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Comparison of hyperbolic and constant width simultaneous confidence bands in multiple linear regression under MVCS criterion

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ABSTRACT

A simultaneous confidence band provides useful information on the plausible range of the unknown regression model, and different confidence bands can often be constructed for the same regression model. For a simple regression line, Liu and Hayter [W. Liu, A.J. Hayter, Minimum area confidence set optimality for confidence bands in simple linear regression, J. Amer. Statist. Assoc. 102 (477) (2007) pp. 181–190] proposed the use of the area of the confidence set corresponding to a confidence band as an optimality criterion in comparison of confidence bands; the smaller the area of the confidence set, the better the corresponding confidence band. This minimum area confidence set (MACS) criterion can be generalized to a minimum volume confidence set (MVCS) criterion in the study of confidence bands for a multiple linear regression model. In this paper hyperbolic and constant width confidence bands for a multiple linear regression model over a particular ellipsoidal region of the predictor variables are compared under the MVCS criterion. It is observed that whether one band is better than the other depends on the magnitude of one particular angle that determines the size of the predictor variable region. When the angle and hence the size of the predictor variable region is small, the constant width band is better than the hyperbolic band but only marginally. When the angle and hence the size of the predictor variable region is large the hyperbolic band can be substantially better than the constant width band.

1. Introduction

Consider the multiple linear regression model

$$\mathbf{Y} = X\mathbf{b} + \mathbf{e}$$

where $\mathbf{Y}_{n\times 1}$ is the vector of observed responses, $X_{n\times p}$ is the design matrix whose first column is given by $(1, \ldots, 1)^{\mathrm{T}}$ and whose jth ($2 \le j \le p$) column is given by $(x_{1,j}, \ldots, x_{n,j})^{\mathrm{T}}$, $\mathbf{b} = (b_1, \ldots, b_p)^{\mathrm{T}}$ is the vector of regression coefficients, and $\mathbf{e}_{n\times 1}$ is an additive error vector with $\mathbf{e} \sim N(0, \sigma^2 I)$ and σ^2 unknown. Assume $X^{\mathrm{T}}X$ is non-singular, so the least squares estimator of $\mathbf{b}$ is given by $\hat{\mathbf{b}} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\mathbf{Y}$. Let $\hat{\sigma}^2$ denote the mean square error with degrees of freedom $\nu = n - p$. Then $\hat{\sigma}^2 \sim \sigma^2\chi^2_\nu/\nu$ and is independent of $\hat{\mathbf{b}}$.

Let $\mathbf{x} = (1, x_2, \ldots, x_p)^{\mathrm{T}}$ and $\mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}}$. A simultaneous confidence band for the regression function

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} = b_1 + b_2x_2 + \cdots + b_px_p$$

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on a given region $\mathcal{X}$ of the $p-1$ predictor variables $\mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}}$ provides useful information on where the true but unknown regression model lies; a linear regression function is a plausible candidate for the unknown regression model if and only if it is contained completely inside the confidence band. There are several recent papers considering various applications of confidence bands; see for example [1–5].

Construction of simultaneous confidence bands has a history going back to Working and Hotelling [6]. Scheffé [7] first provided the well known two-sided hyperbolic simultaneous confidence band over the whole space $\mathcal{X} = R^{p-1}$ of the $p-1$ predictor variables. More useful in practice, however, is construction of confidence bands over some finitely-bounded subset of R^{p-1} that corresponds to relevant values of the predictor variables. For $p = 2$, that is, when there is only one predictor variable, construction of various exact simultaneous confidence bands incorporating interval restrictions on x_2 has been considered by Bowden and Graybill [8], Graybill and Bowden [9], Wynn and Bloomfield [10], Bohrer and Francis [11], and Uusipaikka [12] among others. In particular, Gafarian [13] was the first to suggest use of *constant width* confidence bands when x_2 is restricted to a finite interval. See a recent review by [14].

For $p > 2$, construction of exact confidence bands over a finite region $\mathcal{X}$ of the predictor variables is more difficult. When $p > 2$ there are at least two predictor variables and the region $\mathcal{X}$ may assume various forms. One useful region $\mathcal{X}$ is the rectangular set

$$\mathcal{X}_r = \{\mathbf{x}_{(1)}{}^{\mathrm{T}} : a_i \le x_i \le b_i,\ i = 2, \ldots, p\},$$

where $-\infty \le a_i < b_i \le \infty, i = 2, \ldots, p$ are given constants. (We assume that $-\infty < a_i < b_i < \infty$ for at least one value of i.) Construction of two-sided hyperbolic confidence bands over $\mathcal{X}_r$ has been considered by Knafl et al. [15], Naiman [16, 17] and Sun and Loader [18] among others. All these confidence bands are either conservative or approximate, however. A simulation-based method for constructing a two-sided hyperbolic confidence band over $\mathcal{X}_r$ for a general $p \ge 2$ is given recently in [19]; the critical constant can be calculated as accurately as one requires if the number of replications in the simulation is set sufficiently large. Construction of a two-sided constant width confidence band over $\mathcal{X}_r$ for a general $p \ge 2$ is considered in [20] by using a combination of both numerical integration and simulation.

