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Simultaneous Confidence Bands and Simultaneous Tolerance Bands in Linear Regression

by

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ABSTRACT

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SIMULTANEOUS CONFIDENCE BANDS AND SIMULTANEOUS TOLERANCE BANDS IN LINEAR REGRESSION

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Construction of simultaneous confidence bands for a percentile line in linear regression has been considered by several authors. But only conservative symmetric bands, which use critical constants over the whole covariate range $(-\infty, \infty)$, are available in the literature. New methods allow the construction of exact symmetric bands for a percentile line over a finite interval of the covariate x. The exact symmetric bands can be substantially narrower than the corresponding conservative symmetric bands available in the literature so far. Several exact symmetric confidence bands are compared under the average band width criterion. Furthermore, new asymmetric confidence bands for a percentile line are proposed. They are uniformly and can be very substantially narrower than the corresponding exact symmetric bands. Therefore, asymmetric bands should always be used under the average band width criterion. The proposed methods are illustrated with a real example. One-side simultaneous confidence bands have also been studied.

Construction of simultaneous tolerance bands for calibration in linear regression models has been studied by many researchers. The $(p, 1-\alpha)$-simultaneous tolerance bands are first addressed by Lieberman and Miller (1963), and there are three construction methods in the literature so far. In this thesis, the construction of exact two-sided $(p, 1-\alpha)$-simultaneous tolerance bands is considered. The methods are demonstrated with an example.

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Declaration of Authorship

I, YANG HAN, declare that the thesis entitled

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and the work presented in it are my own and has been generated by me as the result of my own original research. I confirm that:

1. This work was done wholly or mainly while in candidature for a research degree at this University;
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3. Where I have consulted the published work of others, this is always clearly attributed;
4. Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work;
5. I have acknowledged all main sources of help;
6. Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;
7. parts of this work have been published as:

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Signed ....

Date ....

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Chapter 1

Introduction

The method of least squares which is the earliest form of regression was published by Legendre (1805) and Gauss (1809). The term 'regression' was first proposed by Galton (1885) and used to describe a biological phenomenon. From then on, regression analysis has been widely used for prediction and forecasting in many fields such as biology, chemistry, astronomy, agriculture and other practical aspects of both social and natural science. Many statistical methodologies and tools are from or related to the study of linear regression. We are looking at two of them, the simultaneous confidence bands and simultaneous tolerance bands.

One of the main purposes of this research is to construct simultaneous confidence bands for a percentile line over a given covariate interval which can be finite or the whole range $(-\infty, \infty)$ as a special case, and to compare the bands under the average width criterion. The construction of simultaneous confidence bands for a percentile line has been studied by Steinhorst and Bowden (1971), Kabe (1976), Turner and Bowden (1977), Turner and Bowden (1979), Thomas and Thomas (1986), Odeh and Mee (1990). A simultaneous confidence band can quantify the plausible range of the percentile line. Any straight line that lies inside the simultaneous confidence band is deemed, by this band, as a plausible candidate for the true percentile line. It is intuitive that the narrower the band is, the better it is. Hence the average width is used as an optimality criterion.

The other main purpose of this thesis is to construct exact two-sided $(p, 1-\alpha)$-simultaneous tolerance bands. Construction of simultaneous tolerance bands for calibration has been considered by many researchers. It is first addressed by Lieberman and Miller (1963), and there are three construction methods in the literature so far. The first is the probability set method by Wilson (1967) and Limam and Thomas (1988). These bands are conservative and two-sided. The second is the construction of central p-proportion simultaneous confidence bands by Lieberman and Miller (1963), Lieberman et al. (1967) and Scheffé (1973). These bands are also conservative and two-sided. The third is an exact method by Mee et al. (1991)

for two-sided bands and Odeh and Mee (1990) for one-sided bands. Since the first two methods are conservative while Mee et al. (1991) method is exact, the two-sided bands of Mee et al. (1991) are usually narrower and so better than the conservative bands, as demonstrated numerically in Mee et al. (1991). Different bands can be compared under the average width criterion.

In this chapter we give a review of linear regression models, simultaneous confidence bands and simultaneous tolerance bands, and present preliminary results necessary throughout the thesis.

1.1 Linear regression model

Linear regression analysis is a simple but very useful statistical technique for evaluating the relationship between a dependent variable Y and one or more independent variables $x_1, \cdots, x_p$. The model takes the form

$$Y = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + e, \tag{1.1}$$

where $\beta_0, \cdots, \beta_p$ are unknown regression coefficients and e is an unobservable random error which has the distribution $N(0, \sigma^2)$. Let x_i denote the ith variable in the model (1.1) and x_{ji} be the jth observation of the variable x_i. Similarly, Y_j indicates the jth observation of independent variable Y. Denote $\boldsymbol{Y} = (Y_1, \cdots, Y_n)'$ and $\boldsymbol{x}_i = (x_{1i}, \cdots, x_{ni})$ as n observations on Y and x_i, $i = 1, \cdots, p$, respectively. Then the jth observation satisfies

$$Y_j = \beta_0 + \beta_1 x_{j1} + \cdots + \beta_p x_{jp} + e_j, \quad j = 1, \cdots, n.$$

Here the unknown regression coefficients $\beta_0, \cdots, \beta_p$ are the same for all the observations and the errors $e_1, \cdots, e_n$ are assumed to be independent. This model can also be expressed as the matrix form

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}, \tag{1.2}$$

where $\boldsymbol{X} = (\mathbf{1}, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_p)$, $\mathbf{1}$ is a column vector of size n with all elements equal to 1, $\boldsymbol{\beta} = (\beta_0, \beta_1 \cdots, \beta_p)'$ and $\boldsymbol{e} = (e_1, \cdots, e_n)'$.

1.2 A simple linear regression model, parameter estimation and basic results

Considering the simple case of linear regression model (1.2) with $p = 1$, we have

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e} = [\mathbf{1}, \boldsymbol{x}_1]\boldsymbol{\beta} + \boldsymbol{e}, \tag{1.3}$$

where $\boldsymbol{X}$ is the $n\times 2$ design matrix of rank 2, $\boldsymbol{x}_1 = (x_{11}, x_{21}, \cdots, x_{n1})'$ are n observations on x_1, $\boldsymbol{\beta} = (\beta_0, \beta_1)'$ is the vector of unknown regression coefficients and $\boldsymbol{e}$ is the error vector which has the distribution $N_n(0, \sigma^2 I)$ with σ^2 unknown. Without loss of generality, it is assumed that the design matrix $\boldsymbol{X}$ is of full column rank 2 and so $\boldsymbol{X}'\boldsymbol{X}$ is non-singular. The unique least squares estimator of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1)' = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}.$$

The vector of residuals is defined by

$$\hat{\boldsymbol{e}} = (\hat{e}_1, \cdots, \hat{e}_n)' = \boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}} = \boldsymbol{Y} - \hat{\boldsymbol{Y}}.$$

Denote the unbiased estimator of σ^2 is based on the residual sum of squares

$$SS_E = \sum_{j=1}^{n} \hat{e}_j^2 = \|\hat{\boldsymbol{e}}\|^2 = \|\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}\|^2.$$

Define

$$\hat{\sigma}^2 = SS_E/(n-2) = \|\hat{\boldsymbol{e}}\|^2/(n-2).$$

For notation simplicity, we denote $\nu = n-2$. It is well known that the random variables $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are independent, and

$$\hat{\boldsymbol{\beta}} \sim N_2(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}), \quad \hat{\sigma}^2 \sim \frac{\sigma^2}{\nu}\chi^2_\nu,$$

and so $\hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$. Denote $U = \hat{\sigma}/\sigma$. Then the probability density function of U is given by

$$f_{\frac{\hat{\sigma}}{\sigma}}(u) = 2^{1-\nu/2}\nu^{\nu/2}u^{\nu-1}\exp(-\frac{\nu}{2}u^2)/\Gamma(\nu/2), \quad u > 0. \tag{1.4}$$

It follows directly that $E(\hat{\sigma}^2) = \sigma^2$ and $E(\frac{\hat{\sigma}}{\sigma}) = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$.

Throughout this thesis, without loss of generality, let $\boldsymbol{x}_1'\boldsymbol{1} = \boldsymbol{0}$, i.e., the column $\boldsymbol{x}_1$ is mean adjusted. Then we have

$$(\boldsymbol{X}'\boldsymbol{X})^{-1} = \begin{pmatrix} 1/n & 0 \\ 0 & (\boldsymbol{x}_1'\boldsymbol{x}_1)^{-1} \end{pmatrix}.$$

Let $\boldsymbol{P}$ be the unique square root matrix of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$. The matrix $\boldsymbol{P}$ is used only in the derivations but not the final formula of the simultaneous confidence level. The 2×2

matrix $\boldsymbol{P}$ is given by

$$\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}, \tag{1.5}$$

where $P_1 = \sqrt{\boldsymbol{x}_1'\boldsymbol{x}_1}$. Denote $\boldsymbol{N} = (N_1, N_2)' = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma$. It is clear that $\boldsymbol{N} \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$. It is straight forward to show that the two components of $\boldsymbol{N}$ are given by $N_1 = \frac{\sqrt{n}(\hat{\beta}_0 - \beta_0)}{\sigma}$, $N_2 = \frac{P_1(\hat{\beta}_1 - \beta_1)}{\sigma}$.

As in several published papers on this topic, we focus on the simple linear regression model throughout this thesis. Our approach, however, can readily be generalized to polynomial regression and multiple linear regression where the covariates are assumed to have no functional relationships among them. Since we just look at a simple case of the linear regression model (1.1) with only one predictor variable x_1, then we suppressed the subscript "1" of x_1 and use x instead below.

1.3 Percentile lines

A regression percentile line is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma = \beta_0 + \beta_1 x + z_\gamma\sigma, \tag{1.6}$$

where $\boldsymbol{x} = (1, x)'$ and z_γ denotes the 100γth percentile of the standard normal distribution, i.e.,

$$\int_{-\infty}^{z_\gamma} (2\pi)^{-\frac{1}{2}} \exp\{-\frac{1}{2}x^2\} dx = \gamma.$$

For any specific point $\boldsymbol{x}_0$, denote $Z_0 = \boldsymbol{x}_0'\boldsymbol{\beta} + e$. Then we have

$$P(Z_0 \leq \boldsymbol{x}_0'\boldsymbol{\beta} + z_\gamma\sigma) = \gamma. \tag{1.7}$$

Note that the regression line $\boldsymbol{x}'\boldsymbol{\beta}$ is a special case of the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ with $z_\gamma = 0$ and so $\gamma = 0.5$.

1.4 Simultaneous confidence bands

One focus of this thesis is the construction of simultaneous confidence bands for the percentile line in (1.6) and the comparison of different bands.

Construction of simultaneous confidence bands for regression line $\boldsymbol{x}'\boldsymbol{\beta}$ has a history dating back to Working and Hotelling (1929) and Scheffé (1953). For $\gamma = 0.5$, a two-sided hyperbolic confidence band over an interval (a, b) is given by

$$\boldsymbol{x}'\boldsymbol{\beta} \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a, b). \tag{1.8}$$

The band width is proportional to the standard error of the estimated regression function $\boldsymbol{x}'\hat{\boldsymbol{\beta}}$. Working and Hotelling (1929) first considered the band in (1.8) for the special case $(a, b) = (-\infty, \infty)$. Wynn and Bloomfield (1971) and Uusipaikka (1983) presented two methods of finding critical constant c of the hyperbolic band. Bohrer and Francis (1972) provided exact one-sided hyperbolic bands. Pan et al. (2003) studied one-sided bands via the method given by Uusipaikka (1983). Besides hyperbolic bands, Gafarian (1964) presented a two-sided constant-width band over an given interval. Bowden and Graybill (1966) proposed a two-sided three-segment band.
Graybill and Bowden (1967) considered a two-sided three-segment band.

The problem of constructing simultaneous confidence bands for a percentile line

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$$

where z_γ is the 100γth percentile of the standard normal distribution, has been considered by many researchers including Steinhorst and Bowden (1971), Turner and Bowden (1977), Turner and Bowden (1979) and Thomas and Thomas (1986). Recently, several articles have considered various applications of confidence bands for inferential purposes; see for instance, Spurrier (1999), Al-Saidy et al. (2003), Liu et al. (2004), Bhargava and Spurrier (2004), Piegorsch et al. (2005), Liu et al. (2007) and Liu et al. (2009). It can also be used for statistical discrimination as considered by Eastling (1969). In this thesis, the focus is on the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ for $\gamma \neq 0.5$. In some practical problems, for example, drug stability studies, the percentile function may be of more interest than the regression function $\boldsymbol{x}'\boldsymbol{\beta}$. Drug stability studies are routinely carried out in the pharmaceutical industry in order to measure the degradation over time of an active pharmaceutical ingredient of a drug product. From the patients' point of view, it is expected that a large proportion (e.g., $100(1-\gamma)\%$ with $\gamma = 0.05$) of dosage units (e.g., tablets, capsules, vials) should have drug content level above a certain threshold, say, 98 (in percentage) before a specified expiry date, say, 2 years. It is thus of interest to estimate where the 100γth percentile line lies with a two-sided simultaneous confidence band. Comparing the lower part of the confidence band with the threshold 98, we can assess whether no more than 5% of all the dosage units have drug content level below 98, for any given point in the time interval $(0, 2)$. Similarly, comparing the upper part of the confidence band with the threshold 98, we can evaluate whether more than 5% of all the dosage units have drug content level below 98, for any time point in $(0, 2)$. More details of this example are given in Chapter 3. Extensive discussions on the usefulness of percentile points or percentile lines can be found in

Harris and Boyd (1995), Gilchrist (2000), Koenker (2005) and Liu et al. (2013).

We first consider the two-sided symmetric confidence bands of the form

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma \hat{\sigma}/\theta \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2 \xi} \quad \text{for all } x \in (a, b) \tag{1.9}$$

where $\boldsymbol{x} = (1, x)'$, (a, b) is a given covariate interval over which a confidence band is required, and the given constants $\theta \neq 0$ and ξ are chosen to give different specific confidence bands. At a given x, the center of the band is $\boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma \hat{\sigma}/\theta$ while the width of the band is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2 \xi}$. Hence the centre of the band depends on θ, while the width of the band depends on ξ. The central question is how to compute the critical constant c to give the specified confidence level $1 - \alpha$ (for example, chosen as 0.75, 0.95 or 0.99).

All the published bands (e.g. , Turner and Bowden (1977, 1979) and Thomas and Thomas (1986)) are of form (1.9) with a particular pair of θ and ξ values. However, methods available in the literature so far are only for computing the conservative critical constants c over the whole covariate range $(a, b) = (-\infty, \infty)$. As linear regression models often hold for only a finite covariate range, it is important to consider a finite interval (a, b). A confidence band over a finite interval can be substantially narrower and so more efficient than a band over the whole range $(-\infty, \infty)$. Our methods allow the computation of the exact critical constant c of the general form (1.9) for any given interval (a, b), finite or infinite.

Various choices of (θ, ξ) in (1.9) have been studied in the literature in the hope of reducing the average width of a band. In this thesis, we propose new asymmetric confidence bands which are uniformly narrower than the corresponding symmetric bands. Corresponding to each symmetric band of form (1.9), an asymmetric band will be constructed whose width is smaller than the width of the symmetric band at any $x \in (a, b)$ and can be substantially smaller especially when γ is either close to zero or one.

It has to be emphasized that the construction of exact $1 - \alpha$ simultaneous confidence bands (either symmetric or asymmetric) for the percentile line of the standard linear regression models is the focus of this thesis. The standard linear regression model assumption (including normality) is crucial to the particular form (1.6) of the percentile line. As soon as one goes beyond the standard linear regression models, only approximate simultaneous confidence bands for a percentile line can be constructed. For example, one can use the large sample asymptotic normality of quantile regression (cf. Koenker (2005)) to construct only an approximate simultaneous band for a percentile curve.

A $1-\alpha$ one-sided confidence band for a percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ is just the one-sided $(1 - \alpha, \gamma)$ tolerance band for the simple linear model. One-sided confidence band for a percentile line has been studied by Turner and Bowden (1979) and Odeh and Mee (1990). Another related problem that is of interest is calibration. Mee et al. (1991) and Mee and Eberhardt (1996) constructed of simultaneous tolerance intervals and applied them to calibration.

To compare different confidence bands, two criteria are used in the statistical literature: average width criterion and minimum area confidence set criterion. The average width of a simultaneous confidence band has been widely used as an optimality criterion for the comparison of different confidence bands. Gafarian (1964) used the average width as an optimality criterion for the first time. Liu and Hayter (2007) first proposed minimum area confidence set optimality criterion. We compare the average band widths over an interval (a, b) of both asymmetric and symmetric bands.

1.5 Calibration and simultaneous tolerance bands

Calibration, also known as discrimination or the reverse prediction, has been widely used in measurement science and other applications. Statistical calibration with regression has a history dating back to Eisenhart (1939). Suppose one has the training data set $\mathcal{E} := \{(x_j, y_j), j = 1, \cdots, n\}$ which is used to fit a regression line of Y on x. Assume x is a desirable but expensive or difficult measurement and Y represents a cheaper and more conveniently obtainable instrument response. After fitting the linear regression model based on the training data set, for each given future Y-value, one can get the confidence set for the corresponding x, from a simultaneous tolerance band. For example, x is the true alcohol level in blood stream while Y is the reading on a breathalyzer, of a driver; more details on this example are provided in Chapter 5.

Let $Y(x) = \boldsymbol{x}'\boldsymbol{\beta} + e_x$ denote a future observation at x with $e_x \sim N(0, \sigma^2)$. Assume $Y(x)$ is independent of $\boldsymbol{Y}$ in (1.3). For a given x value, a $(p, 1-\alpha)$-tolerance interval for $Y(x)$ contains at least $100p\%$ proportion of the $Y(x)$ distribution with $1-\alpha$ confidence level. In some practical problems, one may be interested in infinite future observations corresponding to x values in a prespecified covariate interval (a, b) based on the same training data set $\mathcal{E} := \{(x_j, y_j), j = 1, \cdots, n\}$, or equivalently $(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\sigma}})$. This is the motivation of constructing simultaneous tolerance bands over a constrained covariate interval. Based on the same training data set, a $(p, 1-\alpha)$-simultaneous tolerance band for infinite future observations $Y(x)$ over $x \in (a, b)$ contains at least $100p\%$ proportion of the $Y(x)$ distribution for any $x \in (a, b)$ simultaneously with confidence level $1 - \alpha$.

The $(p, 1-\alpha)$-simultaneous tolerance bands $[L(x; \mathcal{E}), U(x; \mathcal{E})]$ over the interval $x \in (a, b)$ satisfy

$$P_{\mathcal{E}}\{P_{Y(x)}\{L(x; \mathcal{E}) < Y(x) < U(x; \mathcal{E}) | \mathcal{E}, x\} \geq p \text{ for all } x \in (a, b)\} \geq 1 - \alpha,$$

where $Y(x)$ denotes a future Y-value corresponding to x and $Y(x)$ is independent of the training data $\mathcal{E}$. The probability $P_{Y(x)}$ is with respect to $Y(x)$ and conditional on $\mathcal{E}$, and the probability $P_{\mathcal{E}}$ is with respect to $\mathcal{E}$. Then for each future Y the confidence set $C(Y)$ for the corresponding x is defined as

$$C(Y) = \{x \in (a, b) : L(x; \mathcal{E}) < Y < U(x; \mathcal{E})\}.$$

It is shown in Scheffé(1973, Appendix B) that for an infinite sequence of future Y-values, at least p proportion of confidence sets $C(Y)$ contain the true x-values with confidence level $1 - \alpha$.

There are three construction methods in the literature so far. More details are given in Chapter 5. The construction of exact two-sided $(p, 1 - \alpha)$-simultaneous tolerance bands is studied in this thesis.

1.6 Outline of the thesis

In Chapter 2, we study the two-sided exact symmetric simultaneous confidence bands SB, TBU, TBE V, UV and TT. The details of the definitions of the six bands are given in Chapter 2. Band SB is a new exact band which has the same form as the conservative band constructed in Steinhorst and Bowden (1971). Bands TBU and TBE are new exact bands with the same forms as the conservative bands in Turner and Bowden (1977). Band TT is a new exact band with the same form as the conservative band in Thomas and Thomas (1986). The forms of bands V and UV have not been considered before. We provide thorough comparison of these six exact bands under the average width criterion. In Chapter 3, we propose a method of constructing an asymmetric confidence band corresponding to each symmetric confidence band given in Chapter 2. The asymmetric confidence bands are uniformly better the corresponding exact symmetric bands for any non-trivial situation. In particular, we investigate the extent to which the asymmetric confidence bands improve over the corresponding symmetric confidence bands in terms of average width. In Chapter 4, we consider the one-sided simultaneous confidence bands for a percentile line which is just the one-sided simultaneous tolerance bands for the simple linear model. In Chapter 5, we study the two-sided simultaneous tolerance bands. The construction of exact two-sided simultaneous tolerance bands over any finite interval is proposed.

Chapter 2

Two-sided Symmetric Simultaneous Confidence Bands for a Percentile Line

A two-sided simultaneous confidence band for the percentile function $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ over the interval $x \in (a, b)$ has the general form

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2 \xi} \text{ for all } x \in (a, b). \tag{2.1}$$

Here the constants $\theta \neq 0$ and ξ can be chosen to give different specific confidence bands. For given constants θ and ξ, the critical constant c is determined to satisfy the specified confidence level $1 - \alpha$. Particularly, when $\gamma = 0.5$ and so $z_\gamma = 0$, the band in (2.1) becomes

$$\boldsymbol{x}'\boldsymbol{\beta} \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a, b).$$

Working and Hotelling (1929) considered this band for the special case $(a, b) = (-\infty, \infty)$. In this section, we focus on the bands of the form (2.1) with $\xi = 0$, denoted as Form I:

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a, b). \tag{2.2}$$

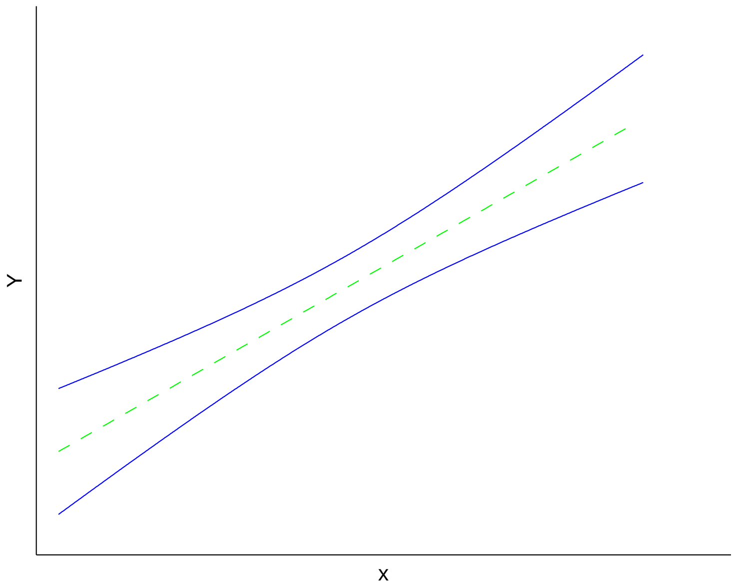
In Section 2.2, we will look at the bands of the form (2.1) with $\xi \neq 0$, since mathematical treatments of these two forms are slightly different.

2.1 Symmetric bands of Form I

Several candidates for θ have been considered in the literature. Steinhorst and Bowden (1971) used $\theta = 1$ for the band over $x \in (-\infty, \infty)$. Turner and Bowden (1977) generalized the procedure of Steinhorst and Bowden (1971) by using several different values for θ (see details below).

Figure 2.1 illustrates the shape of the confidence bands in (2.2). The center of the band at x is given by $\boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta}\hat{\sigma}$. The lower and upper parts of the band are symmetric about the estimated percentile line. The width at x is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$, which is proportional to $\sqrt{\mathrm{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}})}$ since $\boldsymbol{x}'\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{x}'\boldsymbol{\beta}, \sigma^2\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x})$. Furthermore, the width of the band is the smallest at $x=\bar{x}$, the mean of the observed covariate values, and increases as x moves away from $\bar{x}$ on either sides. The upper part of the band, $x'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$ for $x \in (a,b)$, is convex, while the lower part of the band is concave.

Figure 2.1: *The shape of the bands in (2.2)*



We consider three different bands in this chapter. All of them are special cases of the form (2.2). A two-sided simultaneous confidence band can be used to quantify the plausible range of the true percentile line. The intuitive idea is that the narrower the band is, the better the band is. Since for any given x, the width of each band in (2.2) is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$, then the band with the smallest critical constant c is the narrowest.

The first simultaneous confidence band, denoted as *SB*, uses $\theta = 1$ in (2.2) as considered by Steinhorst and Bowden (1971) but over an interval (a,b) which can be finite or the whole range $x \in (-\infty,\infty)$ and is more useful in practise. Specifically, it has the form

$$\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}}+z_\gamma\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b). \tag{2.3}$$

The second band, denoted as *TBU*, uses $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$, where $\nu = n-2$ in (2.2) and is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b). \tag{2.4}$$

Note that θ is chosen so that $E(\frac{\hat{\sigma}}{\theta}) = \sigma$ and therefore $\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma}$ is the uniformly minimum variance unbiased estimator(UMVUE) of $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$. This form was studied by Turner and Bowden (1977), but only over the whole range $x \in (-\infty, \infty)$.

The third band, denoted as *TBE*, uses $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ and is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}, \text{ for all } x \in (a,b). \tag{2.5}$$

This choice of θ was also proposed by Turner and Bowden (1977). Again, they only considered this band over the whole range $x \in (-\infty, \infty)$. From their investigation, they recommended this band among the several bands they studied.

It is noteworthy that all the bands considered in the past by Steinhorst and Bowden (1971), Turner and Bowden (1977) and Thomas and Thomas (1986) are all over the whole range $x \in (-\infty, \infty)$. As an extension, we consider the bands over a given interval (a, b) which is more general and includes the whole range as a special case.

Next we consider the computation of the critical constant c in the band (2.2). For this, it is necessary to find an expression of the simultaneous confidence level of the band that is amenable to computation.

The simultaneous confidence level of this band is given by

$$\begin{aligned}
& P\left\{\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b)\right\} \\
= & P\left\{\max_{x\in(a,b)} \frac{|\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \le c\right\} \\
= & P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c\right\} \\
= & P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N} + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c\right\} \\
= & P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c\right\},
\end{aligned} \tag{2.6}$$

where the matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$$

is the unique square root of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ and defined in (1.5),

$$\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$$

and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$. Note that $\boldsymbol{Px} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}$ and so (2.6) is further equal to

$$P\left\{ \max_{x\in(a,b)} \frac{\left| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix} \right|}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \le c \right\}$$

$$= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{ \max_{x\in(a,b)} \frac{\left| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ N_2/u \end{pmatrix} \right|}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \le c \right\} du, \quad (2.7)$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

Next we give two different methods for computing the critical constant c.

2.1.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \max_{x\in(a,b)} \frac{\left| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} n_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ n_2/u \end{pmatrix} \right|}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (2.7) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{k(\boldsymbol{v}) \le c \text{ for all } x\in(a,b)\}} d\boldsymbol{v}, \quad (2.8)$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$ and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Since $N_1 \sim N(0,1)$, $N_2 \sim N(0,1)$ and $U \sim \sqrt{\chi^2_\nu/\nu}$ are independent and from (1.4), we have

$$f(\boldsymbol{v}) = \pi^{-1} e^{-(n_1^2+n_2^2+\nu u^2)/2} 2^{-\nu/2} \nu^{\nu/2} u^{\nu-1}/\Gamma(\nu/2). \quad (2.9)$$

Expression (2.8) involves a three-dimensional integration and can be used to compute the simultaneous confidence level for a given c via numerical quadrature. Also, for a given confidence level, the value of critical constant c can be found numerically by using this method. Based on adaptive Simpson rule, the MATLAB built-in function `triplequad` can be used for three-dimensional integration .

Our experience shows this method of computing the exact value of critical constant c takes substantially longer computation time than the simulation method introduced in the following section. The numerical quadrature method can be used to cross check with the simulation method. However, we don't have to do this every time. The numerical integration method and the simulation method agree on all the results we have tried. So we can just use the simulation method.

