and are close
 136 to $1 - \alpha$ if n is large enough.

137 3.3 Interval and band based on the bootstrap method

138 This method is based on the famous resampling method called the bootstrap
 139 method (Efron and Tibshirani, 1993). Many statistics can be estimated with this
 140 method, particularly the construction of confidence intervals, as clearly described
 141 in Huet et al. (2004, page 138). We only give the results here:

$$PI_B(y_0, x_0, \alpha) = \left[\hat{y}_0 - b_{1-\alpha/2} h_{x_0}^{1/2}(\hat{\theta}) ; \hat{y}_0 - b_{\alpha/2} h_{x_0}^{1/2}(\hat{\theta}) \right] \quad (11)$$

142 where $b_{1-\alpha/2}$ and $b_{\alpha/2}$ are the $1 - \alpha/2$ -percentile and $\alpha/2$ -percentile, respectively,
 143 of the bootstrap distribution of $\hat{y}_0$. Generally, for a given n (not infinity), it can
 144 be assumed that PB_B will be narrower than PB_t and PB_F for a confidence level
 145 close to $1 - \alpha$.

4 A new prediction band

4.1 The X -region

Because the PB_X is based on an exact confidence region for the parameters of a nonlinear regression model – the X -region fully described in Vila and Gauchi (2007) – we have included the following definition for the reader's information:

Definition 1 *Let $C(\theta^*)$ be the covering probability of θ^* . The confidence region of nominal level α for θ^* is then said to be approximate if $C(\theta^*) \approx 1 - \alpha$, asymptotic if $\lim_{n \rightarrow \infty} C(\theta^*) = 1 - \alpha$, conservative if $C(\theta^*) \geq 1 - \alpha$, and exact if $C(\theta^*) = 1 - \alpha$, $\forall n$.*

The X -region we used is defined as:

$$\mathfrak{R}_X(\theta^*, y) = \{\theta \in \Theta : R_X(\theta) \leq \mathcal{F}_{p, \nu; \alpha}\} \quad (12)$$

where $R_X(\theta) = (y - \eta_\theta)^T P_\theta (y - \eta_\theta) / ps_\nu^2$ with $P_\theta = J_{X, \theta} (J_{X, \theta}^T J_{X, \theta})^{-1} J_{X, \theta}^T$, the usual projector onto the plane, tangent at η_θ , on the model response surface (see Bates and Watts, 1988, p.36, for a clear presentation), and s_ν^2 an estimate of σ^2 , based on ν degrees of freedom (d.o.f.). $\mathcal{F}_{p, \nu; \alpha}$ is the α -percentile of the Fisher-Snedecor distribution $\mathcal{F}_{p, \nu}$ with p and ν d.o.f. If s_ν^2 is not available, it will be replaced by the mean square error (and, thus, $\nu = n - p$ in this case) of the regression procedure. A graph of this region is displayed in Vila and Gauchi (2007). It may look very

different from the ellipsoidal confidence region often used as an approximative region.

We would like to remind the reader here of some important properties of the X -region (Vila and Gauchi, 2007): the X -region does not depend on intrinsic and parametric nonlinearities of the model $\eta(\cdot)$, and the true Θ is taken into account in its construction. These properties are enhanced if n is small and σ is large. Consequently, the PB_X will benefit from these properties of the X -region, to the contrary of the preceding PBs . Indeed, we know that these two conditions make the usual first-order approximation involved in PI_t and PI_F inadequate.

4.2 The PB_X

We can now construct the PB_X . This band is formed by joining K (see Subsection 3.1) adjacent PI_X . A PI_X for y_i is then built by means of the four steps of the following simple algorithm based on Monte Carlo samplings:

Step 1

If $p \leq 3$: uniformly sample a large number Q of vectors $\tilde{\theta}_u \in \Theta$, $u = 1, \dots, Q$ (typically $Q = 1000$ for $p = 1$, $Q = 10^4$ for $p = 2$, $Q = 5 \times 10^4$ for $p = 3$, since these values are now easily attainable with powerful modern computers). Among the Q vectors $\tilde{\theta}_u$, only Q^* satisfy the inequality in (12). Thus, the set of these Q^* vectors $\tilde{\theta}_u$ forms an approximation of the volume of (12).