For $p > 2$, another useful region $\mathcal{X}$ is given by the ellipsoidal region $\mathcal{X}_e$ in (1) below. Let $X_{(1)}$ be the $n \times (p-1)$ matrix produced from the design matrix X by deleting the first column of 1's from X. Let $x_{\cdot j} = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$ be the mean of the observed values of the jth predictor variable ($2 \le j \le p$), and let $\bar{\mathbf{x}}_{(1)} = (x_{\cdot 2}, \ldots, x_{\cdot p})^{\mathrm{T}}$. Define the $(p-1) \times (p-1)$ matrix

$$S = \frac{1}{n}\left(X_{(1)} - \underline{1}\bar{\mathbf{x}}_{(1)}{}^{\mathrm{T}}\right)^{\mathrm{T}}\left(X_{(1)} - \underline{1}\bar{\mathbf{x}}_{(1)}{}^{\mathrm{T}}\right) = \frac{1}{n}\left(X_{(1)}^{\mathrm{T}}X_{(1)} - n\bar{\mathbf{x}}_{(1)}\bar{\mathbf{x}}_{(1)}{}^{\mathrm{T}}\right)$$

where $\underline{1}$ is an n-vector of 1's. Note that matrix S is just the sample variance–covariance matrix of the $p-1$ predictor variables, and it is non-singular whenever X is assumed to be of full column rank. With this, the ellipsoidal region is defined to be

$$\mathcal{X}_e = \left\{\mathbf{x}_{(1)} : \left(\mathbf{x}_{(1)} - \bar{\mathbf{x}}_{(1)}\right)^{\mathrm{T}} S^{-1}\left(\mathbf{x}_{(1)} - \bar{\mathbf{x}}_{(1)}\right) \le a^2\right\} \tag{1}$$

where $a > 0$ is a given constant. It is clear that this region is centered at $\bar{\mathbf{x}}_{(1)}$ and has an ellipsoidal shape in $\mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}} \in R^{p-1}$. One important feature of $\mathcal{X}_e$ is that the variance of the fitted regression model at $\mathbf{x}$, $\mathrm{Var}(\mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}})$, is a constant for all the $\mathbf{x}_{(1)}$ on the surface of the ellipsoid $\mathcal{X}_e$. Construction of an approximate two-sided hyperbolic confidence band over $\mathcal{X}_e$ was first considered by Halperin and Gurian [21]. Construction of exact hyperbolic confidence bands over $\mathcal{X}_e$ has since been considered by Bohrer [22], Casella and Strawderman [23], Seppanen and Uusipaikka [24] and Liu and Lin [25] among others.

The purpose of this paper is to compare the two most popular band forms: the Scheffé-type hyperbolic and Gafarian-type constant width confidence bands over $\mathcal{X}_e$ under the minimum area (volume) confidence set optimality criterion proposed in [26]. We take advantage of the fact that any $1-\alpha$ confidence band for the regression model $\mathbf{x}^{\mathrm{T}}\mathbf{b}$ corresponds to a $1-\alpha$ confidence set in R^p for the regression coefficients $\mathbf{b}$. The minimum area (volume) confidence set optimality criterion prefers a confidence band whose confidence set has a smaller area (volume). For $p = 2$, various confidence bands for a regression line have been assessed and compared in [26] under the minimum area confidence set criterion. Indeed, before the appearance of the minimum area (volume) confidence set criterion, (weighted) average width of a confidence band was the primary optimality criterion for selection of confidence bands; see e.g., [27–29]. In particular, the hyperbolic and constant width bands over $\mathcal{X}_e$ were compared by Naiman [27] under the average width criterion.

In Section 2 the hyperbolic and constant width confidence bands and their corresponding confidence sets are presented. In Section 3, comparisons between the confidence bands under the minimum volume confidence set criterion are given. The notation of Liu and Lin [25] is adopted throughout this paper.

2. Confidence bands and confidence sets

In this section the hyperbolic and constant width confidence bands over $\mathcal{X}_e$ are detailed and the corresponding confidence sets are identified. The two-sided hyperbolic confidence band is given by

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} \in \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} \pm c_{h,2}\hat{\sigma}\sqrt{\mathbf{x}^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}} \in \mathcal{X}_e \tag{2}$$

where $\mathcal{X}_e$ is defined in (1) and $c_{h,2}$ is a suitably chosen critical constant so that the simultaneous confidence level of the band is equal to $1-\alpha$.

As in Liu and Lin [25], define p-vector $\mathbf{z} = \sqrt{n}(1, \bar{\mathbf{x}}_{(1)}^{\mathrm{T}})^{\mathrm{T}}$, and let $p \times (p-1)$ matrix Z satisfy $(\mathbf{z}, Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}(\mathbf{z}, Z) = I_p$. It follows therefore that $\mathbf{T} = (\mathbf{z}, Z)^{-1}(X^{\mathrm{T}}X)(\hat{\mathbf{b}} - \mathbf{b})/\hat{\sigma}$ is a standard p-dimensional t random vector with ν degrees of freedom; see e.g., [30] for a full description of the multivariate t distributions. Note that

$$1-\alpha = \mathrm{P}\left\{\sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} \frac{|\mathbf{x}^{\mathrm{T}}(\hat{\mathbf{b}}-\mathbf{b})|}{\hat{\sigma}\sqrt{\mathbf{x}^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}}} \le c_{h,2}\right\}$$
$$= \mathrm{P}\left\{\sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} \frac{\left|\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}^{\mathrm{T}}\left\{(\mathbf{z},Z)^{-1}(X^{\mathrm{T}}X)(\hat{\mathbf{b}}-\mathbf{b})/\hat{\sigma}\right\}\right|}{\sqrt{\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}^{\mathrm{T}}\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}}} \le c_{h,2}\right\}.$$