2.1.2 Simulation method

From (2.6), let

$$\begin{aligned} S &= \max_{x\in(a,b)} \frac{|\boldsymbol{x}'(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})+z_\gamma(\hat{\sigma}/\theta-\sigma)|}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \\ &= \max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U+z_\gamma(1/\theta-1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}}. \end{aligned} \tag{2.10}$$

The simultaneous confidence level is therefore given by

$$P\{S\le c\}.$$

Hence, the critical constant c of the $1-\alpha$ simultaneous confidence band is just the $100(1-\alpha)$ percentile of the random variable S. This population percentile can be approximated by the sample percentile using simulation in the following way. We first generate independent standard bivariate normal random vectors $\boldsymbol{N}_i$ and variables $U_i\sim\sqrt{\chi^2_\nu/\nu}$, $i=1,2,\cdots,R$. Then we calculate

$$S_i=\max_{x\in(a,b)}\frac{|(P\boldsymbol{x})'\boldsymbol{N}_i/U_i+z_\gamma(1/\theta-1/U_i)|}{\sqrt{(P\boldsymbol{x})'(P\boldsymbol{x})}},\quad i=1,\cdots,R.$$

Finally c is approximated by the $\langle(1-\alpha)R\rangle$th largest of the R replicates of S : $S_1,\cdots,S_R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$. The computation methods available in the literature are: projection method, turning point method and quadratic programming method, see Liu (2010). Next we introduce the three computation methods for calculating S from $\boldsymbol{N}$ and U.

2.1.2.1 Projection method

From (2.10), we have

$$S = \max_{x\in(a,b)} \frac{|(\boldsymbol{Px})'\boldsymbol{Z}|}{\|(\boldsymbol{Px})\|},$$

where

$$\boldsymbol{Z} = \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} = \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix}$$

and $\|\cdot\|$ means the Euclidean norm of a vector. Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$ and $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$. Then $\boldsymbol{Px}_1 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}a \end{pmatrix}$ and $\boldsymbol{Px}_2 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}b \end{pmatrix}$. When x changes over the interval (a,b), $\boldsymbol{Px}$ forms a cone bounded by $\boldsymbol{Px}_1$ and $\boldsymbol{Px}_2$. If the projection of $\pm\boldsymbol{Z}$ belongs to the cone, then

$$S = \max_{x\in(a,b)} \frac{|(\boldsymbol{Px})'\boldsymbol{Z}|}{\|\boldsymbol{Px}\|} = \|\boldsymbol{Z}\|.$$

Otherwise,

$$\begin{aligned} S &= \max_{x\in(a,b)} \frac{|(\boldsymbol{Px})'\boldsymbol{Z}|}{\|\boldsymbol{Px}\|} \\ &= \max\left\{\frac{|(\boldsymbol{Px}_1)'\boldsymbol{Z}|}{\|\boldsymbol{Px}_1\|}, \frac{|(\boldsymbol{Px}_2)'\boldsymbol{Z}|}{\|\boldsymbol{Px}_2\|}\right\}. \end{aligned}$$

We have the following way to judge whether the projection of a given vector belongs to the cone bounded by $\boldsymbol{Px}_1$ and $\boldsymbol{Px}_2$ or not. Note that there exist non-zero coefficients λ and κ such that

$$\lambda\boldsymbol{Z} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}\kappa \end{pmatrix}.$$

It is easy to get that

$$\lambda = n^{-1/2}Z_1{}^{-1} \tag{2.11}$$

and

$$\kappa = n^{-1/2}Z_1^{-1}Z_2P_1. \tag{2.12}$$

If $a < \kappa < b$, then the projection of vector $\pm\boldsymbol{Z}$ lies inside the cone spanned by $\boldsymbol{P}\boldsymbol{x}_1$ and $\boldsymbol{P}\boldsymbol{x}_2$. Otherwise, the projection lies outside the cone.

For the special case $(a, b) = (-\infty, \infty)$, S is clearly equal to $\|\boldsymbol{Z}\|$.

2.1.2.2 Turning point method

This method has been considered by Liu (2010). Denote $h(x) = \dfrac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}}$. Then S in (2.10) can be written as

$$S = \max_{x\in(a,b)} h(x) = \max_{x\in(a,b)} \frac{|f(x)|}{\sqrt{g(x)}},$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U), \\ g(x) &= (\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}). \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, then

$$\begin{aligned} f(x) &= P_1^{-1}U^{-1}N_2 x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\ \frac{\mathrm{d}f}{\mathrm{d}x} &= P_1^{-1}U^{-1}N_2, \\ g(x) &= P_1^{-2}x^2 + n^{-1}, \\ \frac{\mathrm{d}g}{\mathrm{d}x} &= 2P_1^{-2}x. \end{aligned}$$

Solving from $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f}{\sqrt{g}}\right)|_{x_t} = 0$, we can find the turning point of the function $\frac{f(x)}{\sqrt{g(x)}}$ is $x_t = \dfrac{P_1 N_2 n^{-1}}{n^{-1/2}N_1 + z_\gamma(U\theta^{-1} - 1)}$. Therefore, if $a < x_t < b$, the maximum value of $h(x)$ is attained at either $x = a$ or b or x_t, otherwise, the maximum value of $h(x)$ is attained at either $x = a$ or b, i.e.,

$$S = \max_{x\in(a,b)} h(x) = \begin{cases} \max\{h(a), h(x_t), h(b)\}, & \text{if } a < x_t < b; \\ \max\{h(a), h(b)\}, & \text{if } x_t \le a \text{ or } x_t \ge b. \end{cases}$$

For the special case $(a, b) = (-\infty, \infty)$,

$$h(-\infty) = h(\infty) = \lim_{x\to\infty} s(x) = |U^{-1}N_2|,$$

hence

$$S = \max_{x\in(-\infty,\infty)} s(x) \quad = \quad \max\left\{|U^{-1}N_2|, h(x_t)\right\}.$$

2.1.2.3 Quadratic programming method

Note that S in (2.10) can be written as

$$\begin{aligned} S &= \max_{x\in(a,b)} \frac{|(\boldsymbol{Px})'\boldsymbol{Z}|}{||\boldsymbol{Px}||} \\ &= \max_{\boldsymbol{v}\in C(\boldsymbol{P},a,b)} \frac{|\boldsymbol{v}'\boldsymbol{Z}|}{\|\boldsymbol{v}\|}, \end{aligned} \tag{2.13}$$

where

$$C(\boldsymbol{P}, a, b) := \{\lambda \boldsymbol{Px} : \lambda > 0, x \in (a,b)\}.$$

Let $\pi(\boldsymbol{z}, \boldsymbol{P}, a, b)$ denote the projection of $\boldsymbol{z}$ to the cone $C(\boldsymbol{P}, a, b)$, i.e., $\pi(\boldsymbol{z}, \boldsymbol{P}, a, b)$ is the $\boldsymbol{z}$ that solves the problem

$$\min_{\boldsymbol{v}\in C(\boldsymbol{P},a,b)} \|\boldsymbol{v}-\boldsymbol{z}\|^2. \tag{2.14}$$

The objective function to minimize, $\|\boldsymbol{v}-\boldsymbol{z}\|^2 = \boldsymbol{v}'\boldsymbol{v} - 2\boldsymbol{z}'\boldsymbol{v} + \boldsymbol{z}'\boldsymbol{z}$, is equivalent to

$$\frac{1}{2}\boldsymbol{v}'\boldsymbol{v} - \boldsymbol{z}'\boldsymbol{z}. \tag{2.15}$$

From Naiman (1987), we know S in (2.13) is further equal to

$$S = \max\{\|\pi(\boldsymbol{Z}, \boldsymbol{P}, a, b)\|, \|\pi(-\boldsymbol{Z}, \boldsymbol{P}, a, b)\|\}.$$

The solution of the problem (2.14), $\pi(\boldsymbol{z}, \boldsymbol{P}, a, b)$, can be found by using quadratic programming under linear constraints $\boldsymbol{v} = \lambda\boldsymbol{Px} = \lambda \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}$, $\lambda \geq 0$ and $x \in (a,b)$. Let $\boldsymbol{e}_j \in \mathbf{R}^3$ have the jth element equal to one and the remaining elements all equal to zero. We have

$$\begin{aligned} (\boldsymbol{e}_2' - e_1'\sqrt{n}P_1^{-1}b)\boldsymbol{v} &\leq 0 \\ (\boldsymbol{e}_1'\sqrt{n}P_1^{-1}a - \boldsymbol{e}_2')\boldsymbol{v} &\leq 0 \\ -\sqrt{n}\boldsymbol{e}_1'\boldsymbol{v} &\leq 0. \end{aligned}$$

These constraints can be expressed as

$$\boldsymbol{A}\boldsymbol{v} \leq \boldsymbol{b}, \tag{2.16}$$

where the 3×3 matrix

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{e}_2' - e_1'\sqrt{n}P_1^{-1}b \\ \boldsymbol{e}_1'\sqrt{n}P_1^{-1}a - \boldsymbol{e}_2' \\ -\sqrt{n}\boldsymbol{e}_1' \end{pmatrix},$$

and $\boldsymbol{b} = \boldsymbol{0}$.

The problem of minimizing the objective function in (2.15) under the constraints in (2.16) is a standard quadratic programming problem and can be solved by the MATLAB built-in function `quadprog`.

2.1.3 Comparison of the numerical quadrature method and the simulation method

As expected, the numerical integration method and the simulation method give almost the same results from our investigation. The numerical integration method takes longer computation time however, and so is not recommended. The simulation method is fast and produces the critical values almost as accurate as the numerical integration method if the number of simulation runs is 100,000 or more. Among the three computation methods provided for simulating S in (2.10), the projection method is faster than the turning point method which, in turn, is faster than the quadratic programming method. Therefore, we recommend the projection method.

2.1.4 Special cases

2.1.4.1 Special case 1

For the special case of $a = b$, the interval (a, b) shrinks to a point a. The width of $1-\alpha$ confidence interval is straightforwardly equal to $2c\hat{\sigma}\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}$, where $\boldsymbol{a} = (1, a)'$. The confidence level becomes

$$P\left\{\frac{\left|\boldsymbol{a}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)\right|}{\hat{\sigma}\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}} \leq c\right\}$$

$$= P\left\{-c - \frac{z_\gamma}{\theta\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}} \leq \frac{\boldsymbol{a}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma - z_\gamma}{\hat{\sigma}/\sigma\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}}\right. \tag{2.17}$$

$$\left.\leq c - \frac{z_\gamma}{\theta\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}}\right\}. \tag{2.18}$$

We provide two methods for computing the confidence level. Due to $\hat{\boldsymbol{\beta}} \sim N_2(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1})$, it is clear that $\dfrac{\boldsymbol{a}'(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})/\sigma}{\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}} \sim N(0,1)$. Let W denote $\dfrac{\boldsymbol{a}'(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})/\sigma - z_\gamma}{\hat{\sigma}/\sigma\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}}$. Since $\hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$, then $W \sim \text{nct}(\nu, -z_\gamma/\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}})$. Here $\text{nct}(\vartheta,\zeta)$ denotes the noncentral t-distribution with degrees of freedom ϑ and noncentrally parameter ζ. Therefore, the confidence level (2.17) is equal to

$$P\left\{-c - \frac{z_\gamma}{\theta\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}} \le W \le c - \frac{z_\gamma}{\theta\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a}}}\right\}. \tag{2.19}$$

We can compute the confidence level by using MATLAB built-in function `nctcdf`. Then we can work out the critical constant c.

Alternatively, the confidence level can be written as

$$\begin{aligned} & P\left\{\frac{\left|\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)\right|}{\sqrt{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]}} \le c\right\} \\ = & \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u)k_1(u)du. \end{aligned} \tag{2.20}$$

Here $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of $U = \hat{\sigma}/\sigma$ and given in (1.4) and

$$\begin{aligned} k_1(u) &= P\left\{\frac{\left|\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\boldsymbol{N}/u + z_\gamma(1/\theta - 1/u)\right|}{\sqrt{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]}} \le c\right\} \\ &= P\left\{\frac{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\boldsymbol{N}}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]} \in \frac{z_\gamma(1-u/\theta)}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]} \pm cu\right\} \end{aligned} \tag{2.21}$$

Note that

$$\text{Var}\left(\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\boldsymbol{N}\right) = \left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right],$$

and so

$$\frac{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\boldsymbol{N}}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]} \sim N(0,1).$$

Denote

$$L(u,c,a,z_\gamma) = \frac{z_\gamma(1-u/\theta)}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]} - cu,$$

and

$$U(u,c,a,z_\gamma) = \frac{z_\gamma(1-u/\theta)}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]} + cu.$$

Then from (2.21) we have

$$\begin{aligned} k_1(u) &= P\left\{L(u,c,a,z_\gamma) \le N(0,1) \le U(u,c,a,z_\gamma)\right\} \\ &= \Phi\left(U(u,c,a,z_\gamma)\right) - \Phi\left(L(u,c,a,z_\gamma)\right), \end{aligned}$$

where $\Phi(\cdot)$ denotes the standard normal distribution function. Therefore, from (2.20), the confidence level becomes

$$\int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u)\left(\Phi(U(u,c,a,z_\gamma)) - \Phi(L(u,c,a,z_\gamma))\right) du.$$

This expression involves only one-dimensional integration. We can get the confidence level and so the critical constant c of special case 1 by using MATLAB built-in function `quad`. Addition to the numerical quadrature, similar to the last section, we can use simulation method to find the critical constant c.

2.1.4.2 Special case 2

For the special case of $(a,b) = (-\infty,\infty)$, from Section 2.1.2.1, the simultaneous confidence level is given by

$$P\{\|\boldsymbol{Z}\| \le c\}. \tag{2.22}$$

Then the simultaneous confidence level can be written as

$$\int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{\left\|\begin{pmatrix} N_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ N_2/u \end{pmatrix}\right\| \le c\right\} du. \tag{2.23}$$

The probability density function of N_1 is $\varphi_{N_1}(n_1) = \frac{1}{\sqrt{2\pi}} e^{-n_1^2/2}$, $n_1 \in (-\infty, \infty)$. So (2.23) is equal to

$$\begin{aligned} & \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) \int_{-\infty}^\infty \varphi_{N_1}(n_1) P\left\{\left\|\begin{pmatrix} n_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ N_2/u \end{pmatrix}\right\| \le c\right\} dn_1 du \\ = & \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) \int_{-\infty}^\infty \varphi_{N_1}(n_1) P\left\{N_2^2 \le u^2c^2 - (n_1 + (u/\theta - 1)\sqrt{n}z_\gamma)^2\right\} dn_1 du \\ = & \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) \int_{-\infty}^\infty \varphi_{N_1}(n_1) \chi_1^2(l) dn_1 du, \end{aligned} \tag{2.24}$$

where $l = u^2c^2 - (n_1 + (u/\theta - 1)\sqrt{n}z_\gamma)^2$. The expression (2.24) involves two-dimensional integration. The value of critical constant c can be calculated by using MATLAB built-in function `dbquad`. Also, we can use simulation method to get the critical constant c.

2.1.5 Numerical examples

Example 2.1. *Blood pressure and age*

Kleinbaum et al. (1998) provided a data set on how systolic blood pressure (Y) changes with age (x) for a group of forty males. The data set is given in Table 2.1. The data points are plotted in Figure 2.2. We have $\bar{x} = 46.92$, $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2 = 8623.5591$ and $\hat{\sigma} = 8.479$ with 38 degrees of freedom. Since the minimum age $\min(x_i) = 18$ and the maximum age $\max(x_i) = 70$, it is sensible to construct a simultaneous confidence band over $x \in (18, 70)$. Also, we study the bands over $x \in (1, 100)$ and the whole region $(-\infty, \infty)$. Even though the age value x cannot be a negative number or infinity and so $x \in (-\infty, \infty)$ has no practical meaning in this example, we are interested in the mathematical results for the interval $x \in (-\infty, \infty)$. Many previous literatures just considered bands over $(-\infty, \infty)$ but we consider a general interval (a, b) including $(-\infty, \infty)$ as a special case in our study.

Consider two cases: $1 - \alpha = 0.90$, $\gamma = 0.75$ and $1 - \alpha = 0.95$, $\gamma = 0.99$ in this example. By using methods introduced above in this section, we can calculate the critical constants of the bands SB, TBU and TBE over the interval $(18, 70)$, $(1, 100)$ and $(-\infty, \infty)$. The width of each band is given by $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Since the data set is given, for any given x, then the width of each band depends only on the corresponding critical constant c. The smaller the critical constant c is, the narrower the band is.

From Table 2.2, we conclude TBE is the best among the three bands for this example. The 90%-simultaneous confidence bands SB, TBU and TBE for the 75th percentile line over $(18, 70)$ are plotted in Figure 2.3. For this particular case, the simultaneous band SB is only $(2.3179-2.3121)/2.3121 = 0.25\%$ wider than the band TBE, and the simultaneous band SB is only $(2.3148 - 2.3121)/2.3121 = 0.12\%$ wider than the band TBE. Therefore these three bands almost overlap each other in Figure 2.3. The 99%-simultaneous confidence bands SB, TBU and TBE for the 95th percentile line over $(18, 70)$ are plotted in Figure 2.4. For this particular case, the simultaneous band SB is only $(4.8295-4.6472)/4.6472 = 3.92\%$ wider than the band TBE, and the simultaneous confidence band SB is only $(4.7677-4.6472)/4.6472 = 2.59\%$ wider than the band TBE. There is no significant difference among three bands in this example. The band TBE is slightly narrower than the other two bands. Therefore these three bands almost overlap each other in Figure 2.4. Intuitively, the bands over $(-\infty, \infty)$ should be wider than the bands over a finite interval. In this example, we can confirm this since the critical constant of one band over $(-\infty, \infty)$ is larger than the critical constants of the band over $(1, 100)$ and $(18, 70)$.

Table 2.1: *Data from Kleinbaum et al. (1998, page 192)*

Person i	Age in years (x)	Blood Pressure (mm Hg) (Y)	Person i	Age in years (x)	Blood Pressure (mm Hg) (Y)
1	41	158	21	38	150
2	60	185	22	52	156
3	41	152	23	41	134
4	47	159	24	18	134
5	66	176	25	51	174
6	47	156	26	55	174
7	68	184	27	65	158
8	43	138	28	33	144
9	68	172	29	23	139
10	57	168	30	70	180
11	65	176	31	56	165
12	57	164	32	62	172
13	61	154	33	51	160
14	36	124	34	48	157
15	44	142	35	59	170
16	50	144	36	40	153
17	47	149	37	35	148
18	19	128	38	33	140
19	22	130	39	26	132
20	21	138	40	61	169

Table 2.2: Critical constants of simultaneous confidence bands SB,TBU and TBE

	$1-\alpha=0.90,\quad \gamma=0.75$			$1-\alpha=0.99,\quad \gamma=0.95$		
Interval	SB	TBU	TBE	SB	TBU	TBE
(18,70)	2.3179	2.3148	2.3121	4.8295	4.7677	4.6472
(1,100)	2.3381	2.3356	2.3326	4.8299	4.7682	4.6475
$(-\infty,\infty)$	2.3431	2.3403	2.3371	4.8300	4.7683	4.6475

Figure 2.2: *The data points, the estimated regression line and the estimated 75th percentile line*

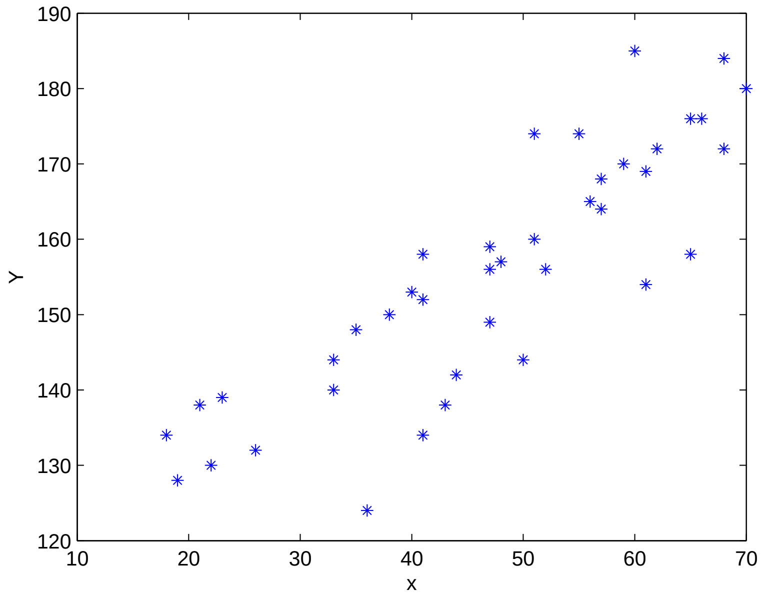


Figure 2.3: *The 90%-simultaneous confidence bands SB, TBU and TBE for the 75th percentile line over* $(18, 70)$

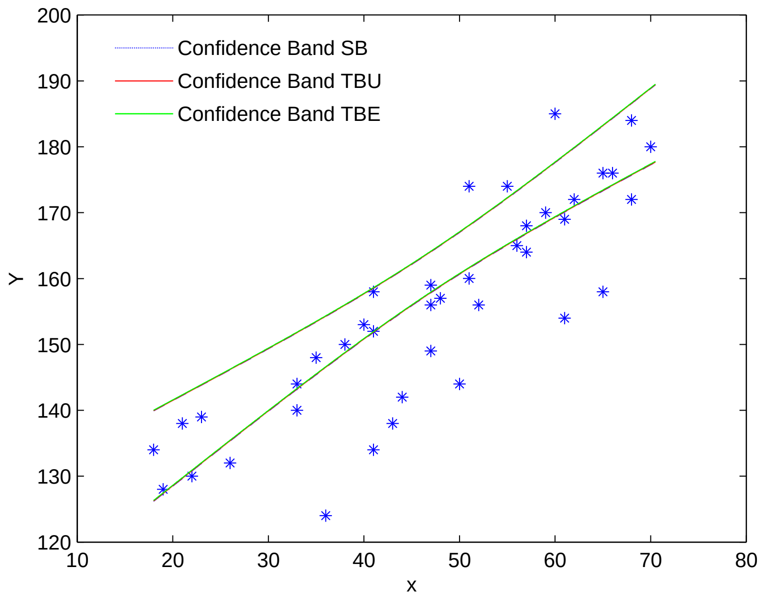
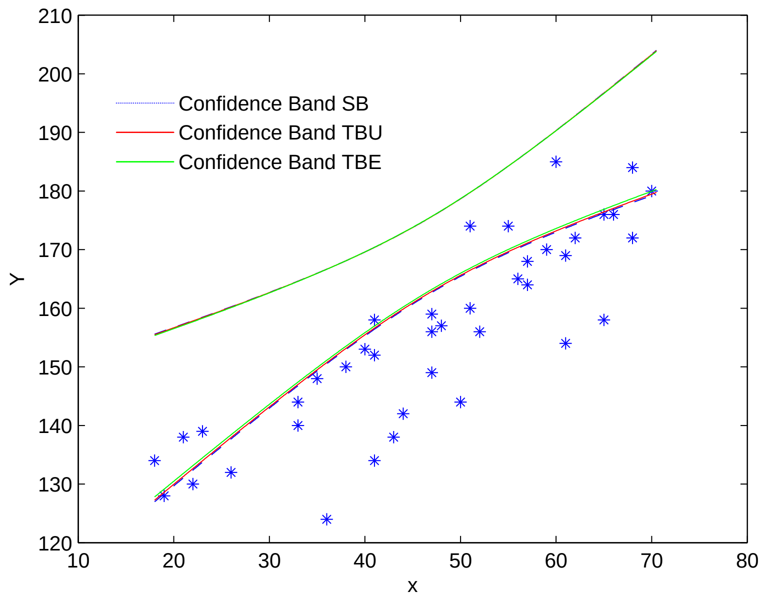


Figure 2.4: *The 99%-simultaneous confidence bands SB, TBU and TBE for the 95th percentile line over* $(18, 70)$



Example 2.2. *Speed and size of rocket engine's orifice*

Consider the example presented originally by Lieberman and Miller (1963) on how speed(Y) in miles per hour changes with the size(x) in inches of a rocket engine's orifice. This example was also discussed by Steinhorst and Bowden (1971) and Turner and Bowden (1977). The data set consists of fifteen pairs of observations $(x_i, y_i), i = 1, \cdots, 15$ and is given in Table 2.3. We have $\bar{x} = 1.3531$, $\bar{y} = 5219.3$, the minimum size of orifice $\min(x_i) = 1.310$, the maximum size of orifice $\max(x_i) = 1.400$, $S_{xx} = \Sigma_{i=1}^{n}(x_i - \bar{x})^2 = 0.011966$, $\hat{\boldsymbol{\beta}} = (-19041.8, 17930)'$ and $\hat{\sigma} = 130.5$ with 13 degrees of freedom.

A two-sided simultaneous confidence band can be used to quantify the plausible range of the true percentile function. Since $\min(x_i) = 1.310$ and $\max(x_i) = 1.400$, it is sensible to construct a simultaneous confidence band over a interval $x \in (a, b)$ which covers the interval $(1.310, 1.400)$. Here we construct two-sided simultaneous confidence bands over the interval $(\bar{x} - 0.060, \bar{x} + 0.060) = (1.2931, 1.4131)$. This interval just covers the observed range and has been considered by Steinhorst and Bowden (1971) and Turner and Bowden (1977). We look at two cases: $1 - \alpha = 0.90$, $\gamma = 0.75$ and $1 - \alpha = 0.95$, $\gamma = 0.99$ in this example. By using the methods introduced above in this section, we can calculate the critical constants of the bands SB, TBU and TBE over the interval $(1.2931, 1.4131)$. (See Table 2.4.) Since a small critical constant means a narrow band, from Table 2.4, we recommend band TBE as its c value is the smallest among the three bands for each case.

Table 2.3: Orifice Speed Data for Lieberman and Miller (1963) Example

Orifice	Speed	Orifice	Speed	Orifice	Speed
1.310	4360	1.340	5070	1.373	5670
1.313	4590	1.347	5230	1.376	5490
1.320	4520	1.355	5080	1.384	5810
1.322	4770	1.360	5550	1.395	6060
1.338	4760	1.364	5390	1.400	5940

Table 2.4: Critical constants of simultaneous confidence bands SB,TBU and TBE

	$1-\alpha=0.90, \quad \gamma=0.75$			$1-\alpha=0.99, \quad \gamma=0.95$		
Interval	SB	TBU	TBE	SB	TBU	TBE
(1.2931, 1.4131)	2.4907	2.4793	2.4656	6.1653	6.0465	5.7894

2.2 Symmetric bands of Form II

In this section, we consider simultaneous confidence bands for the percentile line $\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma$ over the interval $x \in (a, b)$ of the form (2.1) with $\theta \neq 0$ and $\xi \neq 0$ denoted as Form II:

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \text{ for all } x \in (a, b). \tag{2.25}$$

Different from Section 2.1, we focus on the bands with $\xi \neq 0$.

Figure 2.5 illustrates the shape of this confidence band. The lower and upper parts of the band are symmetric about the estimated percentile line $\boldsymbol{x}'\hat{\boldsymbol{\beta}}+z_\gamma\hat{\sigma}$, and the width of the band is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}$.

The constants $\theta \neq 0$ and $\xi \neq 0$ can be chosen to give different specific confidence bands. For a given pair of (θ, ξ), the critical constant c is chose such that the confidence level is equal to $1-\alpha$. We consider three bands in this section. All of them are special cases of form (2.25).

The first band, denoted as V, uses $\theta = 1$ and $\xi = 1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2$ and is given by

$$\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}}+z_\gamma\hat{\sigma}\pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\left(1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2\right)} \text{ for all } x \in (a, b). \tag{2.26}$$

This band has not been considered in the literature before. Here the quantity ξ is chosen so that

$$\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi = \mathrm{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma})/\sigma^2.$$

Note that

$$\begin{aligned}
& \mathrm{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma}) \\
= \; & \mathrm{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}}) + \mathrm{Var}(z_\gamma\hat{\sigma}) & (2.27) \\
= \; & \sigma^2\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2[E(\hat{\sigma}^2) - (E\hat{\sigma})^2] & (2.28) \\
= \; & \sigma^2\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2[\sigma^2 - \sigma^2(E(\frac{\hat{\sigma}}{\sigma}))^2] & (2.29) \\
= \; & \sigma^2\left(\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\left(1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2\right)\right), & (2.30)
\end{aligned}$$

where (2.27) is due to that $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are independent, (2.28) follows directly from the fact that $\boldsymbol{x}'\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{x}'\boldsymbol{\beta}, \sigma^2\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}\right)$. We obtain (2.29) since $\hat{\sigma}^2 \sim \frac{\sigma^2}{\nu}\chi^2_\nu$, $E(\hat{\sigma}^2) = \sigma^2$ and $E(\frac{\hat{\sigma}}{\sigma}) = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$. Hence ξ is equal to $1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2$ from (2.30).

