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Improving Confidence Bands for Non-Linear Regression

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SUMMARY

We propose a simple simulation method for improving the precision of traditional linear confidence bands for non-transformably linear functions in non-linear regression. This method utilises a high order Taylor expansion and allows for finite ranges of predictor variables for the confidence bands. This method also permits self-examination of the performance of linear or high order confidence bands. The proposed method is a case-by-case solution, and thus does not require any prior knowledge of the overall evaluation of the linear bands. Three examples are used to illustrate the technique.

Key words: COVERAGE RATES; LINEAR BANDS; LOGISTIC REGRESSION; QUADRATIC BANDS; SIMULATION; TAYLOR EXPANSION
1. INTRODUCTION

In regression analysis, simultaneous confidence bands are often constructed for certain functions. For linear regression, one can construct confidence bands either using Scheffé's (Seber, 1977) or other methods. When confidence bands are to be constructed for a finite range of predictor variables, Scheffé's method is well known to be conservative, and thus other exact methods have been proposed. For example, Wynn & Bloomfield (1971), Naiman (1987) and Sun & Loader (1994) considered this problem for confidence bands constructed over a constrained range of predictor variables; Uusipaikka (1983) addressed the problem for a union of several disjoint ranges; and Wynn (1984) investigated the issue for one-dimensional polynomial regression.

For non-linear regression, when the expectation of the response is monotonically related to a linear function of regression parameters, i.e., transformably linear (Bates and Watts, 1988), one can still use existing methods to construct confidence bands because of the asymptotic normality of regression parameter estimates (see for example, Hauck, 1983, who considered confidence intervals for the logistic response curve). For generalized linear regression, the expectation of the response often is transformably linear, such as in logistic regression. Kosorok and Qu (1996) proposed a simple simulation method which constructs exact confidence bands for a number of transformably linear functions simultaneously while controlling for finite ranges of predictor variables.

Nevertheless, when the expectation of the response is not transformably linear, construction of exact confidence bands becomes difficult, and first-order Taylor expansion is used to construct approximate bands (Bates and Watts, 1988, and Cox and Ma, 1995). However, the use of the Cauchy-Schwart inequality (Rao 1985) in this method inhibits higher order Taylor approximation, and thus may not give satisfactory precision. In this paper, we propose a simple simulation method which utilises higher orders of the Taylor expansion and thus gives a better approximation. This method also permits self-inspection of the coverage rate, resulting in further improvement of the approximation.
In Section 2, we outline this method. Three examples are given in Section 3, and finally Section 4 concludes our paper with a brief discussion.

**2. CONFIDENCE BANDS**

Let $\theta$ be a $p$-dimensional regression parameter in a non-linear regression model, let $g_x(\theta)$ be the expectation function of the response given $x$, where $x$ is an element of $q$-dimensional Euclidean space, and denote the true parameter value by $\theta_0$. We do not require that $g_x(\theta)$ be transformably linear. Let $0$ be the zero vector of dimension $p$, and let $\hat{\theta}$ be a suitable estimate of $\theta_0$. Under standard regularity conditions, 

$$\sqrt{n} (\hat{\theta} - \theta_0) \sim N(0, V),$$

for large sample size $n$, where $V$ is positive definite and can be consistently estimated by some $\hat{V}$ (Fahrmeir and Kaufmann, 1985, Jennrich, 1969 and Wu, 1981). By the Cauchy-Schwartz inequality, we obtain

$$P\left( \frac{n[(\hat{\theta} - \theta_0)^T u]^2}{u^T \hat{V} u} \leq \chi^2_{p, \nu}, \text{ for all } u \right) \approx 1 - \nu,$$

for large $n$, where superscript $T$ denotes transpose and $\chi^2_{p, \nu}$ is the upper $\nu$ quantile of a chi-square distribution with $p$ degrees of freedom. Let $\Delta_g(\theta) = \partial g_x(\theta)/\partial \theta$ and $\Lambda_g(\theta) = \partial^2 g_x(\theta)/\partial \theta \partial \theta^T$ be the partial derivative and Hessian matrix, respectively, of $g_x(\theta)$ evaluated at $\theta$, where the dependence on $x$ has been suppressed.