Let

$$V_h = \left\{\mathbf{t}: \sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} \frac{\left|\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}^{\mathrm{T}}\mathbf{t}\right|}{\left\|(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\|} \le c_{h,2}\right\} \subset R^p. \tag{3}$$

Then the confidence set for the regression coefficients $\mathbf{b}$ that corresponds to the hyperbolic band in (2) is given by

$$C_{h,2}(\hat{\mathbf{b}}, \hat{\sigma}) = \left\{\mathbf{b}: (\mathbf{z},Z)^{-1}(X^{\mathrm{T}}X)(\mathbf{b}-\hat{\mathbf{b}})/\hat{\sigma} \in V_h\right\}. \tag{4}$$

Let $\mathbf{w} = (\mathbf{z}, Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x} = (w_1, \mathbf{w}_{(1)}^{\mathrm{T}})^{\mathrm{T}}$ where $\mathbf{w}_{(1)} = (w_2, \ldots, w_p)^{\mathrm{T}} = Z^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}$ and $w_1 = \mathbf{z}^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x} = 1/\sqrt{n}$. Then it follows from Liu and Lin [25, expressions (6), (7), (8) and (10)], that V_h can further be expressed as

$$V_h = \left\{\mathbf{t}: \sup_{\mathbf{w}\in\mathcal{W}_e} \frac{|\mathbf{w}^{\mathrm{T}}\mathbf{t}|}{\|\mathbf{w}\|} \le c_{h,2}\right\} \tag{5}$$

where

$$\mathcal{W}_e = \left\{\mathbf{w}: w_1 = 1/\sqrt{n}, \|\mathbf{w}\|^2 \le (1+a^2)/n\right\} \subset R^p. \tag{6}$$

From (4) and the definition of $\mathbf{T}$, the critical constant $c_{h,2}$ can be determined by solving $1-\alpha = \mathrm{P}\{\mathbf{T} \in V_h\}$ which, from Liu and Lin [25, expression (28)], is equivalent to

$$1-\alpha = F_{p,\nu}\left(\frac{c_{h,2}^2}{p}\right)\int_0^{\theta^*} 2k\sin^{p-2}\theta \mathrm{d}\theta + \int_0^{\pi/2-\theta^*} 2k\sin^{p-2}(\theta+\theta^*)\cdot F_{p,\nu}\left\{\frac{c_{h,2}^2}{p\cos^2\theta}\right\}\mathrm{d}\theta$$

where

$$\theta^* = \arccos(1/\sqrt{1+a^2}) \in (0, \pi/2), \tag{7}$$

$k = 1/(\int_0^{\pi}\sin^{p-2}\theta \mathrm{d}\theta)$, and $F_{p,\nu}(\cdot)$ is the cdf of the F distribution with p and ν degrees of freedom.

Now, we turn our attention to the Gafarian-type two-sided constant width band, given by

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} \in \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} \pm c_{c,2}\sqrt{(1+a^2)/n}\,\hat{\sigma} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}} \in \mathcal{X}_e, \tag{8}$$

where $c_{c,2}$ is chosen so that the simultaneous confidence level of the band is equal to $1-\alpha$. Hence

$$1-\alpha = \mathrm{P}\left\{\sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} |\mathbf{x}^{\mathrm{T}}(\hat{\mathbf{b}}-\mathbf{b})|/\hat{\sigma} \le c_{c,2}\sqrt{(1+a^2)/n}\right\}$$
$$= \mathrm{P}\left\{\sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} \left|\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}^{\mathrm{T}}\left\{(\mathbf{z},Z)^{-1}(X^{\mathrm{T}}X)(\hat{\mathbf{b}}-\mathbf{b})/\hat{\sigma}\right\}\right| \le c_{c,2}\sqrt{(1+a^2)/n}\right\}.$$

Let

$$V_c = \left\{\mathbf{t}: \sup_{\mathbf{x}_{(1)}\in\mathcal{X}_e} \left|\left\{(\mathbf{z},Z)^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}\right\}^{\mathrm{T}}\mathbf{t}\right| \le c_{c,2}\sqrt{(1+a^2)/n}\right\} \subset R^p.$$

Then the confidence set for the regression coefficients $\mathbf{b}$ that corresponds to the constant-width band in (8) is given by

$$C_{c,2}(\hat{\mathbf{b}}, \hat{\sigma}) = \left\{\mathbf{b}: (\mathbf{z},Z)^{-1}(X^{\mathrm{T}}X)(\mathbf{b}-\hat{\mathbf{b}})/\hat{\sigma} \in V_c\right\}. \tag{9}$$