182 If $p > 3$: sample a large number Q of uniform random straight half lines $L_k \in \Theta$,
 183 $k = 1, \dots, Q$, whose origins are all located at θ_0 and whose slopes are random
 184 (typically $Q = 10^4$ for $p = 4, 5$, or 6 , $Q = 10^5$ for $6 < p \leq 10$). On each
 185 random line L_k , choose a number q_k of values $\tilde{\theta}_u$, $u = 1, \dots, q_k$, regularly
 186 spaced on this line. The same stepsize is used for all the lines, and each q_k
 187 depends on the proximity of θ_0 from the border of the X -region along the
 188 L_k line. Finally, only Q^* vectors $\tilde{\theta}_u$ among the $\sum_{k=1}^Q q_k$ vectors satisfy the
 189 inequality in (12). It should be observed that the sampling used for $p \leq 3$
 190 would be very ineffective here because it is well-known that the random $\tilde{\theta}_u$
 191 would be increasingly often located in the corners of Θ when the dimension
 192 of Θ increases.

193 **Step 2** Choose x_i as the place in Ξ where we want to make a prediction.

194 **Step 3** Compute the Q^* values $\hat{y}_i^{(u)} = \eta(x_i, \tilde{\theta}_u)$, $u = 1, \dots, Q^*$.

195 **Step 4** Determine the lower bound of the PI_X by $L = \min_u \{\hat{y}_i^{(u)}\}$, and the upper
 196 bound of the PI_X by $U = \max_u \{\hat{y}_i^{(u)}\}$.

197 The exact confidence level of this band is not yet clear but we can assume that it
 198 tends to $\beta \geq 1 - \alpha$ when Q^* increases because the function $\eta(x_i, \theta)$ is surjective
 199 relative to θ . Consequently, the PB_X is a conservative band.

5 Applications to predictive modelling in food science

5.1 A primary growth model: the Baranyi & Roberts model

5.1.1 Definition

The analytic form of this model (the deterministic part) proposed by Baranyi and Roberts (1994, 1995), including four parameters and one explanatory factor, is:

$$\eta(\theta^*, t) = \frac{1}{\ln(10)} [\ln(x_0) + \mu_{\max} A(\theta^*, t) - \ln(B(\theta^*, t))]$$

where

$$A = t + \frac{1}{\mu_{\max}} \ln(A_0)$$

$$A_0 = \exp(-\mu_{\max} t) + \exp(-\mu_{\max} lag) - \exp(-\mu_{\max} t - \mu_{\max} lag)$$

$$B = 1 + \frac{[\exp(\mu_{\max} A)] - 1}{\frac{x_{\max}}{x_0}}$$

with $\mu_{\max}$ (maximum growth rate), lag (lag time before growth, in hours), $x_{\max}$ (maximal number of bacteria), x_0 (initial number of bacteria), the four components

of θ^* , and time t (the explanatory factor). $\eta(\theta^*, t)$ is the number of bacteria (in log units).

5.1.2 Results with simulated data

We first present an illustration with the *a priori* values $\mu_{\max 0} = 1$; $lag_0 = 5$; $x_{\max 0} = 10^8$; $x_{00} = 100$, and $\Theta = [0.5; 1.5]_{\mu_{\max 0}} \times [2; 8]_{lag_0} \times [0.5 \times 10^8; 1.5 \times 10^8]_{x_{\max 0}} \times [50; 150]_{x_{00}}$, and $\Xi = [0, 50]$. With this information (from the SYMPREVIUS Research Group, see Acknowledgements Section) we simulated ten Gaussian y_i values (with standard deviation equal to 0.1) at ten equidistant levels of time. We obtained Fig. 1 after computation of $\hat{\theta} = (1.18 ; 5.44 ; 1.5 \times 10^8 ; 50)^T$ by means of the NLIN procedure of SAS/STAT software.

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Fig. 1: The four bands for the Baranyi-Roberts model for one **simulated** data set (crosses stand for the simulated data). The values of the band areas (calculated with procedures indicated at the end of Subsection 3.1) are: $\mathcal{A}(PB_t) = 21$; $\mathcal{A}(PB_F) = 36$; $\mathcal{A}(PB_B) = 24$; $\mathcal{A}(PB_X) = 42$.

For a more relevant comparison, we simulated 1000 data sets, each data set being defined as the pairs $\{(t_u, \tilde{y}_u) ; u = 1, \dots, 10\}$, where the t_u were always equal to the ten previous levels. Each random $\tilde{y}_u$ was generated by a Gaussian distribution

227 $\mathcal{N}(y_i, \sigma_S)$ where y_i was the previous simulated value. Three values of σ_S were used:
 228 $\sigma_S = 0.05; 0.1; 0.5$, these values being typical of real experimental situations. For
 229 each σ_S -situation, we provide the simulation results in Table 1.