By using a first order Taylor expansion, $g_x(\theta_0) \approx g_x(\hat{\theta}) + \Delta^T_g(\hat{\theta})(\theta_0 - \hat{\theta})$, and by replacing $u$ with $\Delta_g(\hat{\theta})$, we obtain

$$P\left\{ \frac{n[(\hat{\theta} - \theta_0)^T \Delta_g(\hat{\theta})]^2}{\Delta^T_g(\hat{\theta}) \hat{V} \Delta_g(\hat{\theta})} \leq \chi^2_{p, \nu}, \text{ for all } x \right\} \approx 1 - \nu$$

which can be used to form the usual linear confidence bands for $g_x(\theta_0)$:

$$\left\{ g_x(\hat{\theta}) - \left( \chi^2_{p, \nu} \Delta^T_g(\hat{\theta}) \hat{V} \Delta_g(\hat{\theta}) / n \right)^{1/2}, \ g_x(\hat{\theta}) + \left( \chi^2_{p, \nu} \Delta^T_g(\hat{\theta}) \hat{V} \Delta_g(\hat{\theta}) / n \right)^{1/2} \right\}, \quad (1)$$

for all $x$. If the distribution of the random error is Gaussian, and $\hat{\theta}$ is the usual least squares estimate, one can use the quantile of an $F$-distribution, with degrees of freedom $p$ and $n - p$, in (1) (see Chapter 2 of Bates and Watts, 1988). An advantage of this
approximation is its symmetry about $g_x(\hat{\theta})$. When the sample size is large, this approximation gives satisfactory precision. However, when the sample size is not large, the level of precision is unclear and an improvement may be needed.

The band (1) utilises the first-order Taylor expansion and thus the Cauchy-Schwartz inequality by replacing $u$ with $\Delta_g(\hat{\theta})$. Although useful for obtaining approximate confidence bands, the application of the Cauchy-Schwartz inequality prohibits higher than a first-order Taylor approximation to $g_x(\theta)$. Another source of approximation is that $\Delta_g(\hat{\theta})$ does not generally span all of $\mathcal{R}^p$, even when $q \geq p$ and the range of the predictor variable $x$ is all of $\mathcal{R}^q$. In practice, confidence bands are often needed for only a closed subset of the range of $x$, say $U \subset \mathcal{R}^q$. In the following, we propose an improved version of (1) based on the second order Taylor expansion

$$g_x(\theta_0) \approx g_x(\hat{\theta}) + \Delta^T_g(\hat{\theta})(\theta_0 - \hat{\theta}) + \frac{1}{2}(\theta_0 - \hat{\theta})^T \Lambda_g(\hat{\theta})(\theta_0 - \hat{\theta}).$$

Let $r$ be such that

$$P \left( n \left[ (\hat{\theta} - \theta_0)^T \Delta_g(\hat{\theta}) - \frac{1}{2}(\hat{\theta} - \theta_0)^T \Lambda_g(\hat{\theta})(\hat{\theta} - \theta_0) \right] \leq r, \text{ for all } x \text{ in } U \right) = 1 - \nu \quad (2)$$

with $r$ to be determined as follows.

Let $z$ be a vector of $p$ independent and identically distributed normal deviates with mean 0 and variance 1. Since $\sqrt{n}(\hat{\theta} - \theta_0) \sim N(0, \mathbf{V})$, $\sqrt{n}(\hat{\theta} - \theta_0)$ has approximately the same distribution as $\hat{\mathbf{V}}^{1/2} z$. Thus, by Slutsky’s Theorem, (2) is approximately equal to

$$P \left( \frac{[z^T \hat{\mathbf{V}}^{1/2} \Delta_g(\hat{\theta}) + \frac{1}{2} z^T \hat{\mathbf{V}}^{1/2} \Lambda_g(\hat{\theta}) \hat{\mathbf{V}}^{1/2} z/\sqrt{n}]}{\Delta^T_g(\hat{\theta}) \hat{\mathbf{V}} \Delta_g(\hat{\theta})} \leq r, \text{ for all } x \text{ in } U \right) = 1 - \nu, \quad (3)$$

where the probability in (3) is conditional on the sample through $\hat{\theta}$ and $\hat{\mathbf{V}}$, and provided we are willing to ignore the higher order terms in the error resulting from approximating the distribution of $\sqrt{n}(\hat{\theta} - \theta_0)$ with $\hat{\mathbf{V}}^{1/2} z$. Replacing the numerator of the left hand side of the inequality in (2) by $n \left[ g_x(\hat{\theta}) - g_x(\theta_0) \right]^2$, and solving the resulting inequality,
yields the quadratic confidence bands