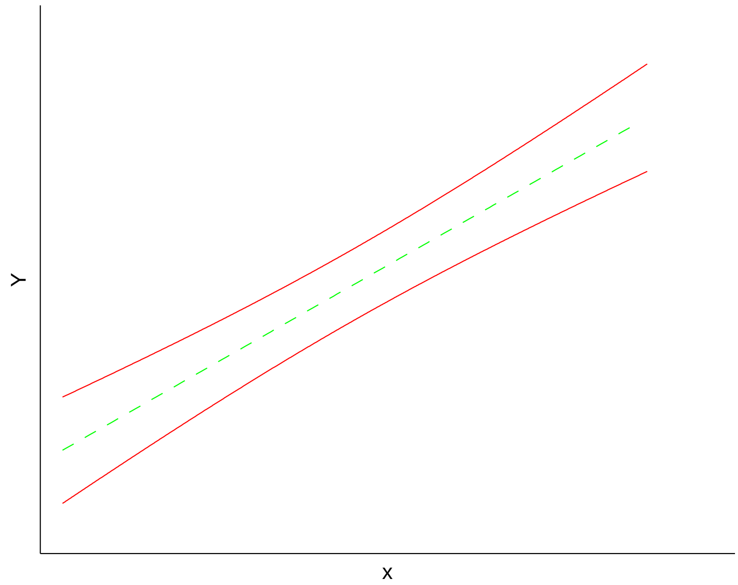


Figure 2.5: *The shape of SCB General Form II*

The second band denoted as UV, uses $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = \frac{\nu}{2}\left(\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$, and is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2(1/\theta^2 - 1)} \text{ for all } x \in (a, b), \tag{2.31}$$

where θ and ξ satisfy $E(\frac{\hat{\sigma}}{\theta}) = \sigma$ and $\text{Var}(\boldsymbol{x}\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma}) = \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi$. This band has not been proposed in the literature before either. Note that θ is chosen so that $E(\frac{\hat{\sigma}}{\theta}) = \sigma$ and therefore $\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma}$ is the uniformly minimum variance unbiased estimator(UMVUE) of $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$. The quantity ξ is chosen so that

$$\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi = \text{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma})/\sigma^2.$$

Similar to (2.27) - (2.29), we have

$$\begin{aligned} & \text{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma}) \\ = \; & \text{Var}(\boldsymbol{x}'\hat{\boldsymbol{\beta}}) + \text{Var}(\frac{z_\gamma}{\theta}\hat{\sigma}) \\ = \; & \sigma^2\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (\frac{z_\gamma}{\theta})^2[E(\hat{\sigma}^2) - (E\hat{\sigma})^2] \end{aligned}$$

$$
\begin{aligned}
&= \sigma^2 \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (\frac{z_\gamma}{\theta})^2[\sigma^2 - \theta^2\sigma^2] \\
&= \sigma^2 \left(\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2 \left(1/\theta^2 - 1\right)\right).
\end{aligned}
$$

Hence ξ is equal to $1/\theta^2 - 1 = \frac{\nu}{2}\left(\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$.

The third band, denoted as TT, uses $\theta = \frac{4\nu - 1}{4\nu}$ and $\xi = \frac{1}{2\nu}$ and is given by

$$
\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{(4\nu-1)/(4\nu)}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2/(2\nu)}, \text{ for all } x \in (a, b). \tag{2.32}
$$

This choice of $(\theta,\ \xi)$ has been considered by Thomas and Thomas (1986). But they only studied the band over the whole region $(-\infty, \infty)$. They claimed this band was more efficient than all the bands studied in Turner and Bowden (1977) over the whole region.

All the bands considered in the past by Steinhorst and Bowden (1971), Turner and Bowden (1977) and Thomas and Thomas (1986) are all over the whole range $x \in (-\infty, \infty)$. Analogous to Section 2.1, we construct the bands over a given interval which is more general and includes the whole range as a special case.

As all these individual bands are special cases of the band (2.25), now we considered the computation of the critical constant c in the band (2.25). For this, it is necessary to find an expression of the simultaneous confidence level of the band that is amenable to computation.

The simultaneous confidence level of this band is given by

$$
\begin{aligned}
& P\left\{\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} \pm c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \text{ for all } x \in (a,b)\right\} \\
= \;& P\left\{\max_{x\in(a,b)} \frac{|\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}} \le c\right\} \\
= \;& P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}) + (z_\gamma)^2\xi}} \le c\right\} \\
= \;& P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N} + z_\gamma(\hat{\sigma}/\theta - \sigma)|}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}) + (z_\gamma)^2\xi}} \le c\right\} \\
= \;& P\left\{\max_{x\in(a,b)} \frac{|(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}) + (z_\gamma)^2\xi}} \le c\right\}, \qquad (2.33)
\end{aligned}
$$

where the matrix $\boldsymbol{P}$ is defined in (1.5), $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$

and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$. Note that (2.33) is further equal to

$$P\left\{\max_{x\in(a,b)} \frac{\left|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}'\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\left\|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}\right\|} \le c\right\}$$

$$= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{\max_{x\in(a,b)} \frac{\left|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}'\begin{pmatrix} \boldsymbol{N}/u \\ (1/\theta - 1/u)/\sqrt{\xi} \end{pmatrix}\right|}{\left\|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}\right\|} \le c\right\} du, \qquad (2.34)$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

Next we give two methods for computing critical constant c.

2.2.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \max_{x\in(a,b)} \frac{\left|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}'\begin{pmatrix} \boldsymbol{n}/u \\ (1/\theta - 1/u)/\sqrt{\xi} \end{pmatrix}\right|}{\left\|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}\right\|},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (2.34) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{k(\boldsymbol{v})\le c \text{ for all } x\in(a,b)\}} d\boldsymbol{v}, \qquad (2.35)$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Expression (2.35) involves a three-dimensional integration and can be used to compute the simultaneous confidence level via numerical integration. We have used the MATLAB built-in function `triplequad` for this purpose. Then the value of critical constant can be found numerically by searching for c so that the simultaneous confidence level is equal to $1 - \alpha$.

2.2.2 Simulation method

Let

$$S = \max_{x\in(a,b)} \frac{|(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}}. \qquad (2.36)$$

From (2.33), the simultaneous confidence level is given by

$$P\{S \le c\}. \tag{2.37}$$

The critical constant c can be determined in a similar way as introduced in the last section. We generate standard bivariate normal random vectors $\boldsymbol{N}_i$ and variables $U_i \sim \sqrt{\frac{\chi^2_\nu}{\nu}}$, $i = 1, 2, \cdots, R$, and then calculate

$$S_i = \max_{x \in (a,b)} \frac{|(P\boldsymbol{x})'\boldsymbol{N}_i/U_i + z_\gamma(1/\theta - 1/U_i)|}{\sqrt{(P\boldsymbol{x})'(P\boldsymbol{x}) + (z_\gamma)^2\xi}}, \quad i = 1, \cdots, R.$$

We choose the $\langle(1-\alpha)R\rangle$th largest of the R replicates of $S : S_1, \cdots, S_R$ as the approximation of critical constant c. Next we give three computation methods for calculating S from N and U.

2.2.2.1 Projection method

S in (2.36) is further equal to

$$S = \max_{x \in (a,b)} \frac{\left| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma \sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right|}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma \sqrt{\xi} \end{pmatrix} \right\|}.$$

Note that $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$ and all the points $\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ for $x \in (-\infty, \infty)$ in the three-dimensional space form a straight line. Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$, $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$, $\boldsymbol{d}_1 = \begin{pmatrix} \boldsymbol{Px}_1 \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ and $\boldsymbol{d}_2 = \begin{pmatrix} \boldsymbol{Px}_2 \\ z_\gamma \sqrt{\xi} \end{pmatrix}$. Note that, for any $x \in (-\infty, \infty)$, $\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma \sqrt{\xi} \end{pmatrix} = \begin{pmatrix} \boldsymbol{P} \begin{pmatrix} 1 \\ x \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ can be expressed as $\begin{pmatrix} \boldsymbol{P} \begin{pmatrix} 1 \\ \omega a + (1-\omega) b \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ for some $\omega \in (-\infty, \infty)$.

For a given ω, we have

$$\begin{aligned}
&\begin{pmatrix} \boldsymbol{P}\begin{pmatrix} 1 \\ \omega a + (1-\omega) b \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix} \\
&= \omega \begin{pmatrix} \boldsymbol{P}\begin{pmatrix} 1 \\ a \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix} + (1-\omega) \begin{pmatrix} \boldsymbol{P}\begin{pmatrix} 1 \\ b \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix} \\
&= \omega \boldsymbol{d}_1 + (1-\omega)\boldsymbol{d}_2.
\end{aligned}$$

It means $\begin{pmatrix} \boldsymbol{P}\begin{pmatrix} 1 \\ \omega a + (1-\omega) b \end{pmatrix} \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ can be written as a linear combination of $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$. So $\begin{pmatrix} \boldsymbol{P}\boldsymbol{x} \\ z_\gamma \sqrt{\xi} \end{pmatrix}$ can be expressed as a linear combination of $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$. Denote the matrix $\boldsymbol{M} = (\boldsymbol{d}_1, \boldsymbol{d}_2)$. Let $\mathcal{L}(\boldsymbol{M})$ be the linear plane spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ and $\boldsymbol{H} = \boldsymbol{M}(\boldsymbol{M}'\boldsymbol{M})^{-1}\boldsymbol{M}'$ be the projection matrix to $\mathcal{L}(\boldsymbol{M})$. If the projection of the vector $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ or $-\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, then

$$S = \left\| \boldsymbol{H} \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|.$$

Otherwise,

$$\begin{aligned}
S &= \max \left(\frac{\left| \boldsymbol{d}_1' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right|}{\|\boldsymbol{d}_1\|}, \quad \frac{\left| \boldsymbol{d}_2' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right|}{\|\boldsymbol{d}_2\|} \right) \\
&= \max \left(\frac{|(\boldsymbol{P}\boldsymbol{x}_1)'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x}_1)'(\boldsymbol{P}\boldsymbol{x}_1) + (z_\gamma)^2\xi}}, \quad \frac{|(\boldsymbol{P}\boldsymbol{x}_2)'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{P}\boldsymbol{x}_2)'(\boldsymbol{P}\boldsymbol{x}_2) + (z_\gamma)^2\xi}} \right).
\end{aligned}$$

We have the following way to judge whether the projection of a given vector, $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ for example, belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ or not.

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$. Then for any x_0,

$$\begin{pmatrix} \boldsymbol{P}\begin{pmatrix} 1 \\ x_0 \end{pmatrix} \\ z_\gamma\sqrt{\xi} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{n} \\ x_0 P_1^{-1} \\ z_\gamma\sqrt{\xi} \end{pmatrix}.$$

The projection of the vector $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ is

$$\boldsymbol{v}_p = \boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}.$$

Then there exist non-zero coefficients λ and κ such that

$$\lambda\boldsymbol{v}_p = \begin{pmatrix} 1/\sqrt{n} \\ \kappa P_1^{-1} \\ z_\gamma\sqrt{\xi} \end{pmatrix}.$$

Note that $\boldsymbol{H}$ can be written as $\begin{pmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{pmatrix}$, then we have

$$\lambda\boldsymbol{v}_p = \lambda\begin{pmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{pmatrix}\begin{pmatrix} N_1/U \\ N_2/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{n} \\ \kappa P_1^{-1} \\ z_\gamma\sqrt{\xi} \end{pmatrix}. \tag{2.38}$$

Two coefficients are therefore solved as

$$\lambda = z_\gamma\sqrt{\xi}/\left(h_{31}N_1/U + h_{32}N_2/U + h_{33}(1/\theta - 1/U)/\sqrt{\xi}\right), \tag{2.39}$$

and

$$\kappa = \lambda P_1\left(h_{21}N_1/U + h_{22}N_2/U + h_{23}(1/\theta - 1/U)/\sqrt{\xi}\right). \tag{2.40}$$

If $a < \kappa < b$, the projection of the vector $\pm\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, otherwise, the projection lies outside the cone.

For the special case of $(a,b) = (-\infty, \infty)$,

$$S = \left\| \boldsymbol{H} \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|. \tag{2.41}$$

2.2.2.2 Turning point method

Denote

$$h(x) = \frac{|(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}}.$$

Then S in (2.36) can be written as

$$S = \max_{x\in(a,b)} h(x) = \max_{x\in(a,b)} \frac{|f(x)|}{\sqrt{g(x)}},$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U), \\ g(x) &= (\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi. \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, and so

$$\begin{aligned} f(x) &= P_1^{-1}U^{-1}N_2x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\ \frac{\mathrm{d}f}{\mathrm{d}x} &= P_1^{-1}U^{-1}N_2, \\ g(x) &= P_1^{-2}x^2 + n^{-1} + (z_\gamma)^2\xi, \\ \frac{\mathrm{d}g}{\mathrm{d}x} &= 2P_1^{-2}x. \end{aligned}$$

Solving from $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f}{\sqrt{g}}\right)|_{x_t} = 0$, we have the turning point $x_t = \dfrac{P_1N_2(n^{-1} + (z_\gamma)^2\xi)}{n^{-1/2}N_1 + z_\gamma(U/\theta - 1)}$. Therefore, if $a < x_t < b$, the minimum value of $h(x)$ is attained at either $x = a$ or b or x_t, otherwise, the minimum value of $h(x)$ is attained at either $x = a$ or b, i.e.,

$$S = \max_{x\in(a,b)} h(x) = \begin{cases} \max\{h(a), h(x_t), h(b)\}, & \text{if } \ a < x_t < b; \\ \max\{h(a), h(b)\}, & \text{if } \ x_t \le a \text{ or } x_t \ge b. \end{cases}$$

For the special case of $(a,b) = (-\infty, \infty)$,

$$h(-\infty) \ = \ h(\infty) = \lim_{x\to\infty} h(x) = |U^{-1}N_2|,$$

hence

$$S = \max_{x\in(a,b)} h(x) \quad = \quad \max\left\{|U^{-1}N_2|, h(x_t)\right\}.$$

2.2.2.3 Quadratic programming method

Note that S in (2.36) can be written as

$$\begin{aligned} S &= \max_{x\in(a,b)} \frac{\left|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\left\|\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}\right\|} \\ &= \max_{v\in C(\boldsymbol{P},z_\gamma,\xi,a,b)} \frac{|\boldsymbol{v}'\boldsymbol{T}|}{\|\boldsymbol{v}\|}, \end{aligned} \tag{2.42}$$

where

$$\boldsymbol{v} = \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}, \boldsymbol{T} = \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$$

and

$$C(\boldsymbol{P}, z_\gamma, \xi, a, b) := \left\{\lambda \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} : \lambda \geq 0, x \in (a,b)\right\}.$$

Let $\pi(\mathbf{t})$ denote the projection of $\boldsymbol{t} \in \mathbf{R}^3$ to the cone $C(\boldsymbol{P}, z_\gamma, \xi, a, b)$, i.e.,$\pi(\mathbf{t})$ is the $\boldsymbol{v} \in \mathbf{R}^3$ that solves the problem

$$\min_{v\in C(\boldsymbol{P},z_\gamma,\xi,a,b)} \|\boldsymbol{v} - \boldsymbol{t}\|^2.$$

The objective function to minimize, $\|\boldsymbol{v} - \boldsymbol{t}\|^2$, can be expressed as $\boldsymbol{v}'\boldsymbol{v} - 2\boldsymbol{t}'\boldsymbol{v} + \boldsymbol{t}'\boldsymbol{t}$, which is equivalent to

$$\frac{1}{2}\boldsymbol{v}'\boldsymbol{v} - \boldsymbol{t}'\boldsymbol{v}. \tag{2.43}$$

It follows from Naiman (1987) that S in (2.42) is further equal to

$$S = \max\{\|\pi(\boldsymbol{T})\|, \|\pi(-\boldsymbol{T})\|\}.$$

The solution $\pi(\mathbf{t})$ can be found by using quadratic programming under linear constraints.

Let $\boldsymbol{e}_j \in \mathbf{R}^3$ have the jth element equal to one and the remaining elements all equal to zero. Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, from the definition of the cone $C(\boldsymbol{P}, z_\gamma, \xi, a, b)$, $\boldsymbol{v} \in C(\boldsymbol{P}, z_\gamma, \xi, a, b)$ implies that

$$\boldsymbol{v} = \lambda \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix}$$

for some $\lambda > 0$. Since $\sqrt{n}\boldsymbol{e}_1'\boldsymbol{v} = (z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3'\boldsymbol{v} = \lambda \geq 0$ and $a \leq x \leq b$, we have

$$\begin{aligned} -(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3'\boldsymbol{v} &\leq 0 \\ -\sqrt{n}\boldsymbol{e}_1'\boldsymbol{v} &\leq 0 \\ (aP_1^{-1}(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3' - \boldsymbol{e}_2')\boldsymbol{v} &\leq 0 \\ (\boldsymbol{e}_2' - bP_1^{-1}(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3')\boldsymbol{v} &\leq 0 \\ (\sqrt{n}\boldsymbol{e}_1' - (z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3')\boldsymbol{v} &= 0. \end{aligned}$$

These constraints can be expressed as

$$\boldsymbol{A}\boldsymbol{v} \leq \boldsymbol{b}, \ \boldsymbol{A}_{eq}\boldsymbol{v} = \boldsymbol{b}_{eq}, \tag{2.44}$$

where the 4×3 matrix

$$\boldsymbol{A} = \begin{pmatrix} -(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3' \\ -\sqrt{n}\boldsymbol{e}_1' \\ aP_1^{-1}(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3' - \boldsymbol{e}_2' \\ \boldsymbol{e}_2' - bP_1^{-1}(z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3' \end{pmatrix},$$

$\boldsymbol{b} = \boldsymbol{0}$, $\boldsymbol{A}_{eq} = \sqrt{n}\boldsymbol{e}_1' - (z_\gamma\sqrt{\xi})^{-1}\boldsymbol{e}_3'$ and $\boldsymbol{b}_{eq} = \boldsymbol{0}$.

The problem of minimizing the objective function in (2.43) under the constraints in (2.44) is a standard quadratic programming problem and can be solved by the MATLAB built-in function `quadprog`.

2.2.3 Special cases

2.2.3.1 Special case 1

For the special case of $a = b$, the interval (a, b) shrinks to a point a. The width of $1 - \alpha$ confidence interval is straightforwardly equal to $2c\hat{\sigma}\sqrt{\boldsymbol{a}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{a} + (z_\gamma)^2\xi}$, where $\boldsymbol{a} = (1, a)'$. The simultaneous confidence level becomes

$$\begin{aligned} 1-\alpha &= P\left\{ \frac{\left| \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \boldsymbol{N}/U + z_\gamma(1/\theta - 1/U) \right|}{\sqrt{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right] + (z_\gamma)^2 \xi}} \le c \right\} \\ &= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) k_2(u) du, \end{aligned} \tag{2.45}$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of $U = \hat{\sigma}/\sigma$ and given in (1.4) and

$$k_2(u) = P\left\{ \frac{\left| \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \boldsymbol{N}/u + z_\gamma(1/\theta - 1/u) \right|}{\sqrt{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right] + (z_\gamma)^2 \xi}} \le c \right\}$$

$$= P\left\{ \frac{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \boldsymbol{N}}{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]} \in \frac{z_\gamma(1 - u/\theta) \pm cu\sqrt{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right] + (z_\gamma)^2 \xi}}{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]} \right\}.$$

Note that

$$\operatorname{Var}\left(\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \boldsymbol{N} \right) = \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right],$$

and so

$$\frac{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \boldsymbol{N}}{\left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]' \left[\boldsymbol{P} \begin{pmatrix} 1 \\ a \end{pmatrix} \right]} \sim N(0, 1).$$

Denote

$$L(u,c,a,z_\gamma) = \frac{z_\gamma(1-u/\theta) - cu\sqrt{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right] + (z_\gamma)^2\xi}}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]},$$

and

$$U(u,c,a,z_\gamma) = \frac{z_\gamma(1-u/\theta) + cu\sqrt{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right] + (z_\gamma)^2\xi}}{\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]'\left[\boldsymbol{P}\begin{pmatrix}1\\a\end{pmatrix}\right]}.$$

Then we have

$$\begin{aligned} k_2(u) &= P\left\{L(u,c,a,z_\gamma) \le N(0,1) \le U(u,c,a,z_\gamma)\right\} \\ &= \Phi\left(U(u,c,a,z_\gamma)\right) - \Phi\left(L(u,c,a,z_\gamma)\right). \end{aligned}$$

Therefore, from (2.45), the confidence level becomes

$$\int_0^\infty f_{\frac{\hat\sigma}{\sigma}}(u)\left(\Phi(U(u,c,a,z_\gamma)) - \Phi(L(u,c,a,z_\gamma))\right) du.$$

This expression involves only one-dimensional integration. We can get the value of critical constant c by using MATLAB built-in function `quad`. Addition to the numerical quadrature, simulation method introduced above also can be utilized to find the critical constant c.

2.2.3.2 Special case 2

For the special case of $(a,b) = (-\infty,\infty)$, the simultaneous confidence level is

$$\begin{aligned} & P\left\{\max_{x\in(-\infty,\infty)} \frac{|(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)|}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}} \le c\right\} \\ = & P\left\{\max_{x\in(-\infty,\infty)} \frac{\left|\begin{pmatrix}\boldsymbol{Px}\\ z_\gamma\sqrt{\xi}\end{pmatrix}'\begin{pmatrix}\boldsymbol{N}/U\\ (1/\theta - 1/U)/\sqrt{\xi}\end{pmatrix}\right|}{\left\|\begin{pmatrix}\boldsymbol{Px}\\ z_\gamma\sqrt{\xi}\end{pmatrix}\right\|} \le c\right\}. \end{aligned} \tag{2.46}$$

Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\boldsymbol{d}_1 = \begin{pmatrix} \boldsymbol{P}\boldsymbol{x}_1 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$ and $\boldsymbol{d}_2 = \begin{pmatrix} \boldsymbol{P}\boldsymbol{x}_2 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$. Let $\mathcal{L}(\boldsymbol{M})$ be the linear space spanned by the two columns of matrix $\boldsymbol{M} = (\boldsymbol{d}_1, \boldsymbol{d}_2)$, and $\boldsymbol{H} = \boldsymbol{M}(\boldsymbol{M}'\boldsymbol{M})^{-1}\boldsymbol{M}'$ be the projection matrix to $\mathcal{L}(\boldsymbol{M})$. It can be shown that (2.46) means the probability of the event that the norm of the projection of the vector $\pm\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ cannot be larger than c. From Section 2.2.2.1, (2.46) is further equal to

$$\begin{aligned} & P\left\{\left\|\boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\| \leq c\right\} \\ = & \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{\left\|\boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/u \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\| \leq c\right\} du. \end{aligned} \tag{2.47}$$

Since N_1, N_2 are $i.i.d. \sim N(0,1)$ and the probability density function of N_1 is $\varphi_{N_1}(n_1) = \frac{1}{\sqrt{2\pi}} e^{-n_1^2/2}$, it is clear that for a fixed u

$$\begin{aligned} & P\left\{\left\|\boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/u \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\| \leq c\right\} \\ = & \int_{-\infty}^\infty \varphi_{N_1}(n_1) P\left\{\left\|\boldsymbol{H}\begin{pmatrix} n_1/u \\ N_2/u \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\| \leq c\right\} dn_1. \end{aligned} \tag{2.48}$$

The 3×3 matrix $\boldsymbol{H}$ can be denoted by $\boldsymbol{H} = (\boldsymbol{H}_1, \boldsymbol{H}_2, \boldsymbol{H}_3)$, where $\boldsymbol{H}_1, \boldsymbol{H}_2, \boldsymbol{H}_3$ are column vectors. Denote $s = z_\gamma(u/\theta - 1)/(z_\gamma\sqrt{\xi})$. Then

$$P\left\{\left\|\boldsymbol{H}\begin{pmatrix} n_1/u \\ N_2/u \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\| \leq c\right\} \tag{2.49}$$

$$\begin{aligned} = & P\left\{\left\|\boldsymbol{H}\begin{pmatrix} n_1/u \\ N_2/u \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right\|^2 \leq c^2\right\} \\ = & P\left\{\left\|(\boldsymbol{H}_1, \boldsymbol{H}_2, \boldsymbol{H}_3)\begin{pmatrix} n_1 \\ N_2 \\ s \end{pmatrix}\right\|^2 \leq u^2c^2\right\} \\ = & P\left\{AN_2^2 + BN_2 + C < 0\right\}, \end{aligned} \tag{2.50}$$

where $A = \boldsymbol{H}_2'\boldsymbol{H}_2$, $B = 2(\boldsymbol{H}_1'\boldsymbol{H}_2 n_1 + \boldsymbol{H}_2'\boldsymbol{H}_3 s)$ and $C = \boldsymbol{H}_1'\boldsymbol{H}_1 n_1^2 + 2\boldsymbol{H}_1'\boldsymbol{H}_3 s n_1 + \boldsymbol{H}_3'\boldsymbol{H}_3 s^2 - u^2c^2$. Let $k(u, n_1, c) = P\{AN_2^2 + BN_2 + C < 0\}$. Therefore,

$$k(u,n_1,c) = \begin{cases} \Phi(\frac{-B+\sqrt{B^2-4AC}}{2A}) - \Phi(\frac{-B-\sqrt{B^2-4AC}}{2A}), & \text{if } B^2-4AC > 0, \\ 0, & \text{if } B^2-4AC \le 0. \end{cases} \tag{2.51}$$

Combining (2.47) - (2.51) gives the confidence level $1-\alpha$ is equal to

$$\int_0^\infty \int_{-\infty}^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u)\varphi_{N_1}(n_1)k(u,n_1,c)dn_1du.$$

This expression involves two-dimensional integration and can be used to calculate the critical constant c . We can use the MATLAB built-in function `dlquad` for this purpose. Also, we can use simulation method to get the critical constant c.

2.2.4 Numerical examples

Example 2.3.

For the data set given in Table 2.1, we also consider two cases: $1-\alpha = 0.90$, $\gamma = 0.75$ and $1-\alpha = 0.95$, $\gamma = 0.99$. By using the methods introduced above in this section, we have computed the critical constants of simultaneous confidence bands V, UV and TT for the percentiles line over $x \in (18, 70)$ and $x \in (1, 100)$ and provide them in Table 2.5. The 90%-simultaneous confidence bands SB, TBU and TBE for the 75th percentile line over $(18, 70)$ are plotted in Figure 2.6. The 99%-simultaneous confidence bands SB, TBU and TBE for the 95th percentile line over $(18, 70)$ are plotted in Figure 2.7. The three bands almost overlap each other in Figures 2.6 and 2.7. There is no significant difference among them. To compare them, We use the average width criterion which is studied in Section 2.3.

Table 2.5: Critical constants of simultaneous confidence bands SB,TBU and TBE

	$1-\alpha = 0.90, \quad \gamma = 0.75$			$1-\alpha = 0.99, \quad \gamma = 0.95$		
Interval	V	UV	TT	V	UV	TT
(18,70)	2.1748	2.1700	2.1708	3.3956	3.3516	3.3558
(1,100)	2.2067	2.2026	2.2034	3.4394	3.4000	3.4033

Figure 2.6: *The 90%-simultaneous confidence bands V, UV and TT for the 75th percentile line over* $(18, 70)$

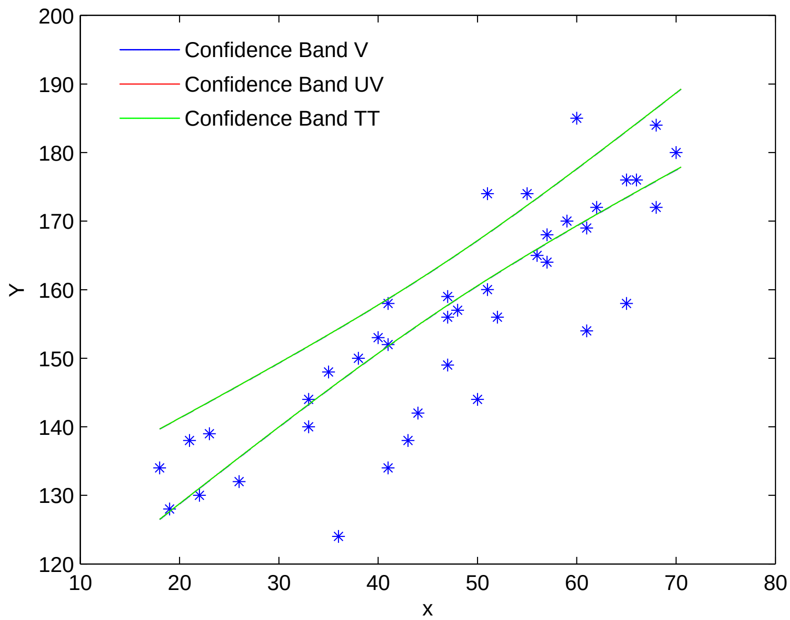
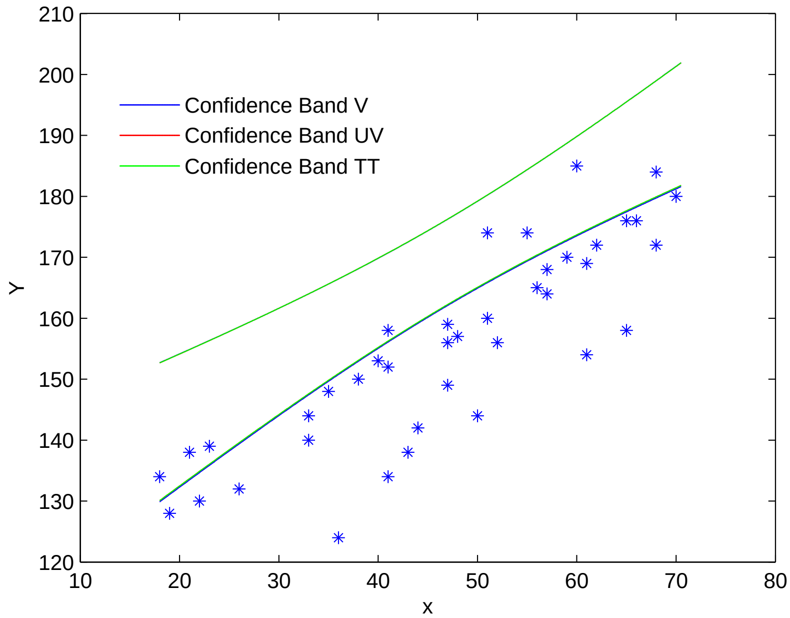


Figure 2.7: *The 99%-simultaneous confidence bands V, UV and TT for the 95th percentile line over* $(18, 70)$



Example 2.4.