Areas	min	max	mean	std	cv%
$\mathcal{A}(PB_t)$	33 ; 31 ; 38	40 ; 44 ; 91	36 ; 37 ; 63	1.5 ; 3 ; 12	4 ; 8 ; 20
$\mathcal{A}(PB_F)$	57 ; 54 ; 66	69 ; 77 ; 159	63 ; 65 ; 110	2.6 ; 5 ; 21	4 ; 8 ; 19
$\mathcal{A}(PB_B)$	60 ; 60 ; 82	86 ; 125 ; 252	78 ; 97 ; 191	6 ; 18 ; 44	7 ; 18 ; 8
$\mathcal{A}(PB_X)$	62 ; 61 ; 46	64 ; 66 ; 71	63 ; 63 ; 61	0.6 ; 1 ; 5	1 ; 1.7 ; 8

231 Table 1: Baranyi-Roberts model: Simulation statistics of the band areas based on
 232 1000 simulated data sets. The figures are given sequentially according to $\sigma_S = 0.05$;
 233 0.1; 0.5, respectively. For example, for $\sigma_S = 0.05$, we obtain $\min(\mathcal{A}(PB_t)) = 33$,
 234 $\max(\mathcal{A}(PB_t)) = 40$, $\text{mean}(\mathcal{A}(PB_t)) = 36$, $\text{std}(\mathcal{A}(PB_t)) = 1.5$, $\text{cv}\%(\mathcal{A}(PB_t)) =$
 235 4.

236 5.1.3 An illustration with real data

237 With real data (obtained from the SYMPREVIUS Research Group, see Acknowl-
 238 edgements Section) we obtained Fig. 2 where the estimated model curve is based
 239 on $\hat{\mu}_{\max} = 0.055$; $\widehat{lag} = 42$; $\hat{x}_{\max} = 1.52 \times 10^8$; $\hat{x}_0 = 4005$; $\Theta = [0.050; 0.060]_{\mu_{\max} 0}$
 240 $\times [30; 54]_{lag 0} \times [38124759; 266660000]_{x_{\max} 0} \times [2715; 5294]_{x_{00}}$, and $\Xi = [0; 310]$.

241 *The figure 2 should be approximately placed here*

Fig. 2: The four bands for the Baranyi-Roberts model for one real data set (crosses stand for the real data). The values of the band areas are: $\mathcal{A}(PB_t) = 70$; $\mathcal{A}(PB_F) = 111$; $\mathcal{A}(PB_B) = 98$; $\mathcal{A}(PB_X) = 166$.

5.1.4 Discussion

We can see on Fig. 1 that the PB_t and PB_F bands are totally inadequate when the model appears as a zero-slope straight line. Indeed, the band is reduced to a single line while the variability of the prediction is not null. On the contrary, the other two bands seem more realistic since their width is not null. Moreover, we can see on Fig. 2 that more data lie outside the PB_t , PB_F and PB_B , contrast to the PB_X . In Table 1, we can observe that the PB_X does not appear to be not very sensitive to the change of the simulation σ_S ; moreover, its area is close to that of the PB_F .

5.2 An inactivation model: the double-Weibull model

5.2.1 Definition

The analytic form of this model (the deterministic part) proposed by Coroller (2006), including five parameters and one explanatory factor, is:

$$\eta(\theta^*, t) = C - \log_{10}(1 + 10^\alpha) + \log_{10} \left[10^{-\left(\frac{t}{\delta_1}\right)^p + \alpha} + 10^{-\left(\frac{t}{\delta_2}\right)^p} \right]$$

where $C = \log_{10} N_0$ (where N_0 is the initial number of bacteria), α and p are shape parameters, δ_1 and δ_2 are treatment times for the first decimal reductions, $\eta(\theta^*, t)$ is the bacteria number (in log units), and t is the time (in hours), the explanatory factor. The vectorial parameter we are interested in is $\theta = (C, \alpha, p, \delta_1, \delta_2)^T$.

5.2.2 Results with simulated data

We first present an illustration with the *a priori* values $C_0 = 5.45$; $\alpha_0 = 3.15$; $p_0 = 3.67$; $\delta_{10} = 5.45$; $\delta_{20} = 17.21$, and $\Theta = [5; 6]_{C_0} \times [2; 4]_{\alpha_0} \times [1.5; 6]_{p_0} \times [4; 7]_{\delta_{20}} \times [12; 20]_{\delta_{20}}$, and $\Xi = [0; 20]$ (Coroller, 2006). Using this information we simulated 20 Gaussian y_i values (with standard deviation equal to 0.1) at 20 equidistant levels of time. We obtained Fig. 3 after computation of $\hat{\theta} = (5.56; 3.15; 2.99; 5.17; 16.50)^T$ by means of the NLIN procedure of SAS/STAT software.