\[ \left\{ g_\epsilon(\hat{\theta}) - r \left( \Delta_\epsilon^T(\hat{\theta}) \hat{V}_\epsilon \Delta_\epsilon(\hat{\theta}) / n \right)^{1/2}, \quad g_\epsilon(\hat{\theta}) + r \left( \Delta_\epsilon^T(\hat{\theta}) \hat{V}_\epsilon \Delta_\epsilon(\hat{\theta}) / n \right)^{1/2} \right\}, \tag{4} \]

for all \( \epsilon \) in \( U \).

Our examples below show that the quadratic bands indeed improve upon the linear bands a great deal. However, the quadratic bands can also be improved upon. Consider approximating \( g_\epsilon(\hat{\theta}) - g_\epsilon(\theta_0) \) by \( g_\epsilon \left( \hat{\theta} + \hat{V}^{1/2} z / \sqrt{n} \right) - g_\epsilon(\hat{\theta}) \). To this end, we have the following lemma:

**Lemma 1** Let \( u_n = \hat{V}^{1/2} z / \sqrt{n} \), and suppose that \( \sqrt{n}(\hat{\theta} - \theta_0) \) and \( \sqrt{n}(u_n) \) converge in distribution to \( z_1 \) and \( z_2 \), respectively, as \( n \to \infty \), where \( z_1 \) and \( z_2 \) are independent multivariate normals with mean zero and variance \( V \). Suppose also that, for each \( \epsilon \in U \),

\[ \lim_{\delta \downarrow 0} \sup_{|\theta - \theta_0| < \delta} |\Lambda_\epsilon(\theta) - \Lambda_\epsilon(\theta_0)| = 0. \]

Then, for each \( \epsilon \in U \),

(i) \( n \left( \Delta_\epsilon^T(\hat{\theta}) u_n - g_\epsilon(\theta_0 + u_n) + g_\epsilon(\theta_0) \right) \) converges in distribution, as \( n \to \infty \), to

\[ z_1^T \Lambda_\epsilon(\theta_0) z_2 - \frac{1}{2} z_2^T \Lambda_\epsilon(\theta_0) z_2 \tag{5} \]

and

(ii) \( n \left( g_\epsilon(\hat{\theta} + u_n) - g_\epsilon(\hat{\theta}) - g_\epsilon(\theta_0 + u_n) + g_\epsilon(\theta_0) \right) \) converges in distribution, as \( n \to \infty \), to

\[ z_1^T \Lambda_\epsilon(\theta_0) z_2. \tag{6} \]

The proof is given in the Appendix. Since \( g_\epsilon(\hat{\theta}) - g_\epsilon(\theta_0) \) has the same asymptotic distribution as \( g_\epsilon(\theta_0 + u_n) - g_\epsilon(\theta_0) \), this lemma compares the asymptotic bias of the linear approximation in part (i) with the proposed approximation in part (ii). Since the expectation of (5) is \(-\frac{1}{2} \text{trace} \{ \Lambda_\epsilon(\theta_0) V \}\) (generally not zero), while the expectation
of (6) is zero, we might expect the proposed higher order confidence bands to perform better than the linear approximation.

In order to compute the proposed confidence bands, we need to be able to determine the supremum and infimum of

$$\frac{g_x(\hat{\theta} + u) - g_x(\hat{\theta})}{\sqrt{\Delta^2(\hat{\theta})V \Delta_\theta(\hat{\theta})}}$$

(7)

over all \(x \in U\) and for any \(u\) so that

$$P \left( \frac{[g_x(\hat{\theta} + \hat{\theta}_u^{1/2}z/\sqrt{n}) - g_x(\hat{\theta})]^2}{\Delta^2(\hat{\theta})V \Delta_\theta(\hat{\theta})} \leq r, \text{ for all } x \text{ in } U \right) = 1 - \nu$$

can be evaluated and solved for \(r\). Provided that \(U\) is closed and that (7) is continuous in \(x\) and bounded with limits on \(U\), then a finite mesh of points in \(U\) can be examined rather than all of \(U\) and the extrema can be thus determined to within any \(\epsilon > 0\) of the true values. Similar results apply to obtaining the requisite extrema for the linear and quadratic bands. In this manner, the coefficient \(r\) can be determined by simulation, for each of the proposed bands, using the random deviate \(z\). As mentioned earlier, for the Gaussian error setting, \(z\) can be replaced by \(t = z/\sqrt{\chi^2_{n-p}/(n-p)}\) where \(\chi^2_{n-p}\) is a chi-square random variable with \(n - p\) degrees of freedom and which is independent of \(z\). In the next section, we will illustrate the above method by three examples.