For the data set given in Table 2.3, we also consider two cases: $1-\alpha = 0.90$, $\gamma = 0.75$ and $1-\alpha = 0.95$, $\gamma = 0.99$. By using the methods introduced above in this section, we compute the critical constants of simultaneous confidence bands V, UV and TT for the percentiles line over $x \in (1.2931, 1.4131)$ and provide them in Table 2.6.

Table 2.6: Critical constants of simultaneous confidence bands SB,TBU and TBE

	$1-\alpha=0.90,\quad \gamma=0.75$			$1-\alpha=0.99,\quad \gamma=0.95$		
Interval	V	UV	TT	V	UV	TT
(1.2931, 1.4131)	2.0449	2.0281	2.0315	3.9693	3.8508	3.8703

2.3 Comparison of symmetric confidence bands under the average width criterion

The average width of a simultaneous confidence band has been widely used as an optimality criterion for the comparison of different confidence bands. Gafarian (1964) used the average width as an optimality criterion for the first time. Intuitively, a narrower confidence band provides more accurate information about the unknown percentile line. The smaller the average width is, the better the band is. The average width of a confidence band is defined as

$$\int_a^b w(x)dx/(b-a), \tag{2.52}$$

where $w(x)$ denotes the width of the confidence band at x. It is clear that, for a given x the width of the band in (1.9) is

$$2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi},$$

where c is the critical constant to give confidence level $1-\alpha$. Let $\bar{x} = \Sigma_{i=1}^n x_i/n$ and $Sxx = \Sigma_{i=1}^n (x_i - \bar{x})^2$. It can be shown that the average width of the band in (1.9) is given by

$$\begin{aligned}
&\int_a^b 2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}\ dx/(b-a) \\
= \ & c\hat{\sigma}\left[\zeta \ln\left(\tilde{b} + \sqrt{\tilde{b}^2+\zeta}\right) + \tilde{b}\sqrt{\tilde{b}^2+\zeta} - \zeta\ln\left(\tilde{a} + \sqrt{\tilde{a}^2+\zeta}\right)\right. \\
&\left. -\tilde{a}\sqrt{\tilde{a}^2+\zeta}\right]/(\tilde{b}-\tilde{a})
\end{aligned} \tag{2.53}$$

where $\tilde{a} = (a-\bar{x})/\sqrt{Sxx}$, $\tilde{b} = (b-\bar{x})/\sqrt{Sxx}$ and $\zeta = 1/n + (z_\gamma)^2\xi$. The comparisons of bands under the average band width criterion given in Turner and Bowden (1977) and Thomas and Thomas (1986) were not complete due to the fact that critical constants over a finite (a,b) were not available and averages only over a few points were used.

Next we present numerical comparisons of the bands under the average width criterion. Specifically, we consider the case that $a = \bar{x} - \delta$ and $b = \bar{x} + \delta$, i.e., the interval (a,b) is symmetric about $\bar{x}$. Denote $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ and $ss = \delta/\sqrt{S_{xx}}$. Note that for a simultaneous confidence band, the critical constant depends only on ss, γ, n and the confidence level $1-\alpha$. Therefore, the average width of this band also depends only on ss, γ, n and $1-\alpha$. When the design points $x_1, \cdots, x_n$ are given, $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ is fixed. So a large value of δ means a wide interval (a,b). In our numerical comparison, we have used $\alpha = 0.10, 0.01$, $\gamma = 0.75, 0.95$, $n = 10, 20, 30, 50, 100$ and $ss = 0.1, 0.5, 1.0, 10, 50$ and investigated all the combinations of these four factors for each band given in this chapter.

When $\bar{x} = 0$, i.e., the x-values $(x_1, \cdots, x_n)$ are mean adjusted, (2.53) is further equal to

$$\begin{aligned}
& \int_{-\delta}^{\delta} 2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}\; dx/(2\delta) \\
= & \int_{-\delta}^{\delta} c\hat{\sigma}/\delta \sqrt{\frac{1}{n} + \frac{x^2}{S_{xx}} + (z_\gamma)^2\xi}\; dx \\
= & \; c\hat{\sigma}\sqrt{S_{xx}}/\delta \left[\left(\frac{1}{n} + (z_\gamma)^2\xi\right) \ln\left(\frac{\delta}{\sqrt{S_{xx}}} + \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2\xi}\right) \right. \\
& \left. -\frac{1}{2}\left(\frac{1}{n} + (z_\gamma)^2\xi\right) \ln\left(\frac{1}{n} + (z_\gamma)^2\xi\right) + \frac{\delta}{\sqrt{S_{xx}}}\sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2\xi}\right] \qquad (2.54) \\
= & \; c\hat{\sigma}\left[\zeta \ln\left(ss + \sqrt{ss^2 + \zeta}\right) - (\zeta/2)\ln\zeta + ss\sqrt{ss^2 + \zeta}\right]/\delta.
\end{aligned}$$

Recall that for notational convenience, we use the following labels for the bands to be compared:

- SB – the band in (2.3) with $\theta = 1$ and $\xi = 0$;
- TBU – the band in (2.4) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ derived from the uniformly minimum variance unbiased estimator (UMVUE) of $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ and $\xi = 0$;
- TBE – the band in (2.5) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ from Turner and Bowden E band and $\xi = 0$;
- V – the band in (2.26) with $\theta = 1$ and $\xi = 1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2$;
- UV – the band in (2.31) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = 1/\theta^2 - 1$;
- TT – the band in (2.32) with $\theta = \frac{4\nu - 1}{4\nu}$ and $\xi = \frac{1}{2\nu}$.

We can compute the critical constant c of each band over any given interval by using numerical calculation methods provided earlier in this chapter. From (2.54), we can calculate the average width of each band and so the ratio of the average widths of two bands. The ratios of the average bandwidths of SB, TBU, TBE, V, TT relative to UV are given in Tables 2.7-2.10, for some selected combinations of the four factors for the purpose of illustrating what has been observed in our study. It should be emphasized that the bands SB, TBU, TBE and TT compared in Tables 2.7-2.10 are **not** the original conservative bands of Steinhorst and Bowden (1971), Turner and

Bowden (1977, 1979) and Thomas and Thomas (1986) that were on $x \in (-\infty, \infty)$, but the exact bands on given interval (a, b) constructed by using the methods of this thesis.

Note that a smaller entry in Tables 2.7-2.10 means a narrower and so better band. It is clear from the table that SB and TBU are dominated by the other four bands most of the time so they are not recommended. TBE can be better than V, TT and UV but only when ss is small (and so (a, b) is narrow), but the gain of TBE over V, TT and UV is not substantial and is never more than 5%. On the other hand, TBE can be substantially wider than V, TT and UV, by as much as about 40% when $1 - \alpha$, γ and s are large. For this reason, TBE should be used only when (a, b) is narrow. Among the three Form II bands V, TT and UV, V seems always worse than UV (although by a very small margin) and so is not recommended. UV and TT have hardly any difference between them and so either can be used. From hindsight, it is not surprising that UV and TT are very similar because their ξ and θ values are very close when $n \geq 10$.

As all the bands proposed (and compared in Tables 2.7- 2.10) in the paper have coverage probabilities equal $1 - \alpha$, no simulation is required to assess or compare the confidence levels of the bands.

Table 2.7: Ratios of the average widths of the bands relative to UV ($1-\alpha = 0.90$, $\gamma = 0.95$)

n	ss	SB	TBU	TBE	V	TT	UV
	0.1	1.0239	0.9878	0.9506	1.0364	0.9992	1
	0.5	1.0411	1.0076	0.9675	1.0246	0.9984	1
10	1.0	1.1579	1.1212	1.0769	1.0231	0.9996	1
	10.0	1.3904	1.3465	1.2933	1.0301	1.0035	1
	50.0	1.3991	1.3550	1.3014	1.0305	1.0037	1
	0.1	0.9948	0.9828	0.9730	1.0126	0.9998	1
	0.5	1.0697	1.0573	1.0461	1.0096	0.9997	1
20	1.0	1.1916	1.1776	1.1655	1.0110	1.0005	1
	10.0	1.3372	1.3216	1.3080	1.0135	1.0017	1
	50.0	1.3413	1.3256	1.3120	1.0136	1.0018	1
	0.1	0.9864	0.9798	0.9735	1.0066	0.9999	1
	0.5	1.0989	1.0915	1.0854	1.0061	0.9999	1
30	1.0	1.2148	1.2066	1.1999	1.0070	1.0005	1
	10.0	1.3244	1.3154	1.3082	1.0080	1.0012	1
	50.0	1.3271	1.3181	1.3108	1.0080	1.0012	1
	0.1	0.9816	0.9779	0.9744	1.0034	0.9999	1
	0.5	1.1398	1.1354	1.1319	1.0032	1.0002	1
50	1.0	1.2398	1.2350	1.2312	1.0040	1.0004	1
	10.0	1.3161	1.3109	1.3070	1.0043	1.0007	1
	50.0	1.3177	1.3126	1.3086	1.0043	1.0007	1
	0.1	0.9853	0.9837	0.9819	1.0011	0.9999	1
	0.5	1.1915	1.1891	1.1871	1.0015	1.0001	1
100	1.0	1.2648	1.2622	1.2601	1.0019	1.0003	1
	10.0	1.3099	1.3072	1.3050	1.0021	1.0003	1
	50.0	1.3108	1.3080	1.3059	1.0021	1.0003	1

Table 2.8: Ratios of the average widths of bands relative to Band UV ($1-\alpha=0.99$, $\gamma=0.95$)

n	ss	SB	TBU	TBE	V	TT	UV
	0.1	1.0127	0.9909	0.9391	1.0212	0.9994	1
	0.5	1.0963	1.0735	1.0197	1.0178	1.0000	1
10	1.0	1.2567	1.2307	1.1690	1.0205	1.0015	1
	10.0	1.5260	1.4945	1.4196	1.0295	1.0059	1
	50.0	1.5357	1.5039	1.4285	1.0299	1.0060	1
	0.1	1.0065	0.9886	0.9497	1.0175	0.9997	1
	0.5	1.1474	1.1277	1.0847	1.0137	1.0001	1
20	1.0	1.2949	1.2727	1.2243	1.0153	1.0010	1
	10.0	1.4576	1.4326	1.3782	1.0181	1.0026	1
	50.0	1.4620	1.4369	1.3823	1.0181	1.0026	1
	0.1	1.0027	0.9877	0.9562	1.0147	0.9998	1
	0.5	1.1758	1.1583	1.1228	1.0115	1.0000	1
30	1.0	1.3076	1.2880	1.2485	1.0123	1.0007	1
	10.0	1.4279	1.4066	1.3635	1.0137	1.0016	1
	50.0	1.4309	1.4094	1.3663	1.0138	1.0017	1
	0.1	1.0023	0.9910	0.9693	1.0102	0.9999	1
	0.5	1.2111	1.1980	1.1725	1.0084	1.0001	1
50	1.0	1.3188	1.3044	1.2768	1.0080	1.0003	1
	10.0	1.4008	1.3855	1.3562	1.0092	1.0008	1
	50.0	1.4025	1.3873	1.3579	1.0092	1.0009	1
	0.1	1.0128	1.0066	0.9953	1.0055	1.0000	1
	0.5	1.2530	1.2458	1.2319	1.0042	1.0002	1
100	1.0	1.3301	1.3224	1.3077	1.0045	1.0004	1
	10.0	1.3777	1.3697	1.3545	1.0046	1.0004	1
	50.0	1.3786	1.3706	1.3554	1.0046	1.0004	1

Table 2.9: Ratios of the average widths of the bands relative to UV ($1-\alpha = 0.90$, $\gamma = 0.75$)

n	ss	SB	TBU	TBE	V	TT	UV
	0.1	1.0039	0.9952	0.9858	1.0084	0.9997	1
	0.5	1.0054	0.9982	0.9870	1.0066	0.9997	1
10	1.0	1.0352	1.0276	1.0169	1.0081	1.0005	1
	10.0	1.0759	1.0677	1.0567	1.0102	1.0013	1
	50.0	1.0771	1.0689	1.0579	1.0103	1.0014	1
	0.1	0.9971	0.9935	0.9904	1.0035	0.9999	1
	0.5	1.0148	1.0116	1.0080	1.0030	1.0001	1
20	1.0	1.0401	1.0372	1.0333	1.0032	1.0003	1
	10.0	1.0638	1.0610	1.0568	1.0038	1.0005	1
	50.0	1.0644	1.0615	1.0574	1.0038	1.0005	1
	0.1	0.9945	0.9924	0.9906	1.0020	1.0000	1
	0.5	1.0206	1.0192	1.0166	1.0020	1.0001	1
30	1.0	1.0432	1.0415	1.0388	1.0021	1.0003	1
	10.0	1.0605	1.0588	1.0560	1.0025	1.0004	1
	50.0	1.0609	1.0592	1.0564	1.0025	1.0004	1
	0.1	0.9924	0.9916	0.9905	1.0013	0.9999	1
	0.5	1.0288	1.0280	1.0267	1.0010	1.0001	1
50	1.0	1.0471	1.0463	1.0450	1.0013	1.0002	1
	10.0	1.0589	1.0581	1.0567	1.0015	1.0003	1
	50.0	1.0592	1.0584	1.0570	1.0015	1.0003	1
	0.1	0.9923	0.9918	0.9911	1.0003	1.0000	1
	0.5	1.0373	1.0368	1.0360	1.0008	1.0001	1
100	1.0	1.0495	1.0491	1.0483	1.0008	1.0001	1
	10.0	1.0563	1.0558	1.0551	1.0008	1.0001	1
	50.0	1.0564	1.0560	1.0552	1.0008	1.0001	1

Table 2.10: Ratios of the average widths of the bands relative to UV ($1-\alpha=0.99$, $\gamma=0.75$)

n	ss	SB	TBU	TBE	V	TT	UV
	0.1	1.0097	0.9959	0.9641	1.0137	0.9997	1
	0.5	1.0192	1.0083	0.9826	1.0101	0.9998	1
10	1.0	1.0488	1.0386	1.0145	1.0097	1.0003	1
	10.0	1.0910	1.0803	1.0555	1.0128	1.0016	1
	50.0	1.0923	1.0815	1.0567	1.0129	1.0017	1
	0.1	1.0049	0.9958	0.9770	1.0088	0.9999	1
	0.5	1.0283	1.0202	1.0062	1.0071	1.0003	1
20	1.0	1.0542	1.0465	1.0323	1.0073	1.0003	1
	10.0	1.0785	1.0708	1.0570	1.0081	1.0007	1
	50.0	1.0791	1.0714	1.0576	1.0081	1.0007	1
	0.1	1.0000	0.9935	0.9811	1.0066	0.9999	1
	0.5	1.0313	1.0260	1.0156	1.0049	1.0001	1
30	1.0	1.0537	1.0485	1.0375	1.0047	1.0003	1
	10.0	1.0715	1.0663	1.0550	1.0051	1.0003	1
	50.0	1.0719	1.0667	1.0554	1.0052	1.0004	1
	0.1	0.9983	0.9944	0.9865	1.0045	1.0000	1
	0.5	1.0345	1.0314	1.0252	1.0032	1.0001	1
50	1.0	1.0524	1.0495	1.0433	1.0033	1.0002	1
	10.0	1.0643	1.0610	1.0549	1.0034	1.0003	1
	50.0	1.0646	1.0612	1.0551	1.0034	1.0003	1
	0.1	0.9980	0.9959	0.9928	1.0020	1.0000	1
	0.5	1.0429	1.0413	1.0385	1.0015	1.0001	1
100	1.0	1.0549	1.0534	1.0507	1.0014	1.0001	1
	10.0	1.0616	1.0601	1.0573	1.0013	1.0001	1
	50.0	1.0617	1.0620	1.0574	1.0013	1.0001	1

2.3.1 Numerical examples

Example 2.5.

Consider the data set in Example 2.1. Since critical constants have been given in Table 2.2 and 2.5, we can compute the average widths of the bands SB, TBU, TBE, V, TT and UV over $(18, 70)$. We provide the average width of each band over $(18, 70)$ and $(1, 100)$ in Table 2.11 and the ratios of the average widths of the bands relative to the band UV in Table 2.12.

Table 2.11: The average widths of the bands

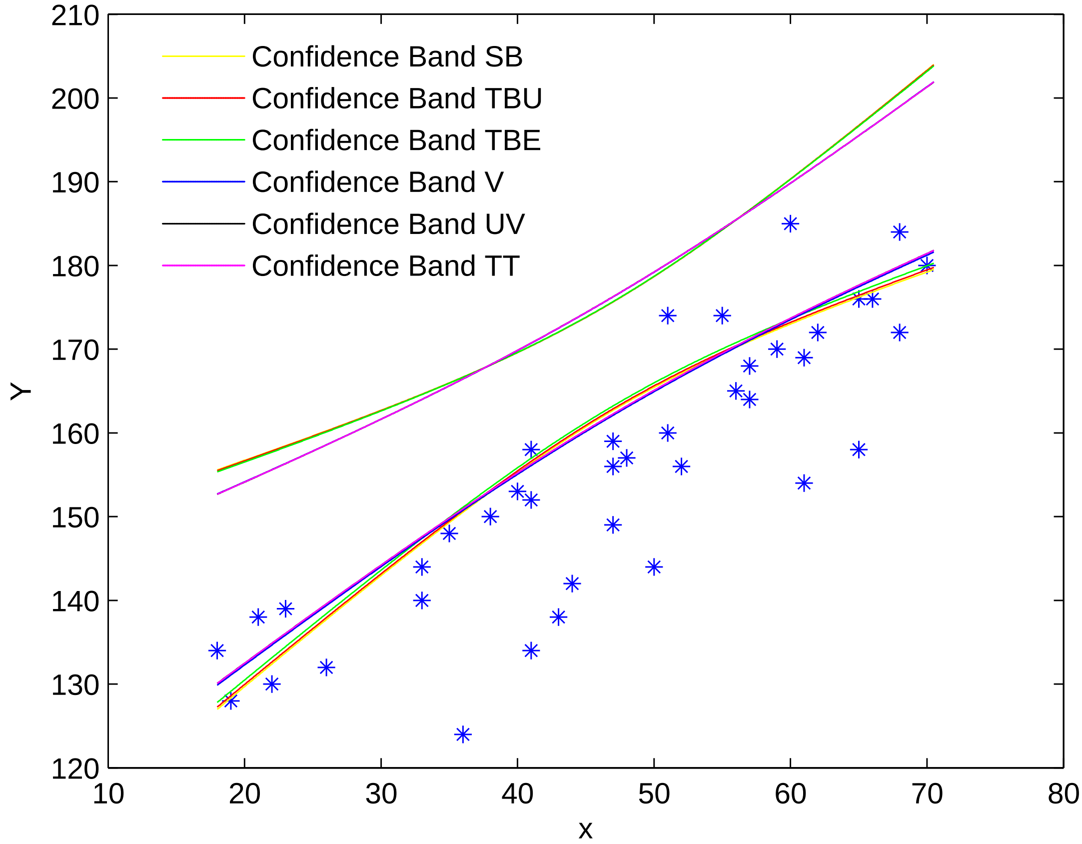
		$1-\alpha=0.90,\quad\gamma=0.75$				
Interval	SB	TBU	TBE	V	TT	UV
(18,70)	8.7248	8.7131	8.7029	8.6892	8.6765	8.6764
(1,100)	12.8693	12.8556	12.8390	12.5374	12.5211	12.5191
		$1-\alpha=0.99,\quad\gamma=0.95$				
Interval	SB	TBU	TBE	V	TT	UV
(18,70)	18.1787	17.9460	17.4925	16.8640	16.6898	16.6917
(1,100)	26.5846	26.2450	25.5806	22.1998	21.9862	21.9838

Table 2.12: Ratios of the average widths of the bands relative to UV

		$1-\alpha=0.90,\quad\gamma=0.75$				
Interval	SB	TBU	TBE	V	TT	UV
(18,70)	1.0055	1.0042	1.0003	1.0015	1.0000	1
(1,100)	1.0280	1.0269	1.0256	1.0015	1.0002	1
		$1-\alpha=0.99,\quad\gamma=0.95$				
Interval	SB	TBU	TBE	V	TT	UV
(18,70)	1.0891	1.0751	1.0480	1.0103	0.9999	1
(1,100)	1.2093	1.1938	1.1636	1.0098	1.0001	1

From Table 2.12, in this example, the bands UV and TT perform well. We recommend band UV when interval (a, b) is large. The 99%-simultaneous confidence bands SB, TBU, TBE, V, UV and TT for the 95th percentile line over $(18, 70)$ are plotted in Figure 2.8. In this example, UV and TT are almost overlap each other. From Figure 2.8, we can see UV and TT are narrower and so better than the other four bands.

Figure 2.8: *The 99%-simultaneous confidence bands for the 95th percentile line over* $(18, 70)$



Example 2.6.

Consider the data set in Example 2.2. Since the critical constants of the bands SB, TBU, TBE, V, UV, TT have been given in Table 2.4 and Table 2.6. Then the average width of each band and the ratio of the average width of each band relative to the band UV can be computed. In this example $\delta = 0.060$, $ss = \delta/\sqrt{Sxx} = 0.5485$ and $n = 15$. Consider two cases: $1 - \alpha = 0.90$, $\gamma = 0.75$ and $1 - \alpha = 0.99$, $\gamma = 0.95$. We provide the ratios in Table 2.13. From this table, we recommend Band UV and TT in these two cases.

Table 2.13: Ratios of the average widths of bands relative to Band UV

Interval	ss	$1-\alpha=0.90$, $\gamma=0.75$ SB	TBU	TBE	V	TT	UV
(1.2931, 1.4131)	0.5485	1.0137	1.0091	1.0035	1.0041	1.0000	1

Interval	ss	$1-\alpha=0.99$, $\gamma=0.95$ SB	TBU	TBE	V	TT	UV
(1.2931, 1.4131)	0.5485	1.1418	1.1198	1.0722	1.0159	1.0001	1

2.4 Conclusions

Two-sided symmetric simultaneous confidence bands have been studied in this chapter. Methods have been given to compute the exact symmetric simultaneous confidence bands for the percentile line over a finite interval of the covariate x. It is observed that the exact symmetric bands can be much narrower than the corresponding conservative symmetric bands. Six bands have been compared under the average width criterion. It is concluded that Bands TT and UV perform better than the other bands most of the time and so recommended.

Chapter 3

Two-sided Asymmetric Simultaneous Confidence Bands for a Percentile Line

It is well known that, for the 100γth percentile of a normal distribution, a confidence interval that is not symmetric about the percentile estimate has a shorter length than the symmetric confidence interval when $\gamma \neq 0.5$, see, for example, Liu et al. (2013). However, all the simultaneous confidence bands for a percentile line available in the statistical literature as discussed above are symmetric. In this chapter, asymmetric simultaneous confidence bands are proposed, and they are uniformly narrower than the corresponding symmetric bands. Corresponding to the symmetric confidence band in (1.9), an asymmetric confidence band for the percentile line $\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma$ has the general form

$$\begin{aligned} & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma}/\theta - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \\ \leq\ & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\ \leq\ & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma}/\theta + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \quad \text{for all } x \in (a,b) \end{aligned} \tag{3.1}$$

where the constants $\theta \neq 0$ and ξ can be chosen to give different specific confidence bands as discussed in Chapter 2. For given constants $\theta \neq 0$ and ξ, there are many solutions of the pair $(c_1,\ c_2)$ which satisfy the specified confidence level $1-\alpha$ requirement. We want to search for the pair $(c_1,\ c_2)$ which minimizes the average width of the band. Since for any given x, the width of the band is $(c_1+c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$, then the smaller is the value of (c_1+c_2), the narrower is the band. Each symmetric band considered in Chapter 2 is a special case of the corresponding asymmetric band with $c_1 = c_2$. This is why the asymmetric band will in general have a smaller average width and be better than the corresponding symmetric bands, and the motivation of the construction of asymmetric bands.

3.1 Asymmetric bands of Form I

In this section, we focus on the bands of the form (3.1) with $\xi = 0$, denoted as Form I:

$$\begin{aligned} & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \\ \le \; & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\ \le \; & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \quad \text{for all } x \in (a,b). \end{aligned} \tag{3.2}$$

In Section 3.2, we will look at the bands of the form (3.1) with $\xi \neq 0$, since the mathematical treatments of these two forms are slightly different.

For each of the three symmetric simultaneous confidence bands in Section 2.1, we have the corresponding asymmetric band. All of them are special cases of form (3.2).

The first asymmetric simultaneous confidence band, denoted as *SBa*, is the asymmetric version of *SB* in (2.3). Specifically, it has the form

$$\begin{aligned} & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \\ \le \; & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\ \le \; & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \quad \text{for all } x \in (a,b). \end{aligned} \tag{3.3}$$

The second band, denoted as *TBUa*, is the asymmetric version of TBU in (2.4) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$, and given by

$$\begin{aligned} & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \\ \le \; & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\ \le \; & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \quad \text{for all } x \in (a,b). \end{aligned} \tag{3.4}$$

The third band, denoted as *TBEa*, is the asymmetric version of TBE in (2.5) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ and given by

$$\begin{aligned} & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \\ \le \; & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\ \le \; & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \quad \text{for all } x \in (a,b). \end{aligned} \tag{3.5}$$

Based on the investigation in Chapter 2 we know TBE is better than the other two bands, so we just look at $TBEa$ in the rest of this chapter.

Next we consider the computation of c_1 and c_2 in (3.2). The simultaneous confidence level of this band is given by

$$\begin{aligned}
& P\left\{\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \le \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \right. \\
& \left. \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b)\right\} \qquad (3.6) \\
= \; & P\left\{-c_2 \le \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \le c_1 \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{-c_2 \le \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c_1 \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{-c_2 \le \frac{(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N} + z_\gamma(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c_1 \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{-c_2 \le \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c_1 \text{ for all } x \in (a,b)\right\}, \qquad (3.7)
\end{aligned}$$

where the matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$$

is the unique square root of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ and defined in (1.5),

$$\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$$

and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$. Note that $\boldsymbol{P}\boldsymbol{x} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}$ and so (3.7) is further equal to

$$P\left\{-c_2 \le \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \le c_1 \text{ for all } x \in (a,b)\right\} \qquad (3.8)$$

$$= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{-c_2 \le \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ N_2/u \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \le c_1 \text{ for all } x \in (a,b)\right\} du,$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

We give two methods for computing the critical constant c_1 and c_2 below.

3.1.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} n_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ n_2/u \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (3.8) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{-c_2 \le k(\boldsymbol{v}) \le c_1 \text{ for all } x \in (a,b)\}} d\boldsymbol{v}, \tag{3.9}$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Expression (3.9) involves a three-dimensional integration and can be used to compute the simultaneous confidence level for given c_1 and c_2 via numerical quadrature. We have used the MATLAB built-in function `triplequad` for this purpose. For a fixed c_2, we can numerically find c_1 so that the simultaneous confidence level is equal to $1 - \alpha$ and then evaluate $c_1 + c_2$. We search numerically for the pair $(c_1,\, c_2)$ which minimizes $c_1 + c_2$.

Our experience shows this method of computing the exact values of (c_1,c_2) takes substantially longer computation time than the simulation method introduced in the following section. The numerical quadrature method can however be used to cross check the results of the simulation method.