Similar to the expression for V_h in (5), V_c can be written as

$$V_c = \left\{ \mathbf{t} : \sup_{\mathbf{w} \in \mathcal{W}_e} |\mathbf{w}^{\mathrm{T}}\mathbf{t}| \le c_{c,2}\sqrt{(1+a^2)/n} \right\} \tag{10}$$

where $\mathcal{W}_e$ is given in (6). Let $\mathbf{t}_{(1)} = (t_2, \ldots, t_p)^{\mathrm{T}}$. Note that

$$\sup_{\mathbf{w} \in \mathcal{W}_e} |\mathbf{w}^{\mathrm{T}}\mathbf{t}| = \sup_{\mathbf{w} \in \mathcal{W}_e} \left| t_1/\sqrt{n} + \mathbf{w}_{(1)}{}^{\mathrm{T}}\mathbf{t}_{(1)} \right| \le |t_1|/\sqrt{n} + \sqrt{a^2/n}\, \|\mathbf{t}_{(1)}\|$$

and the upper bound above is attained at $\mathbf{w} \in \mathcal{W}_e$ with $\mathbf{w}_{(1)} = \mathrm{sign}(t_1)\sqrt{a^2/n}\, \mathbf{t}_{(1)}/\|\mathbf{t}_{(1)}\|$. Hence V_c in (10) can further be expressed as

$$V_c = \left\{ \mathbf{t} : |t_1|/\sqrt{n} + \sqrt{a^2/n}\, \|\mathbf{t}_{(1)}\| \le c_{c,2}\sqrt{(1+a^2)/n} \right\}.$$

Now, using the polar coordinates $(R_{\mathbf{v}}, \theta_{\mathbf{v}1}, \ldots, \theta_{\mathbf{v},p-1})^{\mathrm{T}}$ for a p-dimensional vector $\mathbf{v} = (v_1, \ldots, v_p)^{\mathrm{T}}$

$$\begin{cases} v_1 = R_{\mathbf{v}} \cos\theta_{\mathbf{v}1} \\ v_2 = R_{\mathbf{v}} \sin\theta_{\mathbf{v}1} \cos\theta_{\mathbf{v}2} \\ v_3 = R_{\mathbf{v}} \sin\theta_{\mathbf{v}1} \sin\theta_{\mathbf{v}2} \cos\theta_{\mathbf{v}3} \\ \cdots \quad \cdots \\ v_{p-1} = R_{\mathbf{v}} \sin\theta_{\mathbf{v}1} \sin\theta_{\mathbf{v}2} \cdots \sin\theta_{\mathbf{v},p-2} \cos\theta_{\mathbf{v},p-1} \\ v_p = R_{\mathbf{v}} \sin\theta_{\mathbf{v}1} \sin\theta_{\mathbf{v}2} \cdots \sin\theta_{\mathbf{v},p-2} \sin\theta_{\mathbf{v},p-1} \end{cases} \quad \text{where} \quad \begin{cases} 0 \le \theta_{\mathbf{v}1} \le \pi \\ 0 \le \theta_{\mathbf{v}2} \le \pi \\ \cdots \quad \cdots \\ 0 \le \theta_{\mathbf{v},p-2} \le \pi \\ 0 \le \theta_{\mathbf{v},p-1} \le 2\pi \\ R_{\mathbf{v}} \ge 0 \end{cases}$$

the set V_c can be expressed as

$$V_c = \left\{ \mathbf{t} : |R_{\mathbf{t}} \cos\theta_{\mathbf{t}1}|/\sqrt{n} + \sqrt{a^2/n}\, |R_{\mathbf{t}} \sin\theta_{\mathbf{t}1}| \le c_{c,2}\sqrt{(1+a^2)/n} \right\} = V_{c,1} + V_{c,2} \tag{11}$$

where

$$V_{c,1} = \left\{ \mathbf{t} : 0 \le \theta_{\mathbf{t}1} \le \pi/2,\ R_{\mathbf{t}} \cos(\theta_{\mathbf{t}1} - \theta^*) \le c_{c,2} \right\} \tag{12}$$

$$V_{c,2} = \left\{ \mathbf{t} : \pi/2 \le \theta_{\mathbf{t}1} \le \pi,\ R_{\mathbf{t}} \cos(\pi - \theta_{\mathbf{t}1} - \theta^*) \le c_{c,2} \right\} \tag{13}$$

with θ^* given in (7).

From the definition of $\mathbf{T}$ and expressions (9), (11), (12) and (13), the critical constant $c_{c,2}$ can be solved from

$$\begin{aligned} 1 - \alpha &= \mathrm{P}\{\mathbf{T} \in V_c\} = \mathrm{P}\{\mathbf{T} \in V_{c,1}\} + \mathrm{P}\{\mathbf{T} \in V_{c,2}\} = 2\mathrm{P}\{\mathbf{T} \in V_{c,1}\} \\ &= \int_0^{\pi/2} 2k \sin^{p-2}\theta F_{p,\nu}\left(\frac{c_{c,2}^2}{p\cos^2(\theta - \theta^*)} \right) \mathrm{d}\theta \end{aligned}$$

where the final equality follows immediately from the distributions of $R_{\mathbf{T}}(\sim\sqrt{pF_{p,\nu}})$ and $\theta_{\mathbf{T}1}$ and the independence of $R_{\mathbf{T}}$ and $\theta_{\mathbf{T}1}$ (see e.g., [25, expressions (11) and (12)].)