3. EXAMPLES

3.1 Logistic Regression

Our first example is logistic regression. The expectation of the response in logistic regression is transformably linear and thus permits the construction of exact confidence bands (exact in the sense that we need not use a Taylor expansion to approximate \(g_x(\theta)\)) allowing us to compare the precision of the linear, quadratic and full order to the exact bands in terms of coverage rate and the influence of sample size. The experiment reported by Collett (1991) studied the toxicity of the tobacco budworm *Heliothis virescens*
to doses 1, 2, 4, 8, 16 and 32 in $\mu g$ of the pyrethroid trans-cypermethrin to which the moths were beginning to show resistance. Batches of 20 moths of each sex were exposed for 3 days to the pyrethroid. The number in each batch which were dead or knocked down was recorded as 1, 4, 9, 13, 18, and 20 for males moths. A logistic regression using $\log_2$ (dose) was fit as described in Venable (1994). Let $x$ denote the $\log_2$ (dose). Then the logistic model considered is

$$\text{logit}(p) = \alpha + \beta x$$

with $\theta = (\alpha, \beta)$ and $x = (1, x)^T$. Now consider the construction of 95\% simultaneous bands for the probability of toxicity $g_x(\theta) = e^{\alpha + \beta x}/[1 + e^{\alpha + \beta x}]$ for dose ranging from 0 to 32 $\mu g$ ( $x \in U = [0, 5]$ ). The partial derivative and Hessian matrix of $g_x(\theta)$ are

$$\Delta_g = \frac{e^{\alpha + \beta x}}{(1 + e^{\alpha + \beta x})^2} \begin{pmatrix} 1 \\ x \end{pmatrix}$$

and

$$\Lambda_g = \frac{e^{\alpha + \beta x}(1 - e^{\alpha + \beta x})}{(1 + e^{\alpha + \beta x})^3} \begin{pmatrix} 1 & x \\ x & x^2 \end{pmatrix}.$$ 

The estimates of $\alpha$ and $\beta$ are -2.82 and 1.26 respectively. Using simulation with 1000 replicates of $z$ and a mesh size of 0.1, we have $r = 3.07$ for the quadratic bands and $r = 3.38$ for the full order bands.

The exact confidence bands for $g_x(\theta_0)$ are

$$\left\{ \hat{\theta}^T x - (x_p^2, x \tau V x/n)^{1/2}, \hat{\theta}^T x + (x_p^2, x \tau V x/n)^{1/2} \right\}.$$ 

Figure 1 shows the plots of 95\% linear, quadratic, full order and exact confidence bands. It can be seen that the four bands look quite different.

To evaluate the coverage rates of these four confidence bands, another simulation was performed using -2.82 and 1.26 as true values of $\alpha$ and $\beta$ and the same sample size 120 as in the real data. The simulation was conducted using 1000 replicates, and 1000 normal deviates $z$ for each replicate. The simulated bands are almost identical to those in Figure 1, and thus will not be shown here. The resulting coverage rates are 0.85, 0.91,
0.94 and 0.95 for linear, quadratic, full order and exact bands respectively. It can be seen that the linear bands have a severe loss in the confidence level, and that the high order bands improve the coverage rate greatly. To see the influence of sample size, a third simulation was performed using the same parameter values, replication numbers, and sample sizes 50, 100 and 200. Table 1 shows the coverage rates of the simulation. The coverage rates for linear bands were about 20% and 10% lower than the targeted 95% for sample sizes 50 and 100 respectively, whereas the high order were almost the same as the exact bands, even for sample size 50.