3.1.2 Simulation method

Let

$$S(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})}} \tag{3.10}$$

$$= \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|}. \tag{3.11}$$

The simultaneous confidence level is therefore given by

$$P\{-c_2 \leq S(x) \leq c_1, \text{ for all } x \in (a, b)\}. \tag{3.12}$$

Denote $L = \min_{x \in (a,b)} S(x)$ and $M = \max_{x \in (a,b)} S(x)$. Then (3.12) is equivalent to

$$P\{-c_2 \leq L \text{ and } M \leq c_1, \text{ for all } x \in (a, b)\}.$$

There are many solutions of $(c_1,\ c_2)$ for which the confidence level in (3.12) is equal to $1-\alpha$. But we are only interested in the one pair that satisfies not only the $1-\alpha$ confidence level requirement but also minimizes c_1+c_2 and so the average width of the band in (3.1).

We first generate independent standard bivariate normal random vectors $\boldsymbol{N}_i$ and independent variables $U_i \sim \sqrt{\chi^2_\nu/\nu}$, $i = 1, 2, \cdots, R$. Then we calculate the R replicates

$$S_i(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}_i/U_i + z_\gamma(1/\theta - 1/U_i)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})}},\ i = 1, \cdots, R.$$

Denote $L_i = \min_{x \in (a,b)} S_i(x)$ and $M_i = \max_{x \in (a,b)} S_i(x)$, $i = 1, 2, \cdots, R$. We provide two methods for computing L_i and M_i in the following sections. It is clear that $-c_2 \leq S_i(x) \leq c_1, x \in (a, b)$ is equivalent to

$$\begin{cases} L_i \geq -c_2 \\ M_i \leq c_1. \end{cases}$$

Let the ordered values of $\{L_i,\ i = 1, \cdots, R\}$ be

$$\hat{L}_1 \leq \hat{L}_2 \leq \cdots \leq \hat{L}_i \leq \hat{L}_{i+1} \leq \cdots \leq \hat{L}_R$$

and the corresponding values of $\{M_i,\ i = 1, \cdots, R\}$ be

$$\hat{M}_1, \hat{M}_2, \cdots, \hat{M}_i, \hat{M}_{i+1}, \cdots, \hat{M}_R,$$

which may not be in ascending or descending order. It is noteworthy that each $(\hat{L}_i, \hat{M}_i)$ is equal to $(L_j,\ M_j)$ for some for some $1 \leq j \leq R$.

For a given (initial) value $-\mathring{c}_2$, we want to find $\hat{c}_1$ so that $1-\alpha$ proportion of the R replicates (L_i, M_i) satisfy $\{-\mathring{c}_2 \leq L_i \text{ and } M_i \leq \hat{c}_1\}$. Firstly, it is clear that any $-\mathring{c}_2 < \hat{L}_1$ can be replaced by $\hat{L}_1$ and so we only need to consider $\hat{L}_1 \leq -\mathring{c}_2$. Next, if $\hat{L}_{\langle \alpha R+1 \rangle} < -\mathring{c}_2$ then we cannot find the required $\hat{c}_1$ and so we only need to consider $-\mathring{c}_2 \leq \hat{L}_{\langle \alpha R+1 \rangle}$. Furthermore, any $-\mathring{c}_2$ satisfying $\hat{L}_i < -\mathring{c}_2 < \hat{L}_{i+1}$ for some $1 \leq i \leq \langle \alpha R \rangle$ can be replaced by $\hat{L}_{i+1}$. Hence we only need to consider $-\mathring{c}_2 = \hat{L}_k$ for

$k = 1, \cdots, \langle \alpha R \rangle + 1$.

For a given $-\mathring{c}_2 = \hat{L}_k$, where $1 \le k \le \langle \alpha R \rangle + 1$, a $\hat{c}_1$ satisfying the confidence level requirement can be found in the following way. Sort the $(R - k + 1)$-number subsequence $\{\hat{M}_k, \hat{M}_{k+1}, \cdots, \hat{M}_R\}$ in ascending order $\tilde{M}_1 \le \cdots \le \tilde{M}_{R-k+1}$ and denote the associated $\{\hat{L}_k, \hat{L}_{k+1}, \cdots, \hat{L}_R\}$ as $\{\tilde{L}_1, \tilde{L}_2, \cdots, \tilde{L}_{R-k+1}\}$ which may not be ordered. Set the $\langle (1-\alpha)R \rangle$th value of the ordered sequence $\tilde{M}_1 \le \cdots \le \tilde{M}_{R-k+1}$ as $\hat{c}_1^k$, i.e., $\hat{c}_1^k = \tilde{M}_{\langle (1-\alpha)R \rangle}$.

Note, however, by replacing the initial value $-\mathring{c}_2 = \hat{L}_k$ with the minimum value of the sequence $\{\tilde{L}_1, \tilde{L}_2, \cdots, \tilde{L}_{R-k+1}\}$, denoted as $-\hat{c}_2^k = \min_{1 \le l \le R-k+1} \tilde{L}_l$, the $1-\alpha$ confidence level requirement is still satisfied. Since $-\hat{c}_2^k$ may be larger than $-\mathring{c}_2 = \hat{L}_k$, we have $\hat{c}_1^k + \hat{c}_2^k \le \hat{c}_1^k + \mathring{c}_2$. So it is desirable to replace the initial value $-\mathring{c}_2 = \hat{L}_k$ by $-\hat{c}_2^k$ in order to reduce the average width of the band.

The following three steps are the key to computing $(\hat{c}_1^k, \hat{c}_2^k)$ for a given value $-\mathring{c}_2 = \hat{L}_k$.

Step 1. Sort the sequence $\{\hat{M}_k, \hat{M}_{k+1}, \cdots, \hat{M}_R\}$ in ascending order $\tilde{M}_1 \le \tilde{M}_2 \le \cdots \le \tilde{M}_{R-k+1}$. Denote the corresponding $\{\hat{L}_k, \hat{L}_{k+1}, \cdots, \hat{L}_R\}$ values as $\{\tilde{L}_1, \tilde{L}_2, \cdots, \tilde{L}_{R-k+1}\}$.

Step 2. Set $\hat{c}_1^k = \tilde{M}_{\langle (1-\alpha)R \rangle}$.

Step 3. Set $-\hat{c}_2^k = \min_{1 \le l \le R-k+1} \tilde{L}_l$.

Now repeat Step 1 to Step 3 to compute $(\hat{c}_1^k, \hat{c}_2^k)$ for $k = 1, \cdots, \langle \alpha R \rangle + 1$. Finally we can find the one pair $(\hat{c}_1^m, \hat{c}_2^m)$ such that $\hat{c}_1^m + \hat{c}_2^m \le \hat{c}_1^k + \hat{c}_2^k$ for all $k = 1, \cdots, \langle \alpha R \rangle + 1$ and use them as the critical constants c_1 and c_2. Again, this method can readily be generalized to multiple regression and polynomial regression.

Next we give two computation methods for calculating L and M from $\boldsymbol{N}$ and U.

3.1.2.1 Projection method

From (3.11), we have

$$L = \min_{x \in (a,b)} \frac{(\boldsymbol{Px})' \boldsymbol{Z}}{\|(\boldsymbol{Px})\|} \text{ and } M = \max_{x \in (a,b)} \frac{(\boldsymbol{Px})' \boldsymbol{Z}}{\|(\boldsymbol{Px})\|},$$

where

$$\boldsymbol{Z} = \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} = \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n} z_\gamma \\ N_2/U \end{pmatrix}.$$

Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$ and $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$. Then $\boldsymbol{Px}_1 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} a \end{pmatrix}$ and $\boldsymbol{Px}_2 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} b \end{pmatrix}$. When x changes over the interval (a, b), $\boldsymbol{Px}$ forms a cone bounded by $\boldsymbol{Px}_1$ and $\boldsymbol{Px}_2$.

If $\boldsymbol{Z}$ belongs to the cone, then

$$\begin{aligned} L &= \min\left\{\frac{(\boldsymbol{P}\boldsymbol{x}_1)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_1\|}, \frac{(\boldsymbol{P}\boldsymbol{x}_2)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_2\|}\right\}, \\ M &= \|\boldsymbol{Z}\|. \end{aligned}$$

If $-\boldsymbol{Z}$ belongs to the cone, then

$$\begin{aligned} L &= -\|\boldsymbol{Z}\|, \\ M &= \max\left\{\frac{(\boldsymbol{P}\boldsymbol{x}_1)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_1\|}, \frac{(\boldsymbol{P}\boldsymbol{x}_2)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_2\|}\right\}. \end{aligned}$$

Otherwise,

$$\begin{aligned} L &= \min\left\{\frac{(\boldsymbol{P}\boldsymbol{x}_1)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_1\|}, \frac{(\boldsymbol{P}\boldsymbol{x}_2)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_2\|}\right\}, \\ M &= \max\left\{\frac{(\boldsymbol{P}\boldsymbol{x}_1)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_1\|}, \frac{(\boldsymbol{P}\boldsymbol{x}_2)'\boldsymbol{Z}}{\|\boldsymbol{P}\boldsymbol{x}_2\|}\right\}. \end{aligned}$$

Similar to Section 2.1.2.1, we have the following way to judge whether the projection of a given vector belongs to the cone bounded by $\boldsymbol{P}\boldsymbol{x}_1$ and $\boldsymbol{P}\boldsymbol{x}_2$ or not. Two coefficients λ and κ are given in (2.11) and (5.44). If $a < \kappa < b$ and $\lambda > 0$, then the projection of vector $\boldsymbol{Z}$ lies inside the cone spanned by $\boldsymbol{P}\boldsymbol{x}_1$ and $\boldsymbol{P}\boldsymbol{x}_2$. If $a < \kappa < b$ and $\lambda < 0$, then the projection of vector $-\boldsymbol{Z}$ lies inside the cone spanned by $\boldsymbol{P}\boldsymbol{x}_1$ and $\boldsymbol{P}\boldsymbol{x}_2$. Otherwise, the projections of $\pm\boldsymbol{Z}$ lie outside the cone.

For the special case of $(a, b) = (-\infty, \infty)$, if $\lambda > 0$, then

$$\begin{aligned} L &= -|U^{-1}N_2|, \\ M &= \|Z\|. \end{aligned}$$

Otherwise,

$$\begin{aligned} L &= -\|Z\|, \\ M &= |U^{-1}N_2|. \end{aligned}$$

3.1.2.2 Turning point method

From (3.10), $S(x)$ can be written as

$$S(x) = \frac{f(x)}{\sqrt{g(x)}},$$

where

$$
\begin{aligned}
f(x) &= (\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1-1/U), \\
g(x) &= (\boldsymbol{Px})'(\boldsymbol{Px}).
\end{aligned}
$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$. Then

$$
\begin{aligned}
f(x) &= P_1^{-1}U^{-1}N_2 x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\
\frac{\mathrm{d}f}{\mathrm{d}x} &= P_1^{-1}U^{-1}N_2, \\
g(x) &= P_1^{-2}x^2 + n^{-1}, \\
\frac{\mathrm{d}g}{\mathrm{d}x} &= 2P_1^{-2}x.
\end{aligned}
$$

Solving from $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f}{\sqrt{g}}\right)|_{x_t} = 0$, we have the turning point $x_t = \dfrac{P_1 N_2 n^{-1}}{n^{-1/2}N_1 + z_\gamma(U\theta^{-1} - 1)}$. The maximum value and the minimum value of $S(x)$ are therefore attained at either $x = a$ or $x = b$ or $x = x_t$. If $a < x_t < b$, then

$$
\begin{aligned}
L &= \min_{x\in(a,b)} S(x) = \min\{S(a), S(x_t), S(b)\}, \\
M &= \max_{x\in(a,b)} S(x) = \max\{S(a), S(x_t), S(b)\},
\end{aligned}
$$

otherwise,

$$
\begin{aligned}
L &= \min_{x\in(a,b)} S(x) = \min\{S(a), S(b)\}, \\
M &= \max_{x\in(a,b)} S(x) = \max\{S(a), S(b)\}.
\end{aligned}
$$

For the special case of $(a, b) = (-\infty, \infty)$,

$$
\begin{aligned}
h(-\infty) &= \lim_{x\to-\infty} h(x) = -U^{-1}N_2, \\
h(\infty) &= \lim_{x\to\infty} h(x) = U^{-1}N_2.
\end{aligned}
$$

then

$$
\begin{aligned}
L &= \min_{x\in(-\infty,\infty)} S(x) = \min\left\{-|U^{-1}N_2|, S(x_t)\right\}, \\
M &= \max_{x\in(-\infty,\infty)} S(x) = \max\left\{|U^{-1}N_2|, S(x_t)\right\}.
\end{aligned}
$$

3.1.3 Numerical examples

Example 3.1.

For the data set given in Table 2.1 on how systolic blood pressure (Y) changes with age (x) for a group of forty males, we only consider the asymmetric band $TBEa$ since TBE is the best one among three symmetric bands of Form I. The superiority of TBE compared to SB and TBU has been discussed in Chapter 2. For two cases $1-\alpha = 0.90$, $\gamma = 0.75$ and $1 - \alpha = 0.95$, $\gamma = 0.99$, by using the methods introduced above in this section, we calculate the critical constants c_1 and c_2 of the asymmetric band $TBEa$ over $x \in (18, 70)$ and $x \in (1, 100)$ and provide them in the following Table 3.1. In this table, for each asymmetric band, we also provide c value which is the critical constant of the corresponding symmetric band TBE. For any given x, the width of $TBEa$ is $(c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$ and the width of TBE is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Therefore the percentage of improvement of the average widths from TBE to $TBEa$ is

$$\text{Percentage} = 100[1 - (c_1 + c_2)/(2c)]\%.$$

Table 3.1: Critical constants for simultaneous confidence bands $TBEa$ and TBE and the percentage of improvement

	$1-\alpha = 0.90,\ \gamma = 0.75$					
Interval	$-c_2$	c_1	$c_1 + c_2$	c	$2c$	Percentage
(18,70)	-2.3294	2.2934	4.6228	2.3121	4.6242	0.03%
(1,100)	-2.3618	2.3007	4.6624	2.3326	4.6652	0.06%
	$1-\alpha = 0.99,\ \gamma = 0.95$					
Interval	$-c_2$	c_1	$c_1 + c_2$	c	$2c$	
(18,70)	-4.9062	3.8587	8.7649	4.6472	9.2944	6.04%
(1,100)	-4.9154	3.8559	8.7713	4.6475	9.2950	5.87%

Example 3.2.

For the data set given in Table 2.3 on how systolic blood pressure (Y) changes with age (x) for a group of forty males, we also consider two cases: $1 - \alpha = 0.90$, $\gamma = 0.75$ and $1 - \alpha = 0.95$, $\gamma = 0.99$ and give the results of comparison between $TBEa$ and TBE in Table 3.2.

From these two examples, we can see the asymmetric band $TBEa$ performs better than the symmetric band TBE as expected.

Table 3.2: Critical constants for simultaneous confidence bands $TBEa$ and TBE and the percentage of improvement

	$1-\alpha=0.90, \quad \gamma=0.75$					
Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	Percentage
(1.2931, 1.4131)	-2.5395	2.2854	4.9250	2.4656	4.9312	0.13%
	$1-\alpha=0.99, \quad \gamma=0.95$					
Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	
(1.2931, 1.4131)	-6.0482	3.8843	9.9325	5.7894	11.5788	16.57%

3.2 Asymmetric bands of Form II

We consider two-sided asymmetric simultaneous confidence bands for the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ over the interval $x \in (a, b)$ with $\theta \neq 0$ and $\xi \neq 0$, denoted as Form II

$$\begin{aligned}
& \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \\
\leq\ & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\
\leq\ & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \quad \text{for all } x \in (a, b).
\end{aligned} \tag{3.13}$$

Similar to Section 3.1, for given constants $\theta \neq 0$ and $\xi \neq 0$, there are many solutions of the pair $(c_1,\ c_2)$ which satisfy the specified confidence level $1 - \alpha$ requirement. We want to search for the pair $(c_1,\ c_2)$ which minimizes the average width of the band. Each symmetric band considered in Section 2.2 is a special case of the corresponding asymmetric band with $c_1 = c_2$.

For each of the three symmetric simultaneous confidence bands in Section 2.2 we study the corresponding asymmetric band. All of them are special cases of form (3.13). For any given x, the width of the band is $(c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}$.

The first asymmetric simultaneous confidence band, denoted as Va, is the asymmetric version of V in (2.26) with $\theta = 1$ and $\xi = 1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2$ and given by

$$\begin{aligned}
& \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\left(1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2\right)} \\
\leq\ & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\
\leq\ & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\left(1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2\right)} \\
& \text{for all } x \in (a, b).
\end{aligned} \tag{3.14}$$

The second band, denoted as UVa, is the asymmetric version of UV in (2.31) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = \frac{\nu}{2}\left(\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$ and given by

$$\begin{aligned}
& \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2(1/\theta^2 - 1)} \\
\leq\ & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \\
\leq\ & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2(1/\theta^2 - 1)} \text{ for all } x \in (a, b).
\end{aligned} \tag{3.15}$$

The third band, denoted as TTa, is the asymmetric version of TT in (2.32) with

$\theta = \dfrac{4\nu - 1}{4\nu}$ and $\xi = \dfrac{1}{2\nu}$ and given by

$$
\begin{aligned}
& \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{(4\nu-1)/(4\nu)} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2/(2\nu)} \\
\leq\ & \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \qquad (3.16) \\
\leq\ & \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{(4\nu-1)/(4\nu)} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2/(2\nu)} \quad \text{for all } x \in (a,b).
\end{aligned}
$$

Next we consider the computation of c_1 and c_2 in (3.13). The simultaneous confidence level of this band is given by

$$
\begin{aligned}
& P\left\{\boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} - c_1\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \leq \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \right. \\
& \left. \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c_2\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \text{ for all } x \in (a,b)\right\} \\
= \ & P\left\{-c_2 \leq \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}} \leq c_1 \text{ for all } x \in (a,b)\right\} \\
= \ & P\left\{-c_2 \leq \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}) + (z_\gamma)^2\xi}} \leq c_1 \text{ for all } x \in (a,b)\right\}, \qquad (3.17)
\end{aligned}
$$

where the matrix

$$
\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}
$$

is the unique square root of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ and defined in (1.5),

$$
\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})
$$

and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$. Note that $\boldsymbol{Px} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}$ and so (3.17) is further equal to

$$P\left\{ -c_2 \le \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|} \le c_1 \text{ for all } x \in (a,b) \right\} \quad (3.18)$$

$$= P\left\{ -c_2 \le \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} N_1/U \\ N_2/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|} \le c_1 \text{ for all } x \in (a,b) \right\} \quad (3.19)$$

$$= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{ -c_2 \le \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} N_1/U \\ N_2/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|} \le c_1 \text{ for all } x \in (a,b) \right\} du,$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

Next we give two methods for computing the critical constant c_1 and c_2.

3.2.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} n_1/u \\ n_2/u \\ (1/\theta - 1/u)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (3.19) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{-c_2 \le k(\boldsymbol{v}) \le c_1 \text{ for all } x \in (a,b)\}} d\boldsymbol{v}, \quad (3.20)$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Expression (3.20) involves a three-dimensional integration and can be used to compute the simultaneous confidence level for given c_1 and c_2 via numerical quadrature. For a fixed c_2, we can numerically find c_1 so that the simultaneous confidence level is equal to $1-\alpha$. Then we evaluate c_1+c_2. We search numerically for the pair $(c_1,\, c_2)$ which minimizes c_1+c_2.

3.2.2 Simulation method

From (3.17) and (3.18), let

$$S(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}} \tag{3.21}$$

$$= \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|}. \tag{3.22}$$

The simultaneous confidence level is therefore given by

$$P\{-c_2 \le S(x) \le c_1, \text{ for all } x \in (a,b)\}. \tag{3.23}$$

Denote $L = \min_{x\in(a,b)} S(x)$ and $M = \max_{x\in(a,b)} S(x)$. Then (3.23) is equivalent to

$$P\{-c_2 \le L,\ M \le c_1, \text{ for all } x \in (a,b)\}.$$

There are many solutions of $(c_1,\, c_2)$ for which the confidence level in (3.23) is equal to $1-\alpha$. But we are only interested in the one pair which minimizes c_1+c_2 and so the corresponding confidence band has the smallest average width.

We first generate independent standard bivariate normal random vectors $\boldsymbol{N}_i$ and independent variables $U_i \sim \sqrt{\chi^2_\nu/\nu}$, $i = 1, 2, \cdots, R$. Then we calculate the R replicates

$$S_i(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}_i/U_i + z_\gamma(1/\theta - 1/U_i)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}},\ i = 1, \cdots, R.$$

Denote $L_i = \min_{x\in(a,b)} S_i(x)$ and $M_i = \max_{x\in(a,b)} S_i(x)$, $i = 1, 2, \cdots, R$. Analogues to the last section, the critical constants c_1 and c_2 can be obtained by simulation method. The simulating procedure has been given in Section 3.1.2 in details. Next we give two computation methods for calculating L and M from $\boldsymbol{N}$ and U.

3.2.2.1 Projection method

From (3.22), we have

$$L = \min_{x\in(a,b)} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|}$$

$$M = \max_{x\in(a,b)} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|}$$

Similar to Section 2.2.2.1, denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$, $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$, $\boldsymbol{d}_1 = \begin{pmatrix} \boldsymbol{Px}_1 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$, $\boldsymbol{d}_2 = \begin{pmatrix} \boldsymbol{Px}_2 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$ and the matrix $\boldsymbol{M} = (\boldsymbol{d}_1, \boldsymbol{d}_2)$. Let $\mathcal{L}(\boldsymbol{M})$ be the linear plane spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ and $\boldsymbol{H} = \boldsymbol{M}(\boldsymbol{M}'\boldsymbol{M})^{-1}\boldsymbol{M}'$ be the projection matrix to $\mathcal{L}(\boldsymbol{M})$. If the projection of the vector $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, then

$$\begin{aligned} L &= \min\left(\frac{\boldsymbol{d}_1' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\|\boldsymbol{d}_1\|}, \frac{\left|\boldsymbol{d}_2' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\|\boldsymbol{d}_2\|} \right), \\ M &= \left\| \boldsymbol{H} \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|. \end{aligned}$$

If the projection of the vector $-\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, then

$$\begin{aligned} L &= -\left\| \boldsymbol{H} \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|, \\ M &= \max\left(\frac{\boldsymbol{d}_1' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\|\boldsymbol{d}_1\|}, \frac{\left|\boldsymbol{d}_2' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\|\boldsymbol{d}_2\|} \right). \end{aligned}$$

Otherwise,

$$
\begin{aligned}
L &= \min\left(\frac{\boldsymbol{d}_1'\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\|\boldsymbol{d}_1\|}, \quad \frac{\left|\boldsymbol{d}_2'\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\|\boldsymbol{d}_2\|} \right), \\
M &= \max\left(\frac{\boldsymbol{d}_1'\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\|\boldsymbol{d}_1\|}, \quad \frac{\left|\boldsymbol{d}_2'\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}\right|}{\|\boldsymbol{d}_2\|} \right).
\end{aligned}
$$

Similar to Section 2.2.2.1, we have a way to judge whether the projection of a given vector, $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ for example, belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ or not. Two non-zero coefficients λ and κ are given in (2.39) and (2.40). If $a < \kappa < b$ and $\lambda > 0$, then the projection of vector $\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ lies inside the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$. If $a < \kappa < b$ and $\lambda < 0$, then the projection of vector $-\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ lies inside the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$. Otherwise, the projections of $\pm\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ lie outside the cone.

For the special case of $(a, b) = (-\infty, \infty)$, if $\lambda > 0$, then

$$
\begin{aligned}
L &= -|U^{-1}N_2|, \\
M &= \left\| \boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|.
\end{aligned}
$$

Otherwise,

$$
\begin{aligned}
L &= -\left\| \boldsymbol{H}\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|, \\
M &= |U^{-1}N_2|.
\end{aligned}
$$

3.2.2.2 Turning point method

From (3.21), $S(x)$ can be written as

$$
S(x) = \frac{f(x)}{\sqrt{g(x)}},
$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U), \\ g(x) &= (\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x}) + (z_\gamma)^2\xi. \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$. Then

$$\begin{aligned} f(x) &= P_1^{-1}U^{-1}N_2x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\ \frac{\mathrm{d}f}{\mathrm{d}x} &= P_1^{-1}U^{-1}N_2, \\ g(x) &= P_1^{-2}x^2 + n^{-1} + (z_\gamma)^2\xi, \\ \frac{\mathrm{d}g}{\mathrm{d}x} &= 2P_1^{-2}x. \end{aligned}$$

Solving from $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f}{\sqrt{g}}\right)|_{x_t} = 0$, we have the turning point $x_t = \dfrac{P_1N_2(n^{-1} + (z_\gamma)^2\xi)}{n^{-1/2}N_1 + z_\gamma(U/\theta - 1)}$. The maximum value and the minimum value of $S(x)$ are therefore attained at either $x = a$ or $x = b$ or $x = x_t$. If $a < x_t < b$, then

$$\begin{aligned} L &= \min_{x\in(a,b)} S(x) = \min\{S(a), S(x_t), S(b)\}, \\ U &= \max_{x\in(a,b)} S(x) = \max\{S(a), S(x_t), S(b)\}, \end{aligned}$$

otherwise,

$$\begin{aligned} L &= \min_{x\in(a,b)} S(x) = \min\{S(a), S(b)\}, \\ U &= \max_{x\in(a,b)} S(x) = \max\{S(a), S(b)\}. \end{aligned}$$

For the special case of $(a, b) = (-\infty, \infty)$,

$$h(-\infty) = \lim_{x\to-\infty} h(x) = -U^{-1}N_2,$$
$$h(\infty) = \lim_{x\to\infty} h(x) = U^{-1}N_2.$$

then

$$\begin{aligned} L &= \min_{x\in(-\infty,\infty)} S(x) = \min\left\{-|U^{-1}N_2|, S(x_t)\right\}, \\ M &= \max_{x\in(-\infty,\infty)} S(x) = \max\left\{|U^{-1}N_2|, S(x_t)\right\} \end{aligned}$$

3.2.3 Numerical examples

Example 3.3.

For the data set given in Table 2.1 on how systolic blood pressure (Y) changes with age (x) for a group of forty males, we only consider the bands UV and TT. For two cases $1-\alpha = 0.90$, $\gamma = 0.75$ and $1-\alpha = 0.95$, $\gamma = 0.99$, by using the methods introduced above in this section, we calculate the critical constants c_1 and c_2 of UV and TT over $x \in (18, 70)$ and $x \in (1, 100)$ and provide them in the following Table 3.3 and Table 3.4. In these tables, for each asymmetric band, we also provide c value which is the critical constant of corresponding symmetric band. For any given x, the width of UVa is $(c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2(1/\theta^2 - 1)}$ and the width of UV is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2(1/\theta^2 - 1)}$ while the width of TTa is $(c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2/(2\nu)}$ and the width of TT is $2c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2/(2\nu)}$. Therefore the percentage of improvement of the average widths from a symmetric band to the corresponding asymmetric band is

$$\text{Percentage} = 100[1 - (c_1 + c_2)/(2c)]\%.$$

Table 3.3: Critical constants for simultaneous confidence bands UVa and UV and the percentage of improvement

	$1-\alpha = 0.90, \quad \gamma = 0.75$					
Interval	$-c_2$	c_1	$c_1 + c_2$	c	$2c$	Percentage
(18,70)	-2.2116	2.1213	4.3329	2.1700	4.3400	0.16%
(1,100)	-2.2415	2.1567	4.3991	2.2026	4.4052	0.14%
	$1-\alpha = 0.99, \quad \gamma = 0.95$					
Interval	$-c_2$	c_1	$c_1 + c_2$	c	$2c$	
(18,70)	-3.5438	2.6848	6.2286	3.3516	6.7032	7.62%
(1,100)	-3.5514	2.8522	6.4036	3.4000	6.8000	6.19%

Table 3.4: Critical constants for simultaneous confidence bands TTa and TT and the percentage of improvement

Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	Percentage
	$1-\alpha=0.90,\quad \gamma=0.75$					
(18,70)	-2.2424	2.0890	4.3314	2.1708	4.3416	0.24%
(1,100)	-2.2702	2.1271	4.3973	2.2034	4.4068	0.22%
	$1-\alpha=0.99,\quad \gamma=0.95$					
Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	
(18,70)	-3.5491	2.6874	6.2365	3.3558	6.7116	7.62%
(1,100)	-3.5567	2.8538	6.4105	3.4033	6.8066	6.18%

Example 3.4.

For the data set given in Table 2.3 on how speed (Y) in miles per hour changes with the size(x) in inches of a rocket engine's orifice, we also consider two cases: $1-\alpha=0.90$, $\gamma=0.75$ and $1-\alpha=0.95$, $\gamma=0.99$ and give Table 3.5 and Table 3.6.