Now we consider the one-sided hyperbolic and constant width bands and, without loss of generality, focus on the lower confidence bands. The lower hyperbolic band is given by

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} > \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} - c_{h,1}\hat{\sigma}\sqrt{\mathbf{x}^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}} \in \mathcal{X}_e$$

where $c_{h,1}$ is chosen so that the simultaneous confidence level of the band is equal to $1-\alpha$. From Liu and Lin [25, expression (25)], the critical constant $c_{h,1}$ can be solved from

$$1 - \alpha = \int_0^{\theta^*} k \sin^{p-2}\theta \mathrm{d}\theta \cdot F_{p,\nu}\left(\frac{c_{h,1}^2}{p} \right) + \int_0^{\pi/2} k \sin^{p-2}(\theta + \theta^*) F_{p,\nu}\left(\frac{c_{h,1}^2}{p\cos^2\theta} \right) \mathrm{d}\theta \ + \int_0^{\frac{\pi}{2}-\theta^*} k \sin^{p-2}\theta \mathrm{d}\theta.$$

The lower constant width band is given by

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} > \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} - c_{c,1}\sqrt{(1+a^2)/n}\,\hat{\sigma} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \ldots, x_p)^{\mathrm{T}} \in \mathcal{X}_e,$$

where $c_{c,1}$ is chosen so that the simultaneous confidence level of the band is equal to $1-\alpha$. Similar to the two-sided case, we have

$$1 - \alpha = \mathrm{P}\left\{ \sup_{\mathbf{w} \in \mathcal{W}_e} \mathbf{w}^{\mathrm{T}}\mathbf{T} \le c_{c,1}\sqrt{(1+a^2)/n} \right\} \tag{14}$$

where $\mathbf{T} = (T_1, \mathbf{T}_{(1)}^{\mathrm{T}})^{\mathrm{T}}$ is the same as before. Note that

$$\sup_{\mathbf{w} \in \mathcal{W}_e} \mathbf{w}^{\mathrm{T}}\mathbf{T} = T_1/\sqrt{n} + \sqrt{a^2/n}\, \|\mathbf{T}_{(1)}\|.$$

The probability in (14) is therefore equal to

$$\begin{aligned}
&\mathrm{P}\left\{T_1/\sqrt{n}+\sqrt{a^2/n}\,\|\mathbf{T}_{(1)}\|\le c_{c,1}\sqrt{(1+a^2)/n}\right\}=\mathrm{P}\left\{R_{\mathbf{T}}\cos\theta_{\mathbf{T}1}/\sqrt{n}+\sqrt{a^2/n}\,R_{\mathbf{T}}\sin\theta_{\mathbf{T}1}\le c_{c,1}\sqrt{(1+a^2)/n}\right\}\\
&=\mathrm{P}\left\{R_{\mathbf{T}}\cos(\theta_{\mathbf{T}1}-\theta^*)\le c_{c,1}\right\}\\
&=\mathrm{P}\left\{0\le\theta_{\mathbf{T}1}<\frac{\pi}{2}+\theta^*,\ R_{\mathbf{T}}\cos(\theta_{\mathbf{T}1}-\theta^*)\le c_{c,1}\right\}+\mathrm{P}\left\{\frac{\pi}{2}+\theta^*\le\theta_{\mathbf{T}1}\le\pi\right\}\\
&=\int_0^{\frac{\pi}{2}+\theta^*}k\sin^{p-2}\theta F_{p,\nu}\left(\frac{c_{c,1}^2}{p\cos^2(\theta-\theta^*)}\right)\mathrm{d}\theta+\int_{\frac{\pi}{2}+\theta^*}^{\pi}k\sin^{p-2}\theta\mathrm{d}\theta.
\end{aligned}$$

Substituting this expression in (14), the critical constant $c_{c,1}$ can be computed numerically. All the critical constants $c_{h,2}$, $c_{h,1}$, $c_{c,2}$ and $c_{c,1}$ depend only on θ^*, p, ν and α.

3. Comparisons under the MVCS criterion

In this section we first calculate the volumes of the two-sided confidence sets $c_{h,2}(\hat{\mathbf{b}},\hat{\sigma})$ and $c_{c,2}(\hat{\mathbf{b}},\hat{\sigma})$. We then compare the volumes of these confidence sets to see which is smaller so that the corresponding confidence band is more desirable under the MVCS criterion. Finally, we compare the one-sided hyperbolic and constant width bands in a similar way.

Let $v(R)$ denote the volume of a set $R\subset R^p$, and let $B_p(r)$ denote the ball of radius r in R^p. Note that the Jacobian of the transformation from the Cartesian coordinates to the polar coordinates given in the last section is equal to

$$|J|=R^{p-1}\sin^{p-2}\theta_1\sin^{p-3}\theta_2\cdots\sin\theta_{p-2}.$$

Hence it is clear that

$$v(B_p(r))=\int_{R=0}^{r}\int_{\theta_1=0}^{\pi}\int_{\theta_2=0}^{\pi}\cdots\int_{\theta_{p-2}=0}^{\pi}\int_{\theta_{p-1}=0}^{2\pi}|J|\mathrm{d}R\mathrm{d}\theta_1\cdots\mathrm{d}\theta_{p-1}=c_pr^p$$

where c_p is a constant depending only on p.