3.2 Non-transformably Non-linear Regression

The high order bands outperformed the linear bands a great deal in the previous logistic regression. Because of the monotonic relationship between $g_x(\theta)$ and the linear function $\alpha + \beta x$, we were able to compare the two approximate confidence bands to the exact ones. When $g_x(\theta)$ is not transformably linear, one doesn’t have a gold standard such as the exact bands to compare with for evaluating the effect of sample size. However, it is still possible to compare the linear and high order bands using simulation. If the difference between them is substantial, then the high order bands should be chosen over the linear.

Consider data on the velocity of an enzymatic reaction reported by Treloar (1974). The number of counts per minute of radioactive product from the reaction was measured as a function of substrate concentration in parts per million (ppm); and from these counts, the initial rate, or “velocity,” of the reaction was calculated (counts/min²). The data from the experiment with puromycin treated enzyme are in Table 2. The Michaelis-Menten equation relates the initial velocity of the enzymatic reaction to the substrate concentration $x$ through the model $g_x(\theta) = \theta_1 x / (\theta_2 + x)$ with Gaussian deviates (Bates and Watts 1988).

The estimates of $\theta_1$ and $\theta_2$ are 212.68 and 0.064 respectively, and the standard deviation of the Gaussian deviates is 10.94. The partial derivatives and Hessian matrix of
\( g_x(\theta) \) are

\[
\Delta_x = \left( \frac{x}{\theta_2 + x}, \frac{-\theta_1 x}{(\theta_2 + x)^2} \right)^T
\]

and

\[
\Lambda_x = \frac{x}{(\theta_2 + x)^2} \begin{pmatrix}
0 & -1 \\
-1 & \frac{2\theta_1}{\theta_2 + x}
\end{pmatrix},
\]

respectively.

Using simulation with 1000 replicates of the random deviate \( t \), with \( U = [0.01, 1.20] \) and a mesh size of 0.01, we obtain that \( r = 2.90 \) and 2.95 for the quadratic and full order bands, respectively. Figure 2 shows the 95% linear, quadratic and full order bands. The coefficient for linear bands is 2.86 which is almost the same as those for the quadratic and full order bands. A simulation study was done with 2000 replicates and 212.68, 0.064 and 10.94 as true values of \( \theta_1, \theta_2 \) and the standard deviation, respectively, in the model. The simulated coverage rates are 94% and 96% and 94% for the linear, quadratic and full order bands, respectively. Thus the linear method gives completely satisfactory coverage in this example.

As our last example, we consider data on biochemical oxygen demand (BOD) from Marske (1967). The data consist of six pairs of observations with independent variable time \( x = 1, 2, 3, 4, 5, 7 \) and corresponding response values 8.3, 10.3, 19.0, 16.0, 15.6 and 19.8 for the biochemical oxygen demand. The model for the data is \( g_x(\theta) = \theta_1(1 - \exp(\theta_2 x)) \), as given in Bates and Watts (1988). The estimates of \( \theta_1 \) and \( \theta_2 \) are 19.143 and 0.5311, respectively, and the standard deviation of the Gaussian error is 2.55. Figure 3 shows the linear and high order confidence bands for the mean BOD for \( x \) in [1,7]. It is clear that the three bands are largely different with the full order bands being the widest. The coefficients for the quadratic and full order bands are estimated as 7.76 and 9.57, respectively, using 1000 random replicates with \( U = [1, 7] \) and a mesh size of 0.01. To examine the coverage rate, another simulation study was conducted with 1000 replicates and with 19.143, 0.5311 and 2.55 as the true parameters values of \( \theta_1, \theta_2 \) and standard deviation of the Gaussian error, respectively. The coverage rates were 0.55,
0.90 and 0.91. The difference between the linear and high order band coverage rates is astonishing. Surprisingly, the high order bands performed reasonably well even with six observations in the data, indicating that the normal approximation to the asymptotic distribution of $\hat{\theta} - \theta_0$ is pretty good.

4. DISCUSSION

The method we propose in this paper is simple and can be implemented easily using Monte Carlo simulation. With ever increasing computer capacity, simulation becomes more and more a routine practice in statistical analysis. Our method was presented using a high order Taylor expansion. The precision of confidence bands consists of two components, coverage rate and band width, of which the first might be more important then the second. Certainly, wider bands lead to a higher coverage rate. But the balance between these two components varies from situation to situation.