Table 3.5: Critical constants for simultaneous confidence bands UVa and UV and the percentage of

Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	Percentage
	$1-\alpha=0.90,\quad \gamma=0.75$					
(1.2931, 1.4131)	-2.4315	2.1853	4.6167	2.3191	4.6382	0.47%
	$1-\alpha=0.99,\quad \gamma=0.95$					
Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	
(1.2931, 1.4131)	-4.3237	2.7398	7.0635	4.1268	8.2536	16.85%

Table 3.6: Critical constants for simultaneous confidence bands TTa and TT and the percentage of

Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	Percentage
	$1-\alpha=0.90,\quad \gamma=0.75$					
(1.2931, 1.4131)	-2.4344	2.1873	4.6216	2.3213	4.6426	0.45%
	$1-\alpha=0.99,\quad \gamma=0.95$					
Interval	$-c_2$	c_1	c_1+c_2	c	$2c$	
(1.2931, 1.4131)	-4.3440	2.7440	7.0880	4.1425	8.2850	16.89%

From these two examples, we can see the asymmetric bands UVa and TTa perform better than the corresponding symmetric bands UV and TT as expected.

3.3 Comparison of the symmetric and asymmetric confidence bands under the average width criterion

To compare different asymmetric bands, we also use the average width criterion which has been introduced in Chapter 2. It is clear that, for a given x, the width of the band in (3.1) is

$$(c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi},$$

where c_1 and c_2 are the critical constants to give confidence level $1 - \alpha$. From (2.52), the average width of the band over a specific interval $x \in (a, b)$ is given by

$$\int_a^b (c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}\ dx/(b - a). \tag{3.24}$$

It is noteworthy that each symmetric band is a special case of the corresponding asymmetric band with $c_1 = c_2$.

Specifically, we consider the case that $a = \bar{x} - \delta$ and $b = \bar{x} + \delta$, i.e., the interval (a, b) is symmetric about $\bar{x}$. Denote $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ and $ss = \delta/\sqrt{S_{xx}}$. Note that for a simultaneous confidence band, the critical constants c_1 and c_2 depend only on ss, γ, n and $1 - \alpha$. Therefore, the average width of this band also depends only on ss, γ, n and $1 - \alpha$. When the design points $x_1, \cdots, x_n$ are given, $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ is fixed. So a large value of δ means a wide interval (a, b). In our numerical comparison, we have used α= 0.10, 0.01, γ = 0.75, 0.95, n= 10, 20, 30, 50, 100 and ss = 0.1, 0.5, 1.0, 10, 50 and investigated all the combinations of these four factors for the bands TBE, TT, UV, $TBEa$, TTa, and UVa.

When $\bar{x} = 0$, i.e., the x-values $(x_1, \cdots, x_n)$ are mean adjusted, (3.24) is further equal to

$$\begin{aligned}
&\int_{-\delta}^{\delta} (c_1 + c_2)\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi}\ dx/(2\delta) \\
= &\int_{-\delta}^{\delta} (c_1 + c_2)\hat{\sigma}/(2\delta)\sqrt{\frac{1}{n} + \frac{x^2}{S_{xx}} + (z_\gamma)^2\xi}\ dx \\
= &(c_1 + c_2)\hat{\sigma}\sqrt{S_{xx}}/(2\delta)\left[\left(\frac{1}{n} + (z_\gamma)^2\xi\right)\ln\left(\frac{\delta}{\sqrt{S_{xx}}} + \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2\xi}\right)\right. \\
&\left. -\frac{1}{2}\left(\frac{1}{n} + (z_\gamma)^2\xi\right)\ln\left(\frac{1}{n} + (z_\gamma)^2\xi\right) + \frac{\delta}{\sqrt{S_{xx}}}\sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2\xi}\right].
\end{aligned} \tag{3.25}$$

Recall that for notational convenience, we use the following labels for the bands to be compared:

- *TBE* – the symmetric band in (2.5) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ and $\xi = 0$;

- *TBEa* – the asymmetric band in (3.5) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ and $\xi = 0$;

- *UV* – the symmetric band in (2.31) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = 1/\theta^2 - 1$;

- *UVa* – the asymmetric band in (3.15) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = 1/\theta^2 - 1$;

- *TT* – the symmetric band in (2.32) with $\theta = \frac{4\nu - 1}{4\nu}$ and $\xi = \frac{1}{2\nu}$;

- *TT* – the asymmetric band in (3.16) with $\theta = \frac{4\nu - 1}{4\nu}$ and $\xi = \frac{1}{2\nu}$.

In Chapter 2, we recommend the symmetric bands TBE, TT and UV among the six symmetric bands. In this section, we present numerical comparisons of the bands TBE, TT, UV, $TBEa$, TTa and UVa under the average width criterion. From (3.25), we can calculate the average width of each band and so the ratio of the average widths of any two bands. The ratios of the average bandwidths of TBE, TT, UV, $TBEa$, TTa relative to UV are given in Tables 3.7-3.10.

Note that a smaller entry in the tables means a narrower and so better band. It is clear from the table that an asymmetric band is always no worse than the corresponding symmetric band. From the definition of $ss = \delta/\sqrt{S_{xx}}$, a smaller value of ss means the interval (a, b) is narrower. From Tables 3.7-3.10, we can conclude that when ss is small, i.e., when the interval (a, b) is narrow, $TBEa$ tends to be the best one among the six bands. When ss is large, i.e, the interval (a, b) is wide, UVa is the best, but $TBEa$ can perform very badly. For example, from Table 3.8, we can see $TBEa$ is about 30% wider than UVa when $1 - \alpha = 0.99$, $\gamma = 0.95$ and $ss = 50$. Among the three asymmetric bands, UVa and TTa have hardly any difference between them and are almost always better than $TBEa$. Hence either UVa or TTa are recommended overall if the average band width is of concern.

Table 3.7: Ratios of the average widths of the bands TBE, TT , UV, $TBEa$ and TTa relative to UVa ($1-\alpha=0.90$, $\gamma=0.95$)

n	ss	TBE	TT	UV	$TBEa$	TTa	UVa
	0.1	0.9888	1.0393	1.0402	0.9886	0.9998	1
	0.5	1.0142	1.0446	1.0483	1.0126	0.9991	1
10	1.0	1.1193	1.0391	1.0394	1.1179	0.9999	1
	10.0	1.3171	1.0220	1.0185	1.3159	1.0035	1
	50.0	1.3222	1.0197	1.0160	1.3210	1.0038	1
	0.1	0.9839	1.0110	1.0112	0.9836	0.9999	1
	0.5	1.0603	1.0133	1.0136	1.0598	0.9998	1
20	1.0	1.1792	1.0123	1.0117	1.1786	1.0007	1
	10.0	1.3143	1.0065	1.0048	1.3138	1.0018	1
	50.0	1.3175	1.0060	1.0042	1.3170	1.0018	1
	0.1	0.9805	1.0071	1.0072	0.9802	0.9999	1
	0.5	1.0933	1.0072	1.0072	1.0930	1.0000	1
30	1.0	1.2067	1.0061	1.0056	1.2064	1.0005	1
	10.0	1.3114	1.0037	1.0025	1.3113	1.0012	1
	50.0	1.3137	1.0034	1.0022	1.3135	1.0012	1
	0.1	0.9777	1.0032	1.0033	0.9773	0.9999	1
	0.5	1.1361	1.0039	1.0037	1.1359	1.0002	1
50	1.0	1.2346	1.0031	1.0027	1.2344	1.0005	1
	10.0	1.3081	1.0016	1.0009	1.3080	1.0007	1
	50.0	1.3096	1.0015	1.0008	1.3095	1.0007	1
	0.1	0.9838	1.0019	1.0020	0.9835	1.0000	1
	0.5	1.1892	1.0018	1.0017	1.1889	1.0001	1
100	1.0	1.2614	1.0013	1.0010	1.2611	1.0003	1
	10.0	1.3054	1.0006	1.0003	1.3052	1.0004	1
	50.0	1.3062	1.0005	1.0002	1.3059	1.0003	1

Table 3.8: Ratios of the average widths of the bands TBE, TT , UV, $TBEa$ and TTa relative to UVa ($1-\alpha=0.99$, $\gamma=0.95$)

n	ss	TBE	TT	UV	$TBEa$	TTa	UVa
	0.1	1.2356	1.3159	1.3168	0.9904	0.9998	1
	0.5	1.2860	1.2612	1.2612	1.0319	0.9993	1
10	1.0	1.3886	1.1897	1.1879	1.1226	1.0003	1
	10.0	1.5509	1.0989	1.0925	1.2848	1.0038	1
	50.0	1.5501	1.0917	1.0851	1.2891	1.0043	1
	0.1	1.1120	1.1706	1.1709	0.9868	0.9999	1
	0.5	1.2252	1.1297	1.1295	1.0883	0.9998	1
20	1.0	1.3426	1.0977	1.0966	1.1947	1.0004	1
	10.0	1.4575	1.0603	1.0576	1.3033	1.0018	1
	50.0	1.4572	1.0569	1.0541	1.3038	1.0017	1
	0.1	1.0679	1.1166	1.1168	0.9878	0.9999	1
	0.5	1.2186	1.0852	1.0853	1.1274	1.0000	1
30	1.0	1.3298	1.0658	1.0651	1.2316	1.0006	1
	10.0	1.4210	1.0439	1.0422	1.3188	1.0010	1
	50.0	1.4207	1.0415	1.0398	1.3191	1.0010	1
	0.1	1.0376	1.0703	1.0704	0.9909	0.9999	1
	0.5	1.2269	1.0465	1.0464	1.1719	1.0000	1
50	1.0	1.3243	1.0376	1.0372	1.2655	1.0003	1
	10.0	1.3895	1.0255	1.0246	1.3290	1.0006	1
	50.0	1.3899	1.0244	1.0236	1.3294	1.0007	1
	0.1	1.0263	1.0311	1.0312	1.0045	0.9999	1
	0.5	1.2556	1.0194	1.0192	1.2293	1.0002	1
100	1.0	1.3287	1.0165	1.0161	1.3011	1.0003	1
	10.0	1.3710	1.0126	1.0122	1.3428	1.0003	1
	50.0	1.3714	1.0122	1.0118	1.3431	1.0004	1

Table 3.9: Ratios of the average widths of bands relative to Band UVa ($1-\alpha = 0.90$, $\gamma = 0.75$)

n	ss	TBE	TT	UV	$TBEa$	TTa	UVa
	0.1	0.9956	1.0096	1.0099	0.9955	0.9999	1
	0.5	0.9993	1.0122	1.0124	0.9978	0.9999	1
10	1.0	1.0264	1.0098	1.0093	1.0242	1.0005	1
	10.0	1.0608	1.0052	1.0038	1.0598	1.0015	1
	50.0	1.0614	1.0046	1.0033	1.0605	1.0016	1
	0.1	0.9937	1.0032	1.0033	0.9936	0.9999	1
	0.5	1.0115	1.0035	1.0034	1.0108	1.0001	1
20	1.0	1.0366	1.0035	1.0032	1.0362	1.0004	1
	10.0	1.0581	1.0018	1.0012	1.0580	1.0006	1
	50.0	1.0586	1.0017	1.0011	1.0585	1.0006	1
	0.1	0.9925	1.0019	1.0019	0.9924	0.9999	1
	0.5	1.0188	1.0023	1.0022	1.0184	1.0001	1
30	1.0	1.0404	1.0019	1.0016	1.0401	1.0003	1
	10.0	1.0568	1.0012	1.0008	1.0567	1.0004	1
	50.0	1.0570	1.0011	1.0007	1.0569	1.0003	1
	0.1	0.9917	1.0011	1.0011	0.9941	1.0000	1
	0.5	1.0281	1.0015	1.0014	1.0278	1.0001	1
50	1.0	1.0461	1.0012	1.0011	1.0457	1.0002	1
	10.0	1.0571	1.0007	1.0004	1.0570	1.0003	1
	50.0	1.0573	1.0006	1.0003	1.0572	1.0003	1
	0.1	0.9924	1.0012	1.0013	0.9921	1.0000	1
	0.5	1.0367	1.0008	1.0007	1.0366	1.0001	1
100	1.0	1.0487	1.0005	1.0004	1.0486	1.0001	1
	10.0	1.0552	1.0003	1.0002	1.0551	1.0001	1
	50.0	1.0553	1.0002	1.0001	1.0552	1.0001	1

Table 3.10: Ratios of the average widths of bands relative to Band UVa ($1-\alpha = 0.99$, $\gamma = 0.75$)

n	ss	TBE	TT	UV	$TBEa$	TTa	UVa
	0.1	1.0885	1.1287	1.1290	0.9957	0.9999	1
	0.5	1.0753	1.0941	1.0943	0.9997	0.9999	1
10	1.0	1.0870	1.0718	1.0714	1.0207	1.0002	1
	10.0	1.1001	1.0439	1.0422	1.0519	1.0013	1
	50.0	1.0985	1.0413	1.0396	1.0524	1.0011	1
	0.1	1.0376	1.0619	1.0620	0.9944	0.9999	1
	0.5	1.0478	1.0416	1.0413	1.0105	1.0000	1
20	1.0	1.0661	1.0331	1.0328	1.0333	1.0002	1
	10.0	1.0784	1.0209	1.0202	1.0518	1.0007	1
	50.0	1.0779	1.0200	1.0192	1.0521	1.0007	1
	0.1	1.0185	1.0381	1.0381	0.9938	0.9999	1
	0.5	1.0433	1.0273	1.0272	1.0187	1.0001	1
30	1.0	1.0598	1.0218	1.0215	1.0385	1.0002	1
	10.0	1.0687	1.0133	1.0130	1.0520	1.0003	1
	50.0	1.0684	1.0126	1.0123	1.0521	1.0003	1
	0.1	1.0070	1.0208	1.0208	0.9940	1.0000	1
	0.5	1.0407	1.0153	1.0152	1.0294	1.0002	1
50	1.0	1.0564	1.0128	1.0126	1.0467	1.0002	1
	10.0	1.0642	1.0091	1.0088	1.0564	1.0002	1
	50.0	1.0642	1.0089	1.0086	1.0565	1.0003	1
	0.1	1.0037	1.0109	1.0109	0.9958	1.0000	1
	0.5	1.0453	1.0066	1.0066	1.0395	1.0001	1
100	1.0	1.0561	1.0052	1.0051	1.0511	1.0001	1
	10.0	1.0615	1.0040	1.0039	1.0575	1.0001	1
	50.0	1.0615	1.0039	1.0038	1.0576	1.0001	1

3.4 Example

To understand the degradation over time of a drug product, stability studies are routinely carried out in the pharmaceutical industry. *Guideline for Stability Testing ICHQ1*, which is harmonized among the US, the EU and Japan, can be viewed at http://www.ich.org/products /guidelines/quality/article/quality-guidelines.html. These studies usually consist of a random sample of dosage units (e.g., tablets, capsules, vials) from a given batch stored under controlled temperature and humidity conditions. Individual dosage units are taken at predetermined time points and assayed for the active pharmaceutical ingredient (drug) content. One frequently used statistical model is the simple linear regression of drug content (Y) on time (x): $Y = \beta_0 + \beta_1 x + e$. For illustration, let us consider the observations on the first batch of Experiment One in Ruberg and Hsu (1992): $(x_1, \ldots, x_9) = (0.014, 0.280, 0.514, 0.769, 1.074, 1.533, 2.030, 3.071, 4.049)$ (in years) and $(Y_1, \ldots, Y_9) = (100.4, 100.3, 99.7, 99.2, 98.9, 98.2, 97.3, 95.7, 94.5)$ (in percentage). The usual model diagnostic including residual plots shows that the nine observed data points are nicely fitted by a linear regression line with $R^2 = 0.9961$. Note that, so long as the data are assumed to follow a standard linear regression model, the methods proposed in this paper apply to any sample size $n \geq 3$.

Here $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ is the dividing drug content level at time point x, above which $100(1-\gamma)\%$ of all the dosage units are and below which the other $100\gamma\%$ of all the dosage units are. It is reasonable to expect from patients' point of view that a large proportion, $1-\gamma$, of all the dosage units should have drug content level above a prespecified threshold h. It is therefore of interest to learn how $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ changes over time x (for a small value γ, $\gamma = 0.05$ say) and to learn whether or when $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ is above or below the threshold h (e.g., for a hypothetic value $h = 98$). A simultaneous confidence band for $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma$ can help us to learn these. As the expiry date required by the United States Food and Drug Administration (FDA) to be printed on the package label of the drug is often no longer than two years, it is reasonable to set the time interval $(a, b) = (0, 2)$.

We have written a suite of MATLAB programs, with the inputs $\boldsymbol{Y}$, $\boldsymbol{X}$, (a, b), γ and $1-\alpha$, to compute all the simultaneous confidence bands considered in Sections 2 and 3 and their average band widths. For the given $\boldsymbol{Y}$, $\boldsymbol{X}$, $(a, b) = (0, 2)$, $\gamma = 0.05$ and $1-\alpha = 0.95$, Table 3.11 shows ratios of average band widths among: (i) the conservative symmetric bands $TBEc$, TTc and UVc using the conservative critical constants over $(a, b) = (-\infty, \infty)$ by using the methods given in Turner and Bowden (1977) and Thomas and Thomas (1986), (ii) the symmetric bands TBE, TT and UV using the exact critical constants over $(a, b) = (0, 2)$ by using the methods given in this paper and (iii) the asymmetric bands $TBEa$, TTa and UVa using the exact critical constants over $(a, b) = (0, 2)$ by using the methods given in this paper. For example, the

Table 3.11: Ratios of the average band widths

Bands	Ratio	Bands	Ratio	Bands	Ratio
$\frac{TBEc}{TBE}$	1.015	$\frac{TTc}{TT}$	1.093	$\frac{UVc}{UV}$	1.097
$\frac{TBE}{TBEa}$	1.063	$\frac{TT}{TTa}$	1.156	$\frac{UV}{UVa}$	1.156
$\frac{TBEc}{TBEa}$	1.079	$\frac{TTc}{TTa}$	1.264	$\frac{UVc}{UVa}$	1.268

entry 1.264 means that the conservative symmetric band TTc, which is from Thomas and Thomas (1986), is 26.4% wider than the new asymmetric band TTa. It is clear from the table that the asymmetric bands are often substantially narrower in terms of average band width than the corresponding exact symmetric bands, and even much narrower than the corresponding conservative symmetric bands considered previously in the literature. Our computation for other data sets shows that the asymmetric bands can be narrower than the corresponding exact and conservative symmetric bands by more than the numbers given in Table 3.11. It is clear from the comparison in Section 3.3 and this example that the asymmetric bands UVa or TTa should always be used in order to reduce the average band width.

In Figure 1, the estimated percentile line $\boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma \hat{\sigma}/\theta$, where θ is for the UV band, is shown by the dashed line, the asymmetric band UVa is given by the solid lines, and the conservative symmetric band TTc is given by the broken lines. The UVa band is contained completely inside, and much narrower than, the conservative symmetric band TTc which was recommended in Thomas and Thomas (1986) and claimed as the best band in the literature. For the given $h = 98$, which is given by the dotted line in Figure 1, one can infer from the UVa band that, up to time point $x = 1.326$, the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ is above h and so at least $1-\gamma$ proportion of all the dosage units have drug content above h by this time point. But beyond the time point $x = 1.591$, the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ is below h and so less than $1-\gamma$ proportion of all the dosage units have drug content above h. The time point x at which $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma = h$ can be any where in the interval $(1.326, 1.591)$. The confidence interval for this x from the conservative symmetric band TTc is given by $(1.322, 1.656)$, which is wider than the interval $(1.326, 1.591)$ as expected.

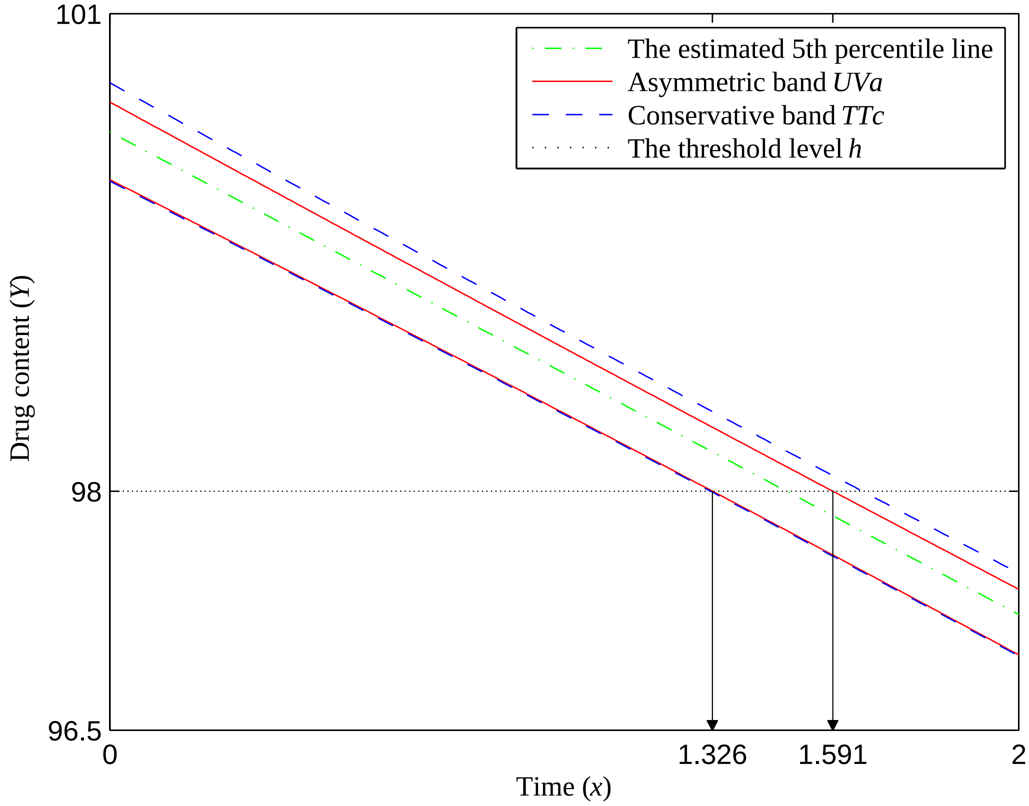


Figure 3.1: *The 95% conservative symmetric band TTc and asymmetric band UVa for the 5th percentile line*

3.5 Conclusions

In this chapter, we have proposed the methods of constructing exact asymmetric simultaneous confidence bands. From results of the thorough comparison and the real example, it is concluded that asymmetric bands are uniformly and can be very substantially narrower than the corresponding exact symmetric bands when $\gamma \neq 0.5$. Therefore, the asymmetric bands should always be used under the average band width criterion.

Chapter 4

One-sided Simultaneous Confidence Bands for a Percentile Line and One-sided Tolerance Bands for the Simple Linear Model

4.1 Introduction

4.1.1 One-sided simultaneous confidence bands

Sometimes, we want to bound the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ from one-side only, either from below or from above. In this case, it is not efficient to use a two-sided band which bounds the percentile line from both sides. One-sided bands are suitable for one-sided inferences. Consider the simple linear regression model given in (1.3). A $1-\alpha$ one-sided lower confidence band $LC(\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{x})$ for the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ over the interval $x \in (a, b)$ satisfies the condition

$$P\{LC(\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{x}) \leq \boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \text{ for all } x \in (a, b)\} = 1 - \alpha, \tag{4.1}$$

and a one-sided upper simultaneous confidence band $UC(\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{x})$ satisfies the condition

$$P\{\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \leq UC(\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{x}) \text{ for all } x \in (a, b)\} = 1 - \alpha. \tag{4.2}$$

In this chapter, we focus on one-sided simultaneous confidence bands for the percentile line $\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma$ over the interval $x \in (a, b)$ of three forms below: Form I, II and III

A one-sided upper band of Form I is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a, b). \tag{4.3}$$

A one-sided upper band of Form II uses constant $\theta \neq 0$ and $\xi \neq 0$ and is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \text{ for all } x \in (a, b). \tag{4.4}$$

A one-sided upper band of Form III is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + c\hat{\sigma}\left(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right) \text{ for all } x \in (a, b). \tag{4.5}$$

Form I and III have been considered by Turner and Bowden (1979) and Odeh and Mee (1990) respectively. They investigated the bands over covariate intervals which are all symmetric about the mean value $\bar{x}$. We consider one-sided confidence bands over any given covariate interval (a, b).

Similarly, a lower band of Form I is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \geq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a, b). \tag{4.6}$$

A lower band of Form II uses constant $\theta \neq 0$ and $\xi \neq 0$ and is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \geq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2\xi} \text{ for all } x \in (a, b). \tag{4.7}$$

A lower band of Form III is given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma \sigma \geq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + c\hat{\sigma}\left(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right) \text{ for all } x \in (a, b). \tag{4.8}$$

Even though a $1 - \alpha$ upper band of any one of these three forms uses a different critical constant from the corresponding $1 - \alpha$ lower band, the methodologies of construction and computation of the lower band and the upper band are similar. We just look up the upper bands in the following sections.

4.1.2 One-sided simultaneous tolerance bands

Let $Y(\boldsymbol{x}) = \boldsymbol{x}'\boldsymbol{\beta} + e_x$ denote a future observation with $e_x \sim N(0, \sigma^2)$ being independent of e in (1.1). Suppose one has the training data set $\mathcal{E} := \{(x_j, y_j), j = 1, \cdots, n\}$ which is used to fit a regression line of Y on x. A $(p, 1 - \alpha)$ lower simultaneous tolerance band $L(x; \mathcal{E})$ for the simple linear model $\boldsymbol{x}'\boldsymbol{\beta} + e$ over $x \in (a, b)$ satisfies the condition

$$P_{\mathcal{E}}\{P_{Y(x)}\{L(x; \mathcal{E}) < Y(x) | \mathcal{E}, x\} \geq p \text{ for all } x \in (a, b)\} = 1 - \alpha, \tag{4.9}$$

while a one-sided upper simultaneous tolerance band $L(x; \mathcal{E})$ satisfies the condition

$$P_{\mathcal{E}}\{P_{Y(x)}\{Y(x) < U(x; \mathcal{E}) | \mathcal{E}, x\} \geq p \text{ for all } x \in (a, b)\} = 1 - \alpha, \tag{4.10}$$

Note that $\Phi(z_\gamma) = \gamma$, we can write (4.9) as

$$P\{L(x;\mathcal{E}) \le \boldsymbol{x}'\boldsymbol{\beta} + z_{(1-p)}\sigma \text{ for all } x \in (a,b)\} = 1-\alpha. \tag{4.11}$$

It is clear from (4.1) and (4.11) that $L(x;\mathcal{E})$ is just a $1-\alpha$ lower confidence band for the $(1-p)$-percentile line. Similarly, we can write (4.10) as

$$P\{\boldsymbol{x}'\boldsymbol{\beta} + z_p\sigma \le U(x;\mathcal{E}) \text{ for all } x \in (a,b)\} = 1-\alpha. \tag{4.12}$$

From (4.2) and (4.12), we can get $U(x;\mathcal{E})$ is just a $1-\alpha$ upper confidence band for the p-percentile line. Therefore, we only need to look at the one-sided confidence bands.

4.2 One-sided bands of Form I

In this section, we focus on Form I. In Section 4.3 and Section 4.4, we will study Form II and III respectively, since mathematical treatments of these two forms are slightly different. The constant $\theta \neq 0$ in (4.3) can be chosen to give different specific confidence bands and the critical constant c is determined to satisfy the specified confidence level $1-\alpha$ for given $\theta \neq 0$. We consider three different bands: SBo, $TBUo$ and $TBEo$. All of them are of Form I given in (4.3).

The band SBo is the one-sided version of the two-sided band SB in (2.3) with $\theta = 1$ and has the form

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + z_\gamma\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b). \tag{4.13}$$

The band $TBUo$ is the one-sided version of the two-sided band TBU in (2.4) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b). \tag{4.14}$$

The band $TBEo$ is the one-sided version of the two-sided band TBE in (2.5) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}$ and given by

$$\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu-1}{2})}}\hat{\sigma} + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}, \text{ for all } x \in (a,b). \tag{4.15}$$

Next, we consider the computation of the critical constant c of the band (4.3). For this, it is necessary to find an expression of the simultaneous confidence level of the band that is amenable to computation.

The simultaneous confidence level of this band is given by

$$\begin{aligned}
& P\left\{\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + \frac{z_\gamma}{\theta}\hat\sigma + c\hat\sigma\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat\sigma/\theta - \sigma)}{\hat\sigma\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_\gamma(\hat\sigma/\theta - \sigma)}{\hat\sigma\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N} + z_\gamma(\hat\sigma/\theta - \sigma)}{\hat\sigma\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \ge -c\right\} \qquad (4.16) \\
= \; & P\left\{-\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})}} \le c\right\},
\end{aligned}$$

where the matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$$

is the unique square root of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ and defined in (1.5),

$$\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$$

and $U = \hat\sigma/\sigma \sim \sqrt{\chi^2_\nu}$.