From Liu and Lin [25, Lemma 4], V_h in (5) can be partitioned into four parts: $V_h=V_{h,1}+V_{h,2}+V_{h,3}+V_{h,4}$ where

$$\begin{aligned}
V_{h,1}&=\{\mathbf{t}:0\le\theta_{\mathbf{t}1}\le\theta^*,\ R_{\mathbf{t}}\le c_{h,2}\},\\
V_{h,2}&=\{\mathbf{t}:\theta^*<\theta_{\mathbf{t}1}\le\frac{\pi}{2},\ R_{\mathbf{t}}\cos(\theta_{\mathbf{t}1}-\theta^*)\le c_{h,2}\},\\
V_{h,3}&=\{\mathbf{t}:\frac{\pi}{2}<\theta_{\mathbf{t}1}\le\pi-\theta^*,\ R_{\mathbf{t}}\cos(\pi-\theta^*-\theta_{\mathbf{t}1})\le c_{h,2}\},\\
V_{h,4}&=\{\mathbf{t}:\pi-\theta^*<\theta_{\mathbf{t}1}\le\pi,\ R_{\mathbf{t}}\le c_{h,2}\}.
\end{aligned}$$

Now $v(V_{h,1})$ is equal to

$$\begin{aligned}
\int_{R=0}^{c_{h,2}}\int_{\theta_1=0}^{\theta^*}\int_{\theta_2=0}^{\pi}\cdots\int_{\theta_{p-2}=0}^{\pi}\int_{\theta_{p-1}=0}^{2\pi}|J|\mathrm{d}R\mathrm{d}\theta_1\cdots\mathrm{d}\theta_{p-1}&=\left(\int_{\theta_1=0}^{\theta^*}\sin^{p-2}\theta_1\mathrm{d}\theta_1\Big/\int_{\theta_1=0}^{\pi}\sin^{p-2}\theta_1\mathrm{d}\theta_1\right)v(B_p(c_{h,2}))\\
&=k\int_{\theta_1=0}^{\theta^*}\sin^{p-2}\theta_1\mathrm{d}\theta_1\ v(B_p(c_{h,2}))
\end{aligned}$$

and $v(V_{h,2})$ is equal to

$$\begin{aligned}
&\int\int_{\substack{R\cos(\theta_1-\theta^*)\le c_{h,2}\\ \theta^*\le\theta_1\le\pi/2}}\int_{\theta_2=0}^{\pi}\cdots\int_{\theta_{p-2}=0}^{\pi}\int_{\theta_{p-1}=0}^{2\pi}|J|\mathrm{d}R\mathrm{d}\theta_1\cdots\mathrm{d}\theta_{p-1}\\
&=\left(\int\int_{\substack{R\cos(\theta_1-\theta^*)\le c_{h,2}\\ \theta^*\le\theta_1\le\pi/2}}R^{p-1}\sin^{p-2}\theta_1\mathrm{d}R\mathrm{d}\theta_1\Big/\int_{R=0}^{c_{h,2}}\int_{\theta_1=0}^{\pi}R^{p-1}\sin^{p-2}\theta_1\mathrm{d}R\theta_1\mathrm{d}\theta_1\right)v(B_p(c_{h,2}))\\
&=k\int_{\theta^*}^{\pi/2}\sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1\ v(B_p(c_{h,2})).
\end{aligned}$$

Furthermore, we have $v(V_{h,3})=v(V_{h,2})$ and $v(V_{h,4})=v(V_{h,1})$. Combining these gives

$$v(V_h)=2k\left(\int_{\theta_1=0}^{\theta^*}\sin^{p-2}\theta_1\mathrm{d}\theta_1+\int_{\theta^*}^{\pi/2}\sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1\right)v(B_p(c_{h,2})).\tag{15}$$

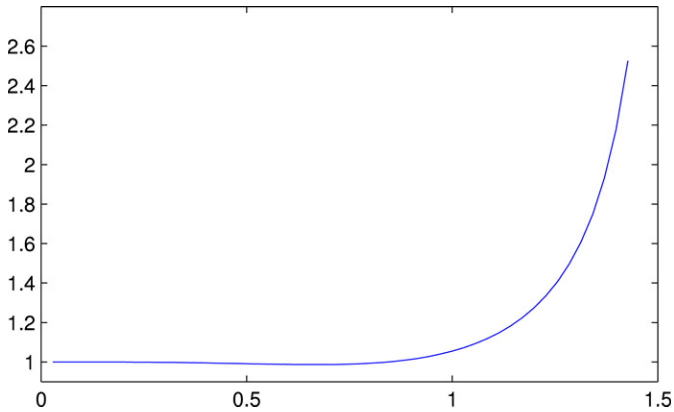

Fig. 1. Plot of the function eff(θ^*) for $p = 3$, $\nu = 15$ and $\alpha = 0.05$.