Our method improves upon existing linear confidence bands and permits inspection of the performance of linear confidence bands. However, our work here is not to evaluate the overall performance of linear bands. What we propose is a case-by-case solution, and thus does not require any prior knowledge of the overall evaluation of linear bands. Since the form of the linear and high order bands are the same, what this method achieves is to improve the coverage rate by appropriately increasing the linear band coefficient. The performance of full order bands seems quite satisfactory. Although not quite as good as the full order bands, the quadratic bands do improve upon the linear bands substantially. In the third example, the full order band coverage rate is still lower than the nominal level 0.95. This might be due to the effect of a small sample size on the normal approximation to the asymptotic distribution of $\hat{\theta} - \theta_0$.

There are a number of ways the proposed bands can be further improved upon. One improvement can be made by considering both the supremum and infemum over $x \in U \subset \mathbb{R}^s$ of (7) and forming confidence bands which are symmetric in probability about $g_x(\hat{\theta})$. Another improvement can result from utilising knowledge about the small
sample distribution of $\hat{\theta} - \theta_0$ since the asymptotic Gaussian assumption can sometimes be seriously violated (see chapter 7 of Bates and Watts, 1988). If we can generate a Markov chain $\{\tilde{u}_k, k = 1 \ldots M\}$ with an equilibrium distribution reasonably close to that of $\hat{\theta} - \theta_0$, then the ergodic theorem allows us to construct confidence bands using the proposed methods after replacing $\hat{V}^{1/2} z / \sqrt{n}$ with $\tilde{u}_k$, $k = 1 \ldots M$.

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APPENDIX: PROOF OF LEMMA 1

For each $\mathbf{u} \in U$, proceed as follows. By Taylor expansion,

$$
n \left( \Delta_g^T(\hat{\theta}) \mathbf{u}_n - g_x(\theta_0 + \mathbf{u}_n) + g_x(\theta_0) \right) = n \left( \left\{ \Delta_g(\hat{\theta}) - \Delta_g(\theta_0) \right\}^T \mathbf{u}_n - \frac{1}{2} \mathbf{u}_n^T \Lambda_g(\theta_x^*) \mathbf{u}_n \right),$$

where $\theta_x^*$ is on the line segment between $\theta_0$ and $\theta_0 + \mathbf{u}_n$, and part (i) follows. Again by Taylor expansion,

$$
n \left( g_x(\hat{\theta} + \mathbf{u}_n) - g_x(\hat{\theta}) - g_x(\theta_0 + \mathbf{u}_n) + g_x(\theta_0) \right) = n \left( \left\{ \Delta_g(\hat{\theta}) - \Delta_g(\theta_0) \right\}^T \mathbf{u}_n + \frac{1}{2} \mathbf{u}_n^T \left\{ \Lambda_g(\theta_x^{**}) - \Lambda_g(\theta_x^*) \right\} \mathbf{u}_n \right),$$

where $\theta_x^*$ is as before and $\theta_x^{**}$ is on the line segment between $\hat{\theta}$ and $\hat{\theta} + \mathbf{u}_n$, and part (ii) follows. □
REFERENCES


Table 1: Simulated coverage rates for logistic regression.

<table>
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<th>sample size</th>
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<th>Quadratic</th>
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Table 2: Data of velocity and substrate concentration for the puromycin experiment.

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<tr>
<td>Velocity</td>
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<td>97, 107</td>
<td>123, 139</td>
<td>159, 152</td>
<td>191, 201</td>
<td>207, 200</td>
</tr>
</tbody>
</table>
Simultaneous 95% Confidence Bands for Probability of Toxicity

Figure 1: Plots of the 95% linear, quadratic, full order and exact confidence bands for the probability of toxicity of the tobacco budworm *Heliothis virescens* for dose in [1, 32] (log$_2$(dose) in [0, 5]) for male moths.
Figure 2: Plots of 95% linear, quadratic and full order confidence bands for mean velocity for substrate concentration in $[0, 1.2]$. The longer dashed-line curve is the estimate of mean velocity.
Simultaneous 95% Confidence Bands for Mean BOD

Figure 3: Plots of 95% linear, quadratic and full order confidence bands for mean biochemical oxygen demand (BOD) for time in [1, 7]. The longer dashed-line curve is the estimate of mean BOD.