Note that $\boldsymbol{P}\boldsymbol{x} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}$ and so (4.16) is further equal to

$$\begin{aligned}
& P\left\{\min_{x\in(a,b)} \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \ge -c\right\} \\
= & \int_0^\infty f_{\frac{\hat\sigma}{\sigma}}(u) P\left\{\min_{x\in(a,b)} \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} N_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ N_2/u \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|} \ge -c\right\} du, \qquad (4.17)
\end{aligned}$$

where $f_{\frac{\hat\sigma}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

The numerical quadrature method and simulation method discussed in two-sided case can be used for one-sided case for computing the critical constant c. We recommend the projection method and the turning point method because they are faster.

4.2.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \min_{x\in(a,b)} \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix}' \begin{pmatrix} n_1/u + (1/\theta - 1/u)\sqrt{n}z_\gamma \\ n_2/u \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}x \end{pmatrix} \right\|},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (4.17) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{k(\boldsymbol{v})\geq -c \text{ for all } x\in(a,b)\}} dn_1 dn_2 du, \tag{4.18}$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Expression (4.18) involves a three-dimensional integration and can be used to compute the simultaneous confidence level for a given c via numerical quadrature. Also, for a given confidence level, the value of critical constant c can be found numerically using this method. Based on adaptive Simpson rule, the MATLAB built-in function `triplequad` can be used for any three-dimensional integration .

Our experience shows this method of computing the exact values of critical constant c takes substantially longer computation time than the simulation method introduced in the following section. The numerical quadrature method can however be used to cross check with the simulation method. The numerical integration method and the simulation method agree on all the results we have tried.

4.2.2 Simulation method

Let

$$S = \min_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})}}. \tag{4.19}$$

The simultaneous confidence level given in (4.16) is therefore given by

$$P\{-S \leq c\}$$

The constant c of the $1-\alpha$ simultaneous confidence band can be found in a similar way as in the last two chapters. We first generate independent standard bivariate normal random vectors $\boldsymbol{N}_i$ and variables $U_i \sim \sqrt{\chi^2_\nu/\nu}$, $i = 1, 2, \cdots, R$. Then we calculate

$$S_i = \min_{x\in(a,b)} \frac{(P\boldsymbol{x})'\boldsymbol{N}_i/U_i + z_\gamma(1/\theta - 1/U_i)}{\sqrt{(P\boldsymbol{x})'(P\boldsymbol{x})}}, \quad i = 1, \cdots, R.$$

Finally c is approximated by the $\langle(1-\alpha)R\rangle$th largest of the R replicates of $-S$: $-S_1, \cdots, -S_R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$. Next we give two computation methods for calculating S from $\boldsymbol{N}$ and U.

4.2.2.1 Projection method

From (4.19), we have

$$S = \min_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{Z}}{\|(\boldsymbol{Px})\|},$$

where

$$\boldsymbol{Z} = \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} = \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n}z_\gamma \\ N_2/U \end{pmatrix}.$$

Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$ and $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$. Then $\boldsymbol{Px}_1 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}a \end{pmatrix}$ and $\boldsymbol{Px}_2 = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}b \end{pmatrix}$. When x changes over the interval (a, b), $\boldsymbol{Px}$ forms a cone bounded by $\boldsymbol{Px}_1$ and $\boldsymbol{Px}_2$. If $-\boldsymbol{Z}$ belongs to the cone, then

$$S = \min_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{Z}}{\|\boldsymbol{Px}\|} = -\|\boldsymbol{Z}\|.$$

Otherwise,

$$\begin{aligned} S &= \min_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{Z}}{\|\boldsymbol{Px}\|} \\ &= \min\left\{\frac{(\boldsymbol{Px}_1)'\boldsymbol{Z}}{\|\boldsymbol{Px}_1\|}, \frac{(\boldsymbol{Px}_2)'\boldsymbol{Z}}{\|\boldsymbol{Px}_2\|}\right\}. \end{aligned}$$

Note that there exist non-zero coefficients λ and κ such that

$$\lambda\boldsymbol{Z} = \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1}\kappa \end{pmatrix}.$$

It is easy to get that

$$\lambda = n^{-1/2} {Z_1}^{-1}$$

and

$$\kappa = n^{-1/2} Z_1^{-1} Z_2 P_1.$$

If $a < \kappa < b$ and $\lambda < 0$, then the vector $-\boldsymbol{Z}$ lies inside the cone spanned by $\boldsymbol{Px}_1$ and $\boldsymbol{Px}_2$. Otherwise, the projection of $-\boldsymbol{Z}$ lies outside the cone.

For the special case of $(a, b) = (-\infty, \infty)$, note that

$$\frac{(\boldsymbol{Px}_1)'\boldsymbol{Z}}{\|\boldsymbol{Px}_1\|} = \lim_{a \to -\infty} \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} a \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n} z_\gamma \\ N_2/U \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} a \end{pmatrix} \right\|} = -N_2/U,$$

and

$$\frac{(\boldsymbol{Px}_2)'\boldsymbol{Z}}{\|\boldsymbol{Px}_2\|} = \lim_{b \to \infty} \frac{\begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} b \end{pmatrix}' \begin{pmatrix} N_1/U + (1/\theta - 1/U)\sqrt{n} z_\gamma \\ N_2/U \end{pmatrix}}{\left\| \begin{pmatrix} 1/\sqrt{n} \\ P_1^{-1} b \end{pmatrix} \right\|} = N_2/U.$$

Therefore,

$$S = \begin{cases} -\|\boldsymbol{Z}\|, & \text{if} \lambda < 0; \\ -|N_2/U|, & \text{if} \lambda > 0. \end{cases}$$

4.2.2.2 Turning point method

Denote $h(x) = \dfrac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})}}$. Then S in (4.19) can be written as

$$S = \min_{x \in (a,b)} h(x) = \min_{x \in (a,b)} \frac{f(x)}{\sqrt{g(x)}},$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U), \\ g(x) &= (\boldsymbol{Px})'(\boldsymbol{Px}). \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, then

$$\begin{aligned}
f(x) &= P_1^{-1}U^{-1}N_2x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\
\frac{\mathrm{d}f}{\mathrm{d}x} &= P_1^{-1}U^{-1}N_2, \\
g(x) &= P_1^{-2}x^2 + n^{-1}, \\
\frac{\mathrm{d}g}{\mathrm{d}x} &= 2P_1^{-2}x.
\end{aligned}$$

Solving from $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f}{\sqrt{g}}\right)|_{x_t} = 0$, we can find the turning point of the function $h(x)$ is $x_t = \dfrac{P_1N_2n^{-1}}{n^{-1/2}N_1 + z_\gamma(U\theta^{-1} - 1)}$. Therefore, if $a < x_t < b$, the minimum value of $h(x)$ is attained at either $x = a$ or b or x_t, otherwise, the minimum value of $h(x)$ is attained at either $x = a$ or b, i.e.,

$$S = \min_{x\in(a,b)} h(x) = \begin{cases} \min\{h(a), h(x_t), h(b)\}, & \text{if } a < x_t < b; \\ \min\{h(a), h(b)\}, & \text{if } x_t \leq a \text{ or } x_t \geq b. \end{cases}$$

For the special case of $(a, b) = (-\infty, \infty)$,

$$\begin{aligned}
h(-\infty) &= \lim_{x\to-\infty} h(x) = -N_2/U, \\
h(\infty) &= \lim_{x\to\infty} h(x) = N_2/U.
\end{aligned}$$

Hence

$$S = \min_{x\in(-\infty,\infty)} h(x) = \min\{-|N_2/U|, h(x_t)\}.$$

4.3 One-sided bands of Form II

Different from Section 4.2, in this section, we focus on the bands of Form II in (4.4) with $\xi \neq 0$. We consider three bands: Vo, UVo and TTo. All of them are of the form (4.4).

The band Vo is the one-sided version of the two-sided band V in (2.26) with $\theta = 1$ and $\xi = 1 - \frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2$, and given by

$$\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}}+z_\gamma\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2\left(1-\frac{2}{\nu}\left(\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\right)^2\right)} \text{ for all } x \in (a,b).$$

The band UV is the one-sided version of the two-sided band UV in (2.31) with $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = \frac{\nu}{2}\left(\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$, and given by

$$\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2(1/\theta^2-1)} \text{ for all } x \in (a,b).$$

The band TTo is the one-sided version of the two-sided band TT in (2.32) with $\theta = \frac{4\nu-1}{4\nu}$ and $\xi = \frac{1}{2\nu}$, and given by

$$\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{(4\nu-1)/(4\nu)}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2/(2\nu)}, \text{ for all } x \in (a,b).$$

Next we consider the computation of the critical constant c in the band (4.4). The simultaneous confidence level of this band is given by

$$\begin{aligned}
& P\left\{\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2\xi} \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})+z_\gamma(\hat{\sigma}/\theta-\sigma)}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2\xi}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})+z_\gamma(\hat{\sigma}/\theta-\sigma)}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})+(z_\gamma)^2\xi}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N}+z_\gamma(\hat{\sigma}/\theta-\sigma)}{\hat{\sigma}\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})+(z_\gamma)^2\xi}} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U+z_\gamma(1/\theta-1/U)}{\sqrt{(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}\boldsymbol{x})+(z_\gamma)^2\xi}} \ge -c\right\},
\end{aligned} \tag{4.20}$$

where the matrix $\boldsymbol{P}$ is defined in (1.5), $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0},\boldsymbol{I})$

and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$.

The confidence level given in (4.20) is further equal to

$$P\left\{\min_{x\in[a,b]} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|} \geq -c \right\}$$

$$= \int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{\min_{x\in[a,b]} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/u \\ (1/\theta - 1/u)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|} \geq -c \right\} du, \tag{4.21}$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

Next we give two different methods for computing the critical constant c.

4.3.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \min_{x\in[a,b]} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{n}/u \\ (1/\theta - 1/u)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|},$$

where $\boldsymbol{v} = (\boldsymbol{n}', u) = (n_1, n_2, u)'$. The simultaneous confidence level (4.21) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{k(\boldsymbol{v})\geq -c\}} d\boldsymbol{v}, \tag{4.22}$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Expression (4.22) involves a three-dimensional integration and can be used to compute the simultaneous confidence level via numerical integration. We have used the MATLAB built-in function `triplequad` for this purpose. Then the value of critical constant can be found numerically by searching for c so that the simultaneous confidence level is equal to $1 - \alpha$.

4.3.2 Simulation method

Let

$$S = \min_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi}}. \tag{4.23}$$

The simultaneous confidence level is therefore given by

$$P\{-S \le c\}.$$

The constant c of the $1-\alpha$ simultaneous confidence band is therefore the $100(1-\alpha)$ percentile of the random variable $-S$. This population percentile can be approximated by the sample percentile by using simulation in the following way. We first generate standard bivariate normal random vectors $\boldsymbol{N}_i$ and variables $U_i \sim \sqrt{\frac{\chi^2_\nu}{\nu}}$, $i = 1, 2, \cdots, R$. Then we calculate

$$S_i = \min_{x\in(a,b)} \frac{(P\boldsymbol{x})'\boldsymbol{N}_i/U_i + z_\gamma(1/\theta - 1/U_i)}{\sqrt{(P\boldsymbol{x})'(P\boldsymbol{x}) + (z_\gamma)^2\xi}}, \quad i = 1, \cdots, R.$$

Finally c is approximated by the $\langle(1-\alpha)R\rangle$th largest of the R replicates of $-S$: $-S_1, \cdots, -S_R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$. Next we give two computation methods for calculating S from $\boldsymbol{N}$ and U.

4.3.2.1 Projection method

S in (4.23) can also be expressed as

$$S = \min_{x\in[a,b]} \frac{\begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix}' \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}}{\left\| \begin{pmatrix} \boldsymbol{Px} \\ z_\gamma\sqrt{\xi} \end{pmatrix} \right\|}.$$

Denote $\boldsymbol{x}_1 = \begin{pmatrix} 1 \\ a \end{pmatrix}$, $\boldsymbol{x}_2 = \begin{pmatrix} 1 \\ b \end{pmatrix}$, $\boldsymbol{d}_1 = \begin{pmatrix} \boldsymbol{Px}_1 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$, $\boldsymbol{d}_2 = \begin{pmatrix} \boldsymbol{Px}_2 \\ z_\gamma\sqrt{\xi} \end{pmatrix}$ and the matrix $\boldsymbol{M} = (\boldsymbol{d}_1, \boldsymbol{d}_2)$. Let $\mathcal{L}(\boldsymbol{M})$ be the linear plane spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ and $\boldsymbol{H} = \boldsymbol{M}(\boldsymbol{M}'\boldsymbol{M})^{-1}\boldsymbol{M}'$ be the projection matrix to $\mathcal{L}(\boldsymbol{M})$. If the projection of the vector $-\begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, then

$$S = -\left\| \boldsymbol{H} \begin{pmatrix} \boldsymbol{N}/U \\ (1/\theta - 1/U)/\sqrt{\xi} \end{pmatrix} \right\|.$$

Otherwise,

$$
\begin{aligned}
S &= \min\left(\frac{\boldsymbol{d}_1'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\|\boldsymbol{d}_1\|}, \quad \frac{\boldsymbol{d}_2'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\|\boldsymbol{d}_2\|}\right)\\
&= \min\left(\frac{(\boldsymbol{Px}_1)'\boldsymbol{N}/U+z_\gamma(1/\theta-1/U)}{\sqrt{(\boldsymbol{Px}_1)'(\boldsymbol{Px}_1)+(z_\gamma)^2\xi}}, \quad \frac{(\boldsymbol{Px}_2)'\boldsymbol{N}/U+z_\gamma(1/\theta-1/U)}{\sqrt{(\boldsymbol{Px}_2)'(\boldsymbol{Px}_2)+(z_\gamma)^2\xi}}\right).
\end{aligned}
$$

Similar to Section 3.2.2.1, we have the following way to judge whether the projection of a given vector, $-\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}$ for example, belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ or not. Two non-zero coefficients λ and κ are given in (2.39) and (2.40) If and only if $a<\kappa<b$ and $\lambda<0$, the projection of the vector $-\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}$ to the plane $\mathcal{L}(\boldsymbol{M})$ belongs to the cone spanned by $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$.

For the special case of $x\in(-\infty,\infty)$, we have

$$
\frac{\boldsymbol{d}_1'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\|\boldsymbol{d}_1\|} = \lim_{a\to-\infty}\frac{\begin{pmatrix}1/\sqrt{n}\\P_1^{-1}a\end{pmatrix}'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\left\|\begin{pmatrix}1/\sqrt{n}\\P_1^{-1}a\end{pmatrix}\right\|} = -N_2/U,
$$

and

$$
\frac{(\boldsymbol{d}_2)'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\|\boldsymbol{d}_2\|} = \lim_{b\to\infty}\frac{\begin{pmatrix}1/\sqrt{n}\\P_1^{-1}b\end{pmatrix}'\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}}{\left\|\begin{pmatrix}1/\sqrt{n}\\P_1^{-1}b\end{pmatrix}\right\|} = N_2/U.
$$

Therefore,

$$
S = \begin{cases} -\left\|\boldsymbol{H}\begin{pmatrix}\boldsymbol{N}/U\\(1/\theta-1/U)/\sqrt{\xi}\end{pmatrix}\right\|, & \text{if}\lambda<0;\\ -|N_2/U|, \quad \text{if}\lambda>0. \end{cases}
$$

4.3.2.2 Turning point method

Denote

$$
h(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}/U+z_\gamma(1/\theta-1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})+(z_\gamma)^2\xi}}.
$$

Then S in (4.23) can be written as

$$S = \min_{x \in (a,b)} h(x) = \min_{x \in (a,b)} \frac{f(x)}{\sqrt{g(x)}},$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{Px})'\boldsymbol{N}/U + z_\gamma(1/\theta - 1/U), \\ g(x) &= (\boldsymbol{Px})'(\boldsymbol{Px}) + (z_\gamma)^2\xi. \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, and so

$$\begin{aligned} f(x) &= P_1^{-1}U^{-1}N_2x + U^{-1}n^{-1/2}N_1 + z_\gamma(\theta^{-1} - U^{-1}), \\ f'(x) &= P_1^{-1}U^{-1}N_2, \\ g(x) &= P_1^{-2}x^2 + n^{-1} + (z_\gamma)^2\xi, \\ g'(x) &= 2P_1^{-2}x. \end{aligned}$$

Solving from $\left(\frac{f}{\sqrt{g}}\right)'|_{x_t} = 0$, we have the turning point of $h(x)$ is $x_t = \dfrac{P_1N_2(n^{-1} + (z_\gamma)^2\xi)}{n^{-1/2}N_1 + z_\gamma(U/\theta - 1)}$. Therefore, if $a < x_t < b$, the minimum value of $h(x)$ is attained at either $x = a$ or b or x_t, otherwise, the minimum value of $h(x)$ is attained at either $x = a$ or b, i.e.,

$$S = \min_{x \in (a,b)} h(x) = \begin{cases} \min\{h(a), h(x_t), h(b)\}, & \text{if } \ a < x_t < b; \\ \min\{h(a), h(b)\}, & \text{if } \ x_t \le a \text{ or } x_t \ge b. \end{cases}$$

For the special case of $(a,b) = (-\infty, \infty)$,

$$h(-\infty) = \lim_{x \to -\infty} h(x) = -N_2/U,$$
$$h(\infty) = \lim_{x \to \infty} h(x) = N_2/U.$$

Hence

$$S = \min_{x \in (a,b)} h(x) \quad = \quad \min\left\{-|N_2/U|, h(x_t)\right\}.$$

4.4 One-sided bands of Form III

In this section, we focus on the band of Form III in (4.5) . The simultaneous confidence level of this band is given by

$$\begin{aligned}
& P\left\{\boldsymbol{x}'\boldsymbol{\beta} + z_\gamma\sigma \le \boldsymbol{x}'\hat{\boldsymbol{\beta}} + c\hat{\sigma}\left(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right) \text{ for all } x \in (a,b)\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) - z_\gamma\sigma}{\hat{\sigma}(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}})} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) - z_\gamma\sigma}{\hat{\sigma}(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}})} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\sigma\boldsymbol{N} - z_\gamma}{\hat{\sigma}(z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}})} \ge -c\right\} \\
= \; & P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U - z_\gamma/U}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \ge -c\right\}, \qquad (4.24)
\end{aligned}$$

where the matrix $\boldsymbol{P}$ is defined in (1.5), $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}_2(\boldsymbol{0}, \boldsymbol{I})$ and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu}$.

Note that (4.24) is further equal to

$$\int_0^\infty f_{\frac{\hat{\sigma}}{\sigma}}(u) P\left\{\min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U - z_\gamma}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \ge -c\right\} du,$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U and given in (1.4).

4.4.1 Numerical quadrature method

Denote

$$k(\boldsymbol{v}) = \min_{x\in(a,b)} \frac{(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}/U - z_\gamma}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}},$$

where $\boldsymbol{v} = (n_1, n_2, u)'$. The simultaneous confidence level (4.21) becomes

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f(\boldsymbol{v}) \boldsymbol{I}_{\{k(\boldsymbol{v}) \ge -c\}} d\boldsymbol{v}, \qquad (4.25)$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$ and is given in (2.9) and $\boldsymbol{I}_{\{A\}}$ is the index function of the set A. Thus, solving for c will require three dimensional numerical quadrature. We can use the MATLAB built-in function `triplequad` for this purpose. But we recommend the simulation method below, turning point method, rather than this numerical quadrature method, since the latter one takes much longer computation time than the former one.

4.4.2 Simulation method

Let

$$S = \min_{x \in (a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{N}/U - z_\gamma/U}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}}. \tag{4.26}$$

The simultaneous confidence level is given by

$$P\{-S \le c\}.$$

To approximate c, we first generate standard bivariate normal random vectors $\boldsymbol{N}_i$ and variables $U_i \sim \sqrt{\frac{\chi^2_\nu}{\nu}}$, $i = 1, 2, \cdots, R$. Then we calculate

$$S_i = \min_{x \in (a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{N}_i/U_i - z_\gamma/U_i}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}}., \quad i = 1, \cdots, R.$$

Finally c is approximated by the $\langle(1-\alpha)R\rangle$th largest of the R replicates of $-S$: $-S_1, \cdots, -S_R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$. Next we give the turning point method for calculating S from $\boldsymbol{N}$ and U.

4.4.2.1 Turning point method

Denote

$$h(x) = \frac{(\boldsymbol{Px})'\boldsymbol{N}/U - z_\gamma/U}{z_\gamma/2 + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}}.$$

Then S in (4.26) can be written as

$$S = \min_{x \in (a,b)} h(x) = \min_{x \in (a,b)} \frac{f(x)}{\sqrt{g(x)}},$$

where

$$\begin{aligned} f(x) &= (\boldsymbol{Px})'\boldsymbol{N}/U - z_\gamma/U, \\ g(x) &= z_\gamma/2 + \sqrt{(\boldsymbol{Px})'(\boldsymbol{Px})}. \end{aligned}$$

Note that $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$, $\boldsymbol{N} = \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$ and $\boldsymbol{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$, and so

$$\begin{aligned} f(x) &= P_1^{-1}U^{-1}N_2x + U^{-1}n^{-1/2}N_1 - z_\gamma U^{-1}, &(4.27)\\ f'(x) &= P_1^{-1}U^{-1}N_2, &(4.28)\\ g(x) &= z_\gamma/2 + \sqrt{P_1^{-2}x^2 + n^{-1}}, &(4.29)\\ g'(x) &= \frac{P_1^{-2}x}{\sqrt{P_1^{-2}x^2 + n^{-1}}}. &(4.30) \end{aligned}$$

The turning point(s) should be the root(s) of the equation

$$\left(\frac{f}{g}\right)' = 0. \tag{4.31}$$

Substituting (4.27) - (4.30) into (4.31) gives

$$N_2 z_\gamma/2\sqrt{n^{-1} + P_1^{-2}x^2} + N_2 n^{-1} = P_1^{-1}(n^{-1/2}N_1 - z_\gamma)x. \tag{4.32}$$

Square both sides of (4.32), we have

$$Ax^2 + Bx + C = 0, \tag{4.33}$$

where $A = P_1^{-2}[N_2^2(z_\gamma)^2/4 - n^{-1}N_1^2 + 2n^{-1/2}N_1 z_\gamma - (z_\gamma)^2]$, $B = 2P_1^{-1}N_2 n^{-1}(n^{-1/2}N_1 - z_\gamma)$ and $C = N_2^2 n^{-1}[(z_\gamma)^2/4 - n^{-1}]$. When $B^2 - AC > 0$, there are two roots of equation (4.33). When $B^2 - AC = 0$, there is only one root of equation (4.33). When $B^2 - AC < 0$, there is no root. Next, we just need to check whether there is/are any root(s) of the equation (4.33) belonging to the covariate interval (a, b). If so, the minimum value of $h(x)$ is then attained at either $x = a$ or $x = b$ or the root(s). Otherwise, the minimum value of $h(x)$ is then attained at either $x = a$ or $x = b$.

There is another idea of finding the turning point(s) of (4.31). Denote $y = P_1^{-1}x$. From (4.32), we have

$$\sqrt{y^2 + n^{-1}} = jy - l, \tag{4.34}$$

where $j = 2(N_1 N_2^{-1} n^{-1/2}/z_\gamma - 1/N_2)$ and $l = 2n^{-1}/z_\gamma$. Then the left-side of (4.34) is the positive part of the hyperbola $z^2 = y^2 + n^{-1}$ and the right-side of (4.34) is a straight line. When $|j| \le 1$, there is no root of (4.34). When $j > 1$ or $j < -1$, there is one root y_t of (4.34). Then we just need to check whether the root belongs to the interval $(P_1^{-1}a, P_1^{-1}b)$. If so, the minimum value of $h(x)$ is then attained at either $x = a$ or $x = b$ or $P_1 y_t$. Otherwise, the minimum value of $h(x)$ is then attained at either $x = a$ or $x = b$.

4.5 Comparison of the one-sided simultaneous bands under the average width criterion

To compare different one-sided simultaneous confidence bands, we use the average width criterion which has been introduced in Chapter 2. Here, we define the 'width' of a one-sided band as the distance between the band and the unbiased estimated line $\boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta_u}\hat{\sigma}$, where $\theta_u=\sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and so $\boldsymbol{x}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta_u}\hat{\sigma}$ is the uniformly minimum variance unbiased estimator of $\boldsymbol{x}'\boldsymbol{\beta}+z_\gamma\sigma$. Hence, for a given $\boldsymbol{x}_0=(1,x_0)'$, the width of the band of form (4.6) is taken as

$$\begin{aligned}&\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0}-\left(\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta_u}\hat{\sigma}\right)\\ = \; & z_\gamma\hat{\sigma}\left(\frac{1}{\theta}-\frac{1}{\theta_u}\right)+c\hat{\sigma}\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0}.\end{aligned}$$

The width of the band of form (4.7) is

$$\begin{aligned}&\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta}\hat{\sigma}+c\hat{\sigma}\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0+(z_\gamma)^2\xi}-\left(\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta_u}\hat{\sigma}\right)\\ = \; & z_\gamma\hat{\sigma}\left(\frac{1}{\theta}-\frac{1}{\theta_u}\right)+c\hat{\sigma}\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0+(z_\gamma)^2\xi}.\end{aligned}$$

The width of the band of form (4.8) is given by

$$\begin{aligned}&\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+c\hat{\sigma}\left(z_\gamma/2+\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0}\right)-\left(\boldsymbol{x}_0{}'\hat{\boldsymbol{\beta}}+\frac{z_\gamma}{\theta_u}\hat{\sigma}\right)\\ = \; & z_\gamma\hat{\sigma}\left(\frac{c}{2}-\frac{1}{\theta_u}\right)+c\hat{\sigma}\sqrt{\boldsymbol{x}_0{}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_0}.\end{aligned}$$

Hence, over a specific covariate interval $x\in(a,b)$, the average width of a band in (4.6) is given by

$$\int_a^b\left[z_\gamma\hat{\sigma}\left(\frac{1}{\theta}-\frac{1}{\theta_u}\right)+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right]\,dx/(b-a). \tag{4.35}$$

The average width of a band in (4.7) is given by

$$\int_a^b\left[z_\gamma\hat{\sigma}\left(\frac{1}{\theta}-\frac{1}{\theta_u}\right)+c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}+(z_\gamma)^2\xi}\right]\,dx/(b-a). \tag{4.36}$$

The average width of a band in (4.8) is given by

$$\int_a^b \left[z_\gamma \hat{\sigma} \left(\frac{c}{2} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \right] \, dx/(b-a) \tag{4.37}$$

$$= \hat{\sigma} z_\gamma \left(\frac{c}{2} - \frac{1}{\theta_u} \right) + \int_a^b c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \, dx/(b-a). \tag{4.38}$$

Specifically, we consider the case that $a = \bar{x} - \delta$ and $b = \bar{x} + \delta$, i.e., the interval (a, b) is symmetric about $\bar{x}$. Denote $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ and $ss = \delta/\sqrt{S_{xx}}$. Note that for a simultaneous confidence band, the critical constant c depends only on ss, γ, n and the confidence level $1 - \alpha$. Therefore, the average width of this band also depends only on ss, γ, n and $1 - \alpha$. When the design points $x_1, \cdots, x_n$ are given, $S_{xx} = \Sigma_{i=1}^n (x_i - \bar{x})^2$ is fixed. So a large value of δ means a wide interval (a, b). In our numerical comparison, we have used α= 0.10, 0.01, γ = 0.75, 0.95, n= 10, 20, 30, 50, 100 and ss = 0.1, 0.5, 1.0, 10, 50 and investigated all the combinations of these four factors for all the one-sided bands of Form I, II and III.