For the two-sided constant width band (8), similar calculation from expressions (11)–(13) shows that

$$v(V_{c,1}) = v(V_{c,2}) = k\int_0^{\pi/2} \sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1\, v(B_p(c_{c,2}))$$

and so

$$v(V_c) = 2k\int_0^{\pi/2} \sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1\, v(B_p(c_{c,2})). \tag{16}$$

Now note that the confidence sets $C_{h,2}$ in (4) and $C_{c,2}$ in (9) are of the form

$$\begin{aligned} C(\hat{\mathbf{b}},\hat\sigma) &= \left\{\mathbf{b} :\ (\mathbf{z}, Z)^{-1}(X^{\mathrm{T}}X)(\mathbf{b}-\hat{\mathbf{b}})/\hat\sigma \in V\right\} \\ &= \hat\sigma(X^{\mathrm{T}}X)^{-1}(\mathbf{z}, Z)V + \hat{\mathbf{b}} \end{aligned}$$

and so

$$v\left(C(\hat{\mathbf{b}},\hat\sigma)\right) = \left|\hat\sigma(X^{\mathrm{T}}X)^{-1}(\mathbf{z}, Z)\right| v(V) = \left|\hat\sigma(X^{\mathrm{T}}X)^{-1/2}\right| v(V).$$

Hence from (15) and (16)

$$\begin{aligned} \mathrm{eff} &:= \frac{v\left(C_{c,2}(\hat{\mathbf{b}},\hat\sigma)\right)}{v\left(C_{h,2}(\hat{\mathbf{b}},\hat\sigma)\right)} = \frac{v(V_c)}{v(V_h)} \\ &= \frac{\int_0^{\pi/2}\sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1}{\int_{\theta_1=0}^{\theta^*}\sin^{p-2}\theta_1\mathrm{d}\theta_1 + \int_{\theta^*}^{\pi/2}\sin^{p-2}\theta_1/\cos^p(\theta_1-\theta^*)\mathrm{d}\theta_1}\left(\frac{c_{c,2}^p}{c_{h,2}^p}\right). \end{aligned} \tag{17}$$

Under the MVCS criterion, the two-sided hyperbolic band is better than the two-sided constant width band if and only if eff > 1.

It can be shown that eff does not change if one of the predictor variables has a linear transformation (i.e. eff is location and scale invariant). It is noteworthy that eff depends only on θ^*, p, ν and α. The size of the region $\mathcal{X}_e$ in (1) is determined by a: the larger is a the bigger is $\mathcal{X}_e$. From the one-to-one relationship (7) between a and θ^*, the size of $\mathcal{X}_e$ is alternatively determined by θ^*; the larger is the angle θ^* the bigger is $\mathcal{X}_e$. When $\theta^* \to 0$ from right, both the hyperbolic and constant width bands approach the two-sided t-confidence interval for $\mathbf{x}^{\mathrm{T}}\mathbf{b}$ at $\mathbf{x}_{(1)} = \bar{\mathbf{x}}_{(1)}$. When $\theta^* \to \pi/2$, the hyperbolic band approaches the Scheffé band over the whole space of the predictor variables. One the other hand, as $\theta^* \to \pi/2$, the critical constant $c_{c,2}$ of the constant width band approaches a finite constant and so the width of the band $2c_{c,2}\sqrt{(1+a^2)/n}\hat\sigma$ and the volume $v(V_c)$ in (16) approach infinity.

We have calculated eff as a function of $\theta^* \in (0, \pi/2)$ for given values of $p = 3(1)8$, $\nu = 15, 40, \infty$ and $\alpha = 0.10, 0.05, 0.01$. The following pattern appears for all the combinations of p, ν and α: The function eff(θ^*) first decreases and then increases over $\theta^* \in (0, \pi/2)$. When θ^* approaches zero from above, eff(θ^*) approaches one. When θ^* approaches $\pi/2$ from below, eff(θ^*) approaches infinity. At a certain threshold value $\theta_0^* = \theta_0^*(p, \nu, \alpha)$, eff($\theta_0^*$) is equal to one. The threshold value $\theta_0^*(p, \nu, \alpha)$ is relatively stable for different values of ν and α we studied, but it increases in p. The value of $\theta_0^*(p, \nu, \alpha)$ is approximately equal to 0.8 for $p = 3$ and 1.1 for $p = 8$. Furthermore, $\min_{\theta^*\in(0,\pi/2)}$ eff(θ^*) is no less than 0.98 for all the combinations studied. Fig. 1 provides a plot of eff(θ^*) for $p = 3$, $\nu = 15$ and $\alpha = 0.05$, the shape of which is typical for all the combinations of p, ν and α.

From these observations, the following conclusions can be drawn. When $0 < \theta^* < \theta_0^*$ (i.e. when the value of a in (1) is smaller than a certain threshold value), the two-sided constant width band improves upon the two-sided hyperbolic band in terms of its MVCS. The advantage of the constant width band over the hyperbolic band in this situation is very limited, however, since $\min_{\theta^* \in (0,\pi/2)} \text{eff}(\theta^*)$ is only very marginally smaller than one. On the other hand, when $\theta_0^* < \theta^* < \pi/2$, the hyperbolic band improves upon the constant width band. Indeed, the advantage of the hyperbolic band over the constant width band can be enormous, especially when θ^* is close to the upper limit $\pi/2$ since $\text{eff}(\theta^*)$ becomes very large when θ^* is close to $\pi/2$.

These observations are consistent with those for a simple linear regression made in [26], where the angle $\theta/2$ plays a similar role there as the angle θ^* does here. In a simple linear regression, however, the interval over which the confidence bands are constructed is not necessarily symmetric about the mean of the observed values of the predictor variable.