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269 *The figure 3 should be approximately placed here*

270 Fig. 3. The four bands for the **Coroller** model for one **simulated** data set (crosses
271 stand for the simulated data). The values of the band areas are: $\mathcal{A}(PB_t) = 7.82$;
272 $\mathcal{A}(PB_F) = 13.97$; $\mathcal{A}(PB_B) = 8.90$; $\mathcal{A}(PB_X) = 13.38$. It should be noted that
273 days appear on the abscisses, but the parameters are given in the text for the time
274 in hours.

275
276 For a more relevant comparison, we simulated 1000 data sets, each data set being
277 defined as the pairs $\{(t_u, \tilde{y}_u); u = 1, \dots, 10\}$ where t_u were always equal to the
278 20 previous levels. We proceded as in Subsection 5.1.2, and we obtained the
279 simulation results given in Table 2.

Areas	min	max	mean	std	cv%
$\mathcal{A}(PB_t)$	8 ; 8 ; 19	10 ; 13 ; 35	9 ; 10 ; 26	0.5 ; 0.96 ; 3.7	5 ; 9 ; 14
$\mathcal{A}(PB_F)$	15 ; 15 ; 33	19 ; 22 ; 62	17 ; 19 ; 47	0.89 ; 1.7 ; 6.6	5 ; 9 ; 14
$\mathcal{A}(PB_B)$	10 ; 11 ; 29	26 ; 42 ; 96	20 ; 32 ; 73	4 ; 8 ; 13	20 ; 24 ; 18
$\mathcal{A}(PB_X)$	31 ; 31 ; 36	33 ; 33 ; 35	32 ; 32 ; 31	0.36 ; 0.54 ; 1.95	1.1 ; 1.7 ; 6

281 Table 2 : Coroller model: Simulation statistics of the band areas. The figures are
282 given sequentially according to $\sigma_S = 0.05$; 0.1; 0.5, respectively. The figures have
283 been rounded off.

5.2.3 An illustration with real data

With real data (Coroller, 2006), we obtained Fig. 4 where the estimated model curve is based on $\hat{C}_0 = 5.39$; $\hat{\alpha} = 3.06$; $\hat{p} = 3.53$; $\hat{\delta}_1 = 5.54$; $\hat{\delta}_2 = 17.44$.

The figure 4 should be approximately placed here

Fig. 4: The four bands for the Coroller model for one real data set (crosses stand for the real data). The values of the band areas are: $\mathcal{A}(PB_t) = 9$; $\mathcal{A}(PB_F) = 15.78$; $\mathcal{A}(PB_B) = 9.33$; $\mathcal{A}(PB_X) = 16.54$.

5.2.4 Discussion

This real application is particularly relevant for demonstrating the usefulness of the PB_X . Indeed, a crucial point here is to have a realistic PCI at the place where the model begins to break down (after about eight days in Fig. 4). At that time, the microbiologist needs a realistic PCI for the log number of bacteria present in the experiment. In this case, we can observe that PI_t and PI_B are completely false. We confirm that the PB_X is not very sensitive to the simulation σ_S . Its area is slightly larger than that of other bands, but that does not prevent its future use.

5.3 Another inactivation model: the Leguerinel et al. model

5.3.1 Definition

The analytic form of this model (the deterministic part) proposed by Leguerinel et al. (2005) for modelling the logarithm of the decreasing number of bacteria, including five parameters and three explanatory factors, is:

$$\eta(\theta; t, pH, Aw) = 5 - \left(\frac{t}{\delta \times 10 \left[\left(\frac{pH - pH_{opt}}{Z_{pH}} \right)^2 + \left(\frac{Aw - 0.985}{Z_{Aw}} \right)^2 \right]} \right)^p$$

where the vector parameter is $\theta = (p, \delta, Z_{pH}, Z_{Aw}, pH_{opt})^T$, and the explanatory factors are t (the time in minutes), pH , and water activity Aw . Because no rigorous design has yet to be found, real data are not available at that moment for the modelling of such a model. However, it is of particular importance to run some simulations for comparing the different regions. The *a priori* values provided by Leguérinel et al. (2005) for the parameters and domains are:

$$p_0 = 5; \delta_0 = 1.8; Z_{pH0} = 2.18; Z_{Aw0} = 0.092; pH_{opt0} = 6.96$$

$$\Theta_0 = [4.5; 5.5]_{p_0} \times [1.6; 2]_{\delta_0} \times [2; 2.5]_{Z_{pH0}} \times [0.0917; 0.0930]_{Z_{Aw0}} \times [6.5; 7.2]_{pH_{opt0}}$$

$$\Xi = [0; 5378]_t \times [4; 9]_{pH} \times [0.9; 1]_{Aw}$$

The 72 simulated values were obtained by forming a 3-dimensional grid on Ξ , with respect for the constraint $\eta(\cdot) \geq 1$ throughout. Table 3 gives the results based on 100 simulated data sets, obtained with $\sigma_S = 0.2$.

Volumes	min	max	mean	std	cv%
$\mathcal{V}(PR_t)$	2.68	2.95	2.82	0.06	2.15
$\mathcal{V}(PR_F)$	4.55	5.01	4.79	0.10	2.14
$\mathcal{V}(PR_X)$	36.50	38.20	37.26	0.74	2.02

Table 3: Inactivation model: simulation statistics of the band areas for $\sigma_S = 0.2$. $\mathcal{V}(PR_B)$ do not appear here because they are too time-consuming (one computation of $\mathcal{V}(PR_B)$ alone requires about ten hours, while $\mathcal{V}(PR_t)$ and $\mathcal{V}(PR_F)$ require less than three minutes, and $\mathcal{V}(PR_X)$ require about one hour; all the computations were carried out under the same conditions on a Pentium IV Personal Computer).

5.3.2 Discussion

This model leads to a larger volume for PR_X but, as in the preceding examples, this **region** is usable mainly because it is a conservative **region**.

324 **6 Conclusion**

325 We now have a relevant and a statistically rigorous PB – the PB_X – for evaluating
326 the global predictive capability of a nonlinear regression model. Since we were
327 able to observe in the preceding examples that its area is not too large, on the
328 one hand, and keeping in mind that it is a conservative band, on the other hand,
329 we are convinced that the PB_X can become a useful tool for the practioner in
330 predictive modelling in food. The two usual bands, PB_t and PB_F , **can lead to a**
331 **weak accuracy and, consequently, can be incorrect**, especially when n and
332 σ^2 are large. The PB_B is based on a second-order approximation, not an exact
333 basis.

334 The algorithm proposed in Subsection 4.2 for determining the PB_X is easy to code
335 and quick to run. Even with five parameters and three explanatory factors in the
336 model (example of Subsection 5.3), less than one hour is necessary on a Pentium
337 IV Personal Computer. The PB_B is too time-consuming, even for $p = 3$.

338 The PB_X could be effectively used for the comparison of two models by considering
339 the eventual overlapping of their bands. If the two bands overlap, then we will
340 assume that these two models are not significantly different for fitting the data
341 collected, and different if no overlapping exists at all. The intermediate case where
342 overlapping is partial obviously remains a difficult case to resolve. More research
343 is needed in this situation. Finally, a complementary study must be carried out

when the variance is heteroscedastic. This work is in progress.

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Fig. 1: The four bands for the Baranyi-Roberts model for one **simulated** data set (crosses stand for the simulated data). The values of the band areas (calculated with procedures indicated at the end of Subsection 3.1) are: $\mathcal{A}(PB_t) = 21$; $\mathcal{A}(PB_F) = 36$; $\mathcal{A}(PB_B) = 24$; $\mathcal{A}(PB_X) = 42$.

Fig. 2: The four bands for the Baranyi-Roberts model for one real data set (crosses stand for the real data). The values of the band areas are: $\mathcal{A}(PB_t) = 70$; $\mathcal{A}(PB_F) = 111$; $\mathcal{A}(PB_B) = 98$; $\mathcal{A}(PB_X) = 166$.

Fig. 3. The four bands for the **Coroller** model for one **simulated** data set (crosses stand for the simulated data). The values of the band areas are: $\mathcal{A}(PB_t) = 7.82$; $\mathcal{A}(PB_F) = 13.97$; $\mathcal{A}(PB_B) = 8.90$; $\mathcal{A}(PB_X) = 13.38$. It should be noted that days appear on the abscisses, but the parameters are given in the text for the time in hours.

Fig. 4: The four bands for the Coroller model for one real data set (crosses stand for the real data). The values of the band areas are: $\mathcal{A}(PB_t) = 9$; $\mathcal{A}(PB_F) = 15.78$; $\mathcal{A}(PB_B) = 9.33$; $\mathcal{A}(PB_X) = 16.54$.