Now we turn our attention to the comparison of the one-sided hyperbolic and constant width bands. Note that the confidence sets for $\mathbf{b}$ that correspond to the one-sided hyperbolic and constant width bands are not bounded and have volumes equal to infinity. To overcome this, we adopt the following approach that is also used for the comparison of one-sided confidence bands or intervals under the average width criterion; see e.g., [27]. Since the $1-\alpha$ level lower and upper hyperbolic (constant width) confidence bands are symmetric about the fitted regression model $\mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}}$, we use half of the volume of the set of $\mathbf{b}$ that corresponds to the band

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} \in \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} \pm c_{h,1}\hat{\sigma}\sqrt{\mathbf{x}^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}\mathbf{x}} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \dots, x_p)^{\mathrm{T}} \in \mathcal{X}_e$$

as a measure for the one-sided hyperbolic band, and half of the volume of the set of $\mathbf{b}$ that corresponds to the band

$$\mathbf{x}^{\mathrm{T}}\mathbf{b} \in \mathbf{x}^{\mathrm{T}}\hat{\mathbf{b}} \pm c_{c,1}\sqrt{(1+a^2)/n}\,\hat{\sigma} \quad \text{for all } \mathbf{x}_{(1)} = (x_2, \dots, x_p)^{\mathrm{T}} \in \mathcal{X}_e$$

as a measure for the one-sided constant width band. Hence the ratio of these two measures, $\text{eff}_1(\theta^*)$, still has the expression (17) except that $c_{h,2}$ and $c_{c,2}$ are replaced by $c_{h,1}$ and $c_{c,1}$ respectively.

We have also calculated eff_1 as a function of $\theta^* \in (0, \pi/2)$ for given values of $p = 3(1)8$, $\nu = 15, 40, \infty$ and $\alpha = 0.10, 0.05, 0.01$. It turns out that $\text{eff}_1(\theta^*)$ has similar shape and properties as $\text{eff}(\theta^*)$.

We therefore recommend that the hyperbolic band should be the default method of choice unless the "constant width" feature of the constant width band is highly desirable for the practical problem under study. One example of when constant width is more desirable than hyperbolic shape is given in [32].

Note that, on the set $\left\{\mathbf{x}_{(1)} : \left(\mathbf{x}_{(1)} - \bar{\mathbf{x}}_{(1)}\right)^{\mathrm{T}} S^{-1} \left(\mathbf{x}_{(1)} - \bar{\mathbf{x}}_{(1)}\right) = b^2\right\}$ for a given b satisfying $0 \le b \le a$, the width of the hyperbolic band is constant. This constant width increases with b and is equal to the width of the constant width band at a particular value of b between 0 and a. As such, the hyperbolic band is narrower than the constant width band when $\mathbf{x}_{(1)}$ is near $\bar{\mathbf{x}}_{(1)}$ and vice versa when $\mathbf{x}_{(1)}$ is near the boundary of $\mathcal{X}_e$. Comparison of the hyperbolic and constant width bands under the average width criterion in [27] leads to conclusions that differ from our observations under the MVCS criterion above in two major ways. First, the average width of the hyperbolic band is always no larger than that of the constant width band. Second, the ratio of the average widths of the two bands is always finite even as $\theta^* \to \pi/2$. Of course, under either form of optimality one is led to recommend use of the hyperbolic bands, so in that sense there is a consistency of direction in both criteria.

Finally, we use a portion of the acetylene data in [31] to briefly illustrate the calculations discussed in this paper. This same data set has also been used for illustration by Casella and Strawderman [23], Naiman [16] and Liu and Lin [25] among others. The two predictor variables are reactor temperature (x_2) and ratio of H_2 to n-Heptane (x_3). The response variable (y) is conversion of n-Heptane to Acetylene. There are sixteen data points, so that $p = 3$, $n = 16$ and $\nu = 13$. The fitted multiple linear regression model is given by $y = -130.69 + 0.134x_2 + 0.351x_3$, with $\hat{\sigma} = 3.624$, and $R^2 = 0.92$.

The observed values of x_2 range from 1100 to 1300 with average $x_{\cdot 2} = 1212.5$, and the observed values of x_3 range from 5.3 to 23 with average $x_{\cdot 3} = 12.4$. So, the ellipsoidal region $\mathcal{X}_e$ is centered at $(x_{\cdot 2}, x_{\cdot 3})^{\mathrm{T}} = (1212.5, 12.4)^{\mathrm{T}}$. The size of $\mathcal{X}_e$ increases with the value of a. For $a = 1.9$ and $\alpha = 0.10$ as considered in [25], the region $\mathcal{X}_e$ is comparable with the range of observations on the predictor variables and our MATLAB program calculates $\theta^* = 1.086$, $c_{h,2} = 2.723$, $c_{c,2} = 2.598$, $c_{h,1} = 2.370$, $c_{c,1} = 2.276$, $\text{eff} = 1.119$ and $\text{eff}_1 = 1.141$. So the two-sided hyperbolic band is about 12% more efficient than the two-sided constant width band in this particular case, and the one-sided hyperbolic band is about 14% more efficient than the one-sided constant width band. The smallest value of eff over $a \in (0, \infty)$ is equal to 0.987, obtained at $a = 0.771$. The smallest value of eff_1 over $a \in (0, \infty)$ is equal to 0.990, attained at $a = 0.761$.

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