When $\bar{x} = 0$, i.e., the x-values $(x_1, \cdots, x_n)$ are mean adjusted and $(a, b) = (-\delta, \delta)$, (4.35) is further calculated to be

$$\begin{aligned}
&\int_{-\delta}^{\delta} \left[z_\gamma \hat{\sigma} \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \right] \, dx/(2\delta) \\
= &\int_{-\delta}^{\delta} z_\gamma \hat{\sigma}/(2\delta) \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) \, dx + \int_{-\delta}^{\delta} c\hat{\sigma}/(2\delta)\sqrt{\frac{1}{n} + \frac{x^2}{S_{xx}}} \, dx \\
= &\hat{\sigma} z_\gamma \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{S_{xx}}/(2\delta) \left[\frac{1}{n} \ln \left(\frac{\delta}{\sqrt{S_{xx}}} + \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n}} \right) \right. \\
&\left. + \frac{1}{2n} \ln n + \frac{\delta}{\sqrt{S_{xx}}} \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n}} \right],
\end{aligned} \tag{4.39}$$

(4.36) is equal to

$$\begin{aligned}
&\int_{-\delta}^{\delta} \left[z_\gamma \hat{\sigma} \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_\gamma)^2 \xi} \right] \, dx/(2\delta) \\
= &\int_{-\delta}^{\delta} z_\gamma \hat{\sigma}/(2\delta) \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) \, dx + \int_{-\delta}^{\delta} c\hat{\sigma}/(2\delta)\sqrt{\frac{1}{n} + \frac{x^2}{S_{xx}} + (z_\gamma)^2 \xi} \, dx \\
= &\hat{\sigma} z_\gamma \left(\frac{1}{\theta} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{S_{xx}}/(2\delta) \left[\left(\frac{1}{n} + (z_\gamma)^2 \xi \right) \ln \left(\frac{\delta}{\sqrt{S_{xx}}} + \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2 \xi} \right) \right. \\
&\left. - \frac{1}{2} \left(\frac{1}{n} + (z_\gamma)^2 \xi \right) \ln \left(\frac{1}{n} + (z_\gamma)^2 \xi \right) + \frac{\delta}{\sqrt{S_{xx}}} \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n} + (z_\gamma)^2 \xi} \right],
\end{aligned} \tag{4.40}$$

and (4.37) is equal to

$$\begin{aligned}
&\int_{-\delta}^{\delta} \left[z_\gamma \hat{\sigma} \left(\frac{c}{2} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \right] \, dx/(2\delta) \\
= &\int_{-\delta}^{\delta} z_\gamma \hat{\sigma}/(2\delta) \left(\frac{c}{2} - \frac{1}{\theta_u} \right) \, dx + \int_{-\delta}^{\delta} c\hat{\sigma}/(2\delta)\sqrt{\frac{1}{n} + \frac{x^2}{S_{xx}}} \, dx \\
= &\hat{\sigma} z_\gamma \left(\frac{c}{2} - \frac{1}{\theta_u} \right) + c\hat{\sigma}\sqrt{S_{xx}}/(2\delta) \left[\frac{1}{n} \ln \left(\frac{\delta}{\sqrt{S_{xx}}} + \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n}} \right) \right. \\
&\left. + \frac{1}{2n} \ln n + \frac{\delta}{\sqrt{S_{xx}}} \sqrt{\frac{\delta^2}{S_{xx}} + \frac{1}{n}} \right]. \qquad (4.41)
\end{aligned}$$

From (4.39) - (4.41), we can calculate the average width of each band and so the ratio of the average widths of any two bands. The ratios of the average bandwidths of SBo, $TBUo$, $TBEo$, Vo, TTo, OMo relative to UVo are given in Tables 4.1-4.4.

We want to choose a band with small entries in the tables. The smaller entries in the tables mean the corresponding band is narrower and so better. From the definition of $ss = \delta/\sqrt{S_{xx}}$, a smaller value of ss means the interval (a, b) is narrower. From Tables 4.1-4.4, we can conclude that if confidence level $1 - \alpha$ is chosen as 0.90 , UVo is the best among the seven bands. However, if we choose a bigger confidence level, 0.99 for example, OMo is the best among the seven bands.

To further compare the band OMo and UVo for the 95th percentile line, we choose three more different confidence level values: 0.95, 0.85, 0.80. We provide the ratios of the average bandwidths of OMo relative to UVo in Tables 4.5. From this table, it is clear that OMo performs better than UVo when we choose a big confidence level, 0.95 for example. However, UVo is better than UVo when confidence level is less than 0.85.

4.6 Conclusions

One-sided simultaneous confidence bands have been studied in this chapter. Methods have been given to compute the exact one-sided simultaneous confidence bands for the percentile line over a finite interval of the covariate x. It is observed that the exact bands can be much narrower than the corresponding conservative bands.

Table 4.1: Ratios of the average widths of bands relative to Band UVo ($1-\alpha = 0.90$, $\gamma = 0.95$)

n	ss	SBo	$TBUo$	$TBEo$	Vo	TTo	OMo	UVo
	0.1	0.9861	0.9869	0.9891	0.9991	0.9998	0.9915	1
	0.5	1.0155	1.0099	0.9992	0.9963	0.9993	0.9899	1
10	1.0	1.1453	1.1266	1.0867	1.0030	1.0005	1.0323	1
	10.0	1.3921	1.3415	1.2287	1.0299	1.0039	1.0372	1
	50.0	1.4025	1.3484	1.2267	1.0331	1.0038	1.0191	1
	0.1	0.9804	0.9813	0.9831	0.9990	0.9999	0.9867	1
	0.5	1.0585	1.0514	1.0366	0.9989	1.0000	1.0106	1
20	1.0	1.1790	1.1619	1.1267	1.0041	1.0005	1.0500	1
	10.0	1.3216	1.2874	1.2170	1.0176	1.0015	1.0376	1
	50.0	1.3259	1.2902	1.2165	1.0194	1.0016	1.0260	1
	0.1	0.9753	0.9762	0.9777	0.9990	0.9999	0.9818	1
	0.5	1.0832	1.0753	1.0597	1.0000	1.0000	1.0236	1
30	1.0	1.1926	1.1767	1.1449	1.0045	1.0005	1.0569	1
	10.0	1.2950	1.2675	1.2124	1.0136	1.0009	1.0375	1
	50.0	1.2972	1.2688	1.2116	1.0146	1.0009	1.0277	1
	0.1	0.9725	0.9729	0.9741	0.9990	1.0000	0.9785	1
	0.5	1.1176	1.1091	1.0930	1.0010	1.0002	1.0391	1
50	1.0	1.2063	1.1925	1.1651	1.0043	1.0004	1.0618	1
	10.0	1.2722	1.2513	1.2103	1.0097	1.0006	1.0364	1
	50.0	1.2733	1.2520	1.2097	1.0105	1.0006	1.0288	1
	0.1	0.9748	0.9747	0.9746	0.9991	0.9999	0.9770	1
	0.5	1.1565	1.1487	1.1337	1.0018	1.0001	1.0562	1
100	1.0	1.2182	1.2073	1.1854	1.0039	1.0002	1.0643	1
	10.0	1.2539	1.2397	1.2109	1.0068	1.0004	1.0349	1
	50.0	1.2542	1.2395	1.2103	1.0072	1.0002	1.0291	1

Table 4.2: Ratios of the average widths of bands relative to Band UVo ($1-\alpha = 0.99$, $\gamma = 0.95$)

n	ss	SBo	$TBUo$	$TBEo$	Vo	TTo	OMo	UVo
	0.1	0.9910	0.9909	0.9914	0.9995	0.9998	0.9978	1
	0.5	1.0783	1.0735	1.0628	0.9998	1.0004	1.0020	1
10	1.0	1.2429	1.2309	1.2027	1.0067	1.0019	0.9968	1
	10.0	1.5241	1.4946	1.4247	1.0275	1.0058	0.8355	1
	50.0	1.5353	1.5040	1.4296	1.0295	1.0059	0.7968	1
	0.1	0.9886	0.9886	0.9886	0.9996	0.9999	0.9972	1
	0.5	1.1344	1.1281	1.1142	1.0006	1.0001	1.0022	1
20	1.0	1.2865	1.2737	1.2455	1.0064	1.0012	0.9796	1
	10.0	1.4567	1.4329	1.3810	1.0168	1.0025	0.8325	1
	50.0	1.4621	1.4372	1.3831	1.0178	1.0026	0.8053	1
	0.1	0.9876	0.9875	0.9875	0.9995	0.9998	0.9963	1
	0.5	1.1677	1.1605	1.1462	1.0013	1.0003	1.0024	1
30	1.0	1.3036	1.2907	1.2647	1.0059	1.0008	0.9693	1
	10.0	1.4285	1.4077	1.3652	1.0131	1.0013	0.8353	1
	50.0	1.4320	1.4105	1.3665	1.0139	1.0013	0.8129	1
	0.1	0.9911	0.9910	0.9904	0.9996	0.9999	0.9964	1
	0.5	1.2095	1.2019	1.1871	1.0020	1.0001	0.9969	1
50	1.0	1.3202	1.3084	1.2850	1.0052	1.0006	0.9599	1
	10.0	1.4032	1.3863	1.3525	1.0091	1.0007	0.8430	1
	50.0	1.4050	1.3877	1.3530	1.0093	1.0009	0.8252	1
	0.1	1.0057	1.0050	1.0036	0.9996	0.9999	0.9987	1
	0.5	1.2539	1.2467	1.2328	1.0021	1.0002	0.9868	1
100	1.0	1.3304	1.3206	1.3016	1.0040	1.0003	0.9457	1
	10.0	1.3767	1.3642	1.3399	1.0060	1.0004	0.8537	1
	50.0	1.3777	1.3650	1.3403	1.0063	1.0004	0.8403	1

Table 4.3: Ratios of the average widths of bands relative to Band UVo ($1-\alpha=0.90$, $\gamma=0.75$)

n	ss	SBo	$TBUo$	$TBEo$	Vo	TTo	OMo	UVo
10	0.1	0.9942	0.9948	0.9966	0.9991	0.9999	0.9951	1
	0.5	0.9967	0.9965	0.9969	0.9983	0.9998	0.9975	1
	1.0	1.0279	1.0233	1.0134	1.0034	1.0005	1.0078	1
	10.0	1.0737	1.0583	1.0242	1.0147	1.0013	0.9945	1
	50.0	1.0753	1.0587	1.0217	1.0156	1.0011	0.9887	1
20	0.1	0.9920	0.9928	0.9945	0.9991	0.9999	0.9917	1
	0.5	1.0079	1.0066	1.0044	1.0001	1.0000	1.0039	1
	1.0	1.0327	1.0281	1.0189	1.0032	1.0003	1.0125	1
	10.0	1.0576	1.0478	1.0272	1.0091	1.0006	1.0037	1
	50.0	1.0585	1.0478	1.0263	1.0097	1.0006	1.0005	1
30	0.1	0.9909	0.9916	0.9931	0.9992	0.9999	0.9900	1
	0.5	1.0147	1.0131	1.0099	1.0010	1.0001	1.0090	1
	1.0	1.0367	1.0322	1.0237	1.0035	1.0002	1.0163	1
	10.0	1.0542	1.0461	1.0296	1.0070	1.0003	1.0074	1
	50.0	1.0547	1.0463	1.0289	1.0075	1.0003	1.0050	1
50	0.1	0.9895	0.9901	0.9915	0.9992	0.9999	0.9880	1
	0.5	1.0217	1.0198	1.0157	1.0013	1.0001	1.0140	1
	1.0	1.0385	1.0346	1.0267	1.0030	1.0001	1.0190	1
	10.0	1.0499	1.0440	1.0317	1.0055	1.0002	1.0113	1
	50.0	1.0502	1.0439	1.0312	1.0056	1.0001	1.0092	1
100	0.1	0.9900	0.9905	0.9914	0.9993	1.0000	0.9884	1
	0.5	1.0296	1.0274	1.0233	1.0015	1.0000	1.0207	1
	1.0	1.0401	1.0372	1.0308	1.0023	1.0001	1.0218	1
	10.0	1.0472	1.0428	1.0339	1.0037	1.0001	1.0149	1
	50.0	1.0472	1.0427	1.0337	1.0039	1.0001	1.0136	1

Table 4.4: Ratios of the average widths of bands relative to Band UVo ($1-\alpha = 0.99$, $\gamma = 0.75$)

n	ss	SBo	$TBUo$	$TBEo$	Vo	TTo	OMo	UVo
	0.1	0.9955	0.9956	0.9964	0.9995	0.9999	1.0012	1
	0.5	1.0111	1.0095	1.0068	1.0005	1.0000	1.0041	1
10	1.0	1.0463	1.0420	1.0310	1.0044	1.0012	0.9754	1
	10.0	1.0925	1.0815	1.0558	1.0124	1.0015	0.8680	1
	50.0	1.0943	1.0824	1.0549	1.0129	1.0016	0.8512	1
	0.1	0.9938	0.9940	0.9947	0.9995	0.9999	1.0022	1
	0.5	1.0245	1.0224	1.0185	1.0015	1.0000	0.9957	1
20	1.0	1.0527	1.0477	1.0382	1.0038	1.0004	0.9593	1
	10.0	1.0791	1.0706	1.0523	1.0080	1.0008	0.8696	1
	50.0	1.0800	1.0709	1.0516	1.0084	1.0007	0.8576	1
	0.1	0.9932	0.9934	0.9941	0.9995	1.0000	1.0038	1
	0.5	1.0306	1.0282	1.0234	1.0015	1.0002	0.9913	1
30	1.0	1.0529	1.0483	1.0395	1.0036	1.0003	0.9521	1
	10.0	1.0722	1.0650	1.0506	1.0066	1.0005	0.8713	1
	50.0	1.0727	1.0650	1.0501	1.0069	1.0004	0.8612	1
	0.1	0.9936	0.9939	0.9944	0.9996	0.9999	1.0055	1
	0.5	1.0349	1.0327	1.0286	1.0009	1.0001	0.9829	1
50	1.0	1.0538	1.0501	1.0432	1.0032	1.0002	0.9436	1
	10.0	1.0648	1.0597	1.0488	1.0048	1.0002	0.8721	1
	50.0	1.0655	1.0599	1.0487	1.0052	1.0003	0.8634	1
	0.1	0.9971	0.9972	0.9975	0.9998	1.0000	1.0088	1
	0.5	1.0427	1.0406	1.0364	1.0014	1.0001	0.9698	1
100	1.0	1.0539	1.0513	1.0450	1.0020	1.0001	0.9320	1
	10.0	1.0598	1.0556	1.0485	1.0028	1.0001	0.8728	1
	50.0	1.0599	1.0556	1.0484	1.0030	1.0001	0.8664	1

Table 4.5: Ratios of the average widths of OMo relative to UVo ($\gamma = 0.95$)

n	ss	$1-\alpha=0.95$	$1-\alpha=0.85$	$1-\alpha=0.80$
	0.1	0.9946	0.9883	0.9851
	0.5	0.9948	0.9830	0.9744
10	1.0	1.0183	1.0406	1.0480
	2.0	1.0145	1.0923	1.1239
	8.0	0.9581	1.1068	1.1698
	10.0	0.9510	1.1051	1.1703
	50.0	0.9240	1.0948	1.1676
	0.1	0.9913	0.9802	0.9737
	0.5	1.0081	1.0100	1.0101
20	1.0	1.0200	1.0742	1.0993
	2.0	1.0023	1.1112	1.1599
	8.0	0.9531	1.1160	1.1891
	10.0	0.9480	1.1147	1.1896
	50.0	0.9292	1.1084	1.1886
	0.1	0.9898	0.9753	0.9671
	0.5	1.0137	1.0310	1.0410
30	1.0	1.0162	1.0922	1.1283
	2.0	0.9933	1.1195	1.1785
	4.0	0.9661	1.1234	1.1967
	8.0	0.9470	1.1207	1.2013
	10.0	0.9426	1.1197	1.2017
	50.0	0.9271	1.1149	1.2013
	0.1	0.9874	0.9690	0.9587
	0.5	1.0174	1.0575	1.0774
50	1.0	1.0087	1.1100	1.1583
	2.0	0.9813	1.1277	1.1962
	8.0	0.9405	1.1263	1.2116
	10.0	0.9369	1.1254	1.2119
	50.0	0.9245	1.1217	1.2115
	0.1	0.9868	0.9676	0.9563
	0.5	1.0172	1.0935	1.1312
100	1.0	0.9959	1.1281	1.1923
	2.0	0.9670	1.1361	1.2161
	8.0	0.9328	1.1319	1.2246
	10.0	0.9301	1.1312	1.2246
	50.0	0.9205	1.1284	1.2244

Chapter 5

Two-sided Simultaneous Tolerance Bands, Prediction and Calibration

The basic model which will be assumed throughout this chapter is the simple linear regression model (1.3). In previous chapters, we study methods of constructing simultaneous confidence bands. This chapter treats the other three problems associated with linear regression analysis: simultaneous prediction intervals, simultaneous tolerance bands and statistical calibration.

5.1 Prediction

For one future observation $Y_{f_0} = \boldsymbol{x}'_{f_0}\boldsymbol{\beta} + e_{f_0}$ at x_{f_0}, a specific value of the independent variable x, where $e_{f_0} \sim N(0, \sigma^2)$, one can construct an exact prediction interval for Y_{f_0}. Since $Y_{f_0} - \boldsymbol{x}'_{f_0}\hat{\boldsymbol{\beta}} = e_f - \boldsymbol{x}'_{f_0}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \sim N(0, \sigma^2(1 + \boldsymbol{x}'_{f_0}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_0})$ where $\boldsymbol{x}_{f_0} = (1, x_{f_0})'$, then $\frac{Y_{f_0} - \boldsymbol{x}'_{f_0}\hat{\boldsymbol{\beta}}}{\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_0}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_0}}}$ has a t distribution with ν degrees of freedom and

$$P\left\{Y_{f_0} \in \boldsymbol{x}'_{f_0}\hat{\boldsymbol{\beta}} \pm t_\nu^{\alpha/2}\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_0}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_0}}\right\} = 1 - \alpha. \qquad (5.1)$$

Thus a $1 - \alpha$ perdition interval for Y_{f_0} is $\boldsymbol{x}'_{f_0}\hat{\boldsymbol{\beta}} \pm t_\nu^{\alpha/2}\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_0}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_0}}$.

One may also wish to predict the values of $k(\geq 2)$ future observations $Y_{f_1}, Y_{f_2}, \cdots,$ Y_{f_k} at k given settings of the independent variable $x_{f_1}, x_{f_2}, \cdots, x_{f_k}$, respectively. The natural predictors are still given by $\boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}},\ i = 1, \cdots, k$. Here $Y_{f_i} = \boldsymbol{x}'_{f_i}\boldsymbol{\beta} + e_{f_i}$ with $e_{f_i} \sim N(0, \sigma^2),\ i = 1, \cdots, k$. The simultaneous prediction intervals for these k future observations can be given by the general form

$$P\left\{Y_{f_i} \in \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} \pm c\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}, \quad i = 1, \cdots, k\right\} = 1 - \alpha. \qquad (5.2)$$

Liberman (1961) chose c as $(kF^{\alpha}_{k,\nu})^{-1/2}$ and so gave the prediction intervals as $Y_{f_i} \in$

$\boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} \pm (kF^{\alpha}_{k,\nu})^{-1/2}\hat{\sigma}\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}$, $i = 1, \cdots, k$, which are conservative. Liberman (1961) also considered the following conservative prediction intervals. The idea is simple. An exact prediction interval for $k = 1$ is given by (5.1). For $k \geq 2$, simply replacing $t_\nu^{\alpha/2}$ by $t_\nu^{\alpha/2k}$ will give the confidence level at least $1 - \alpha$ by using Bonferroni Inequality, that is,

$$P\{Y_{f_i} \in \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} \pm t_\nu^{\alpha/2k}\hat{\sigma}\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}, \quad i = 1, \cdots, k\} > 1-\alpha. \tag{5.3}$$

This can be easily explained by taking the special case $k = 2$. Suppose A and B are two events and $P(A) = P(B) = \alpha/2$. Then $P(A \text{ or B}) = \mathrm{P(A) + P(B) - P(AB)} \leq \mathrm{P(A) + P(B)} = \alpha$. Therefore, $P(A^c \cap B^c) = 1 - P(A \text{ or B}) \geq 1 - \alpha$. Let A be the event that the first future observation fails to fall into its prediction interval, and B be the event that the second future observation fails to fall into its prediction interval. Then $1 - P(A \text{ or B})$ is the probability that both two future observations belong to their corresponding prediction intervals. This probability is greater than $1 - \alpha$. We are able to construct exact prediction intervals for a finite number $k \geq 2$ of future observations in the following way. From (5.2), we have

$$\begin{aligned}
& P\left\{Y_{f_i} \in \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} \pm c\hat{\sigma}\sqrt{1+\boldsymbol{x}'_{f_0}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}, \quad i = 1, \cdots, k\right\} \\
= \; & P\left\{\frac{|Y_{f_i} - \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}}|}{\hat{\sigma}\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \leq c, \quad i = 1, \cdots, k\right\} \\
= \; & P\left\{\max_{i=1,\cdots,k} \frac{|Y_{f_i} - \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}}|}{\hat{\sigma}\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \leq c\right\} \\
= \; & P\left\{\max_{i=1,\cdots,k} \frac{\left|\frac{Y_{f_i} - \boldsymbol{x}'_{f_i}\boldsymbol{\beta}}{\sigma} - \frac{\boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} - \boldsymbol{x}'_{f_i}\boldsymbol{\beta}}{\sigma}\right|}{(\hat{\sigma}/\sigma)\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \leq c\right\}.
\end{aligned} \tag{5.4}$$

Denote $N_{f_i} = \frac{Y_{f_i} - \boldsymbol{x}'_{f_i}\boldsymbol{\beta}}{\sigma}, i = 1, \cdots, k$. It is clear that $N_{f_i} \sim N(0,1)$ for each i. Let $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & P_1^{-1} \end{pmatrix}$ be the square root of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ which is given in (1.5). Denote $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$ and $\boldsymbol{N_0} = (N_{01}, N_{02})' = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}(\boldsymbol{0}, I)$. We have $\frac{\boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} - \boldsymbol{x}'_{f_i}\boldsymbol{\beta}}{\sigma} = (\boldsymbol{P}\boldsymbol{x}_{f_i})'\boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma = (\boldsymbol{P}\boldsymbol{x}_{f_i})'\boldsymbol{N_0} = N_{01}/\sqrt{n} + N_{02}P_1^{-1}x_{f_i}$. Therefore, (5.4) can be written as

$$P\left\{\max_{i=1,\cdots,k} \frac{|N_{f_i} - (\boldsymbol{P}\boldsymbol{x}_{f_i})'\boldsymbol{N_0}|}{U\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \leq c\right\} \tag{5.5}$$

$$= \; P\{S \leq c\}, \tag{5.6}$$

where $S = \max_{i=1,\cdots,k} \frac{|N_{f_i}-(\boldsymbol{P}\boldsymbol{x}_{f_i})'\boldsymbol{N_0}|}{U\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}}$. Similar to Chapter 2-4, we can use simulation method and numerical quadrature method to calculate the critical constant c in (5.5).

In each simulation of S, we first generate independent standard normal vector $\boldsymbol{N_0} \sim \boldsymbol{N}(\boldsymbol{0}, I)$, $N_{f_i} \sim N(0,1), i = 1, \cdots, k$ and $U \sim \sqrt{\chi^2_\nu/\nu}$ and then calculate S from its definition in (5.6). Donnelly (2003) suggested to use simulation to find c.

The probability in (5.5) can also be expressed as

$$\int_{u=0}^{\infty}\int_{n_2=-\infty}^{\infty}\int_{n_1=-\infty}^{\infty} P\left\{\max_{i=1,\cdots,k} \frac{|N_{f_i} - (n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i})|}{u\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \le c\right\} f(\boldsymbol{v})d\boldsymbol{v}, \qquad (5.7)$$

where $f(\boldsymbol{v})$ is the joint probability density function of the random vector of $\boldsymbol{v} = (n_1, n_2, u)'$. Since $N_{01} \sim N(0,1)$, $N_{02} \sim N(0,1)$ and $U \sim \sqrt{\chi^2_\nu/\nu}$ are independent and from (1.4), we have

$$f(\boldsymbol{v}) = \pi^{-1}e^{-(n_1^2+n_2^2+\nu u^2)/2}2^{-\nu/2}\nu^{\nu/2}u^{\nu-1}/\Gamma(\nu/2).$$

Denote $Sxx_i = 1 + \boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}$ and

$$k(\boldsymbol{v}) = P\left\{\max_{i=1,\cdots,k} \frac{|N_{f_i} - (n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i})|}{u\sqrt{1+\boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}}} \le c\right\}.$$

Then

$$\begin{aligned} k(\boldsymbol{v}) &= P\Big\{n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i} - cu\sqrt{Sxx_i} \le N_{f_i} \\ &\le n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i} + cu\sqrt{Sxx_i}, \quad i = 1, \cdots, k\Big\} \\ =& \prod_{i=1}^{k}\left[\Phi\left(n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i} + cu\sqrt{Sxx_i}\right) - \Phi\left(n_1/\sqrt{n} + n_2P_1^{-1}x_{f_i} - cu\sqrt{Sxx_i}\right)\right]. \end{aligned}$$

Expression (5.7) is therefore equal to

$$\int_{u=0}^{\infty}\int_{n_2=-\infty}^{\infty}\int_{n_1=-\infty}^{\infty} k(\boldsymbol{v})f(\boldsymbol{v})d\boldsymbol{v}.$$

It involves a three-dimensional integration and can be used to compute c for a given confidence level $1-\alpha$.

It should be emphasized that the prediction intervals given above are only for a finite number of future observations. If the number of future observations k is very large, these prediction intervals may be very wide. If the number of future observations k is infinite, these prediction intervals cannot be used at all. In some cases, the total number of predictions may be unknown. In these circumstances, we should use simultaneous tolerance bands for prediction, which bracket $100p$ percent proportion of all future observations with a certain confidence level $1-\alpha$.

5.2 Calibration

Calibration, also known as discrimination and the reverse prediction, has been widely used in measurement science and other applications. Statistical calibration with regression has a history dating back to Eisenhart (1939). Suppose one has the training data set $\mathcal{E} := \{(x_j, y_j), j = 1, \cdots, n\}$ which is used to fit a regression line of Y on x. He also has k additional observations $Y_{f_1}, Y_{f_2}, \cdots, Y_{f_k}$. But the corresponding values of independent variable $x_{f_1}, x_{f_2}, \cdots, x_{f_k}$ are unknown. Then calibration intervals can be used to estimate the unknown $x_{f_1}, x_{f_2}, \cdots, x_{f_k}$ and bracket them with a certain confidence level. Comparing with calibration, the prediction problem is the reverse. The values $x_{f_1}, x_{f_2}, \cdots, x_{f_k}$ are known, and the aim is to predict $Y_{f_1}, Y_{f_2}, \cdots, Y_{f_k}$.

5.2.1 Finite number of calibrations

Suppose the value of k is finite. From (5.3), we know that, when $c = t_\nu^{\alpha/2k}$ all the points x which satisfy

$$\boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} - c\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}} \le Y_{f_i} \le \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}} + c\hat{\sigma}\sqrt{1 + \boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}} \qquad (5.8)$$

form a confidence interval for the unknown x_{f_i}. The k confidence sets for the unknown $x_{f_1}, x_{f_2}, \cdots, x_{f_k}$ have a combined probability $1-\alpha$. Note that (5.8) is equivalent to

$$\left(Y_{f_i} - \boldsymbol{x}'_{f_i}\hat{\boldsymbol{\beta}}\right)^2 \le c^2\hat{\sigma}^2\left[1 + \boldsymbol{x}'_{f_i}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_{f_i}\right].$$

The confidence set for each x_{f_i} is the given by

$$C(Y_{f_i}) = \left\{x : \left(Y_{f_i} - \boldsymbol{x}'\hat{\boldsymbol{\beta}}\right)^2 \le c^2\hat{\sigma}^2\left[1 + \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}\right]\right\}.$$

5.2.2 Infinite number of calibrations

When k, the number of calibrations is infinite, simultaneous tolerance bands should be used to give infinitely many calibration sets. Assume x is a desirable but expensive or difficult measurement and Y represents a cheaper and more convenient instrument response obtainable. After fitting the linear regression model based on the training data set, for each given future Y value, one can get the confidence set for the corresponding x, from a simultaneous tolerance band.

Krishnamoorthy (2001) provided a data set from a calibration experiment of breathalyzers which are used to measure blood alcohol concentration. Let x be the true alcohol level in blood stream and Y the reading on a breathalyzer of a driver. Policemen usually use breathalyzer to test drivers blood alcohol concentration values. To test a person's real blood alcohol is expensive and difficult. But to use breathalyzer is convenient. After the fit, from a training data set, for a future breathalyzer reading Y, one can find the corresponding calibration confidence set for x. Denote the confidence set for the unknown x by $C(Y)$. For an infinite sequence of future Y values, the infinite sequence of confidence sets $C(Y)$ have the property that: with confidence level $1-\alpha$ (with respect to the training data set), the proportion of confidence sets $C(Y)$ containing the true x values is at least p, where $0 < 1-\alpha < 1$ and $0 < p < 1$ are pre-specified factors. It has been pointed out that this property is desirable in many applications in the literature, see Lieberman and Miller (1963), Scheffé (1973), Mee et al. (1991) and Mee and Eberhardt (1996). For example, the traffic police who use breathalyzers to catch drunk drivers would require the two factors $1-\alpha$ and p to be close to one. Assume a prior that all the unknown x values corresponding to the future Y-values are in a given interval (a, b). For example, the true blood alcohol level of a person cannot be less than 0 or more than a threshold. The $(p, 1-\alpha)$-simultaneous tolerance bands $[L(x;\mathcal{E}), U(x;\mathcal{E})]$ over the interval $x \in (a, b)$ satisfy

$$P_{\mathcal{E}}\{P_{Y(x)}\{L(x;\mathcal{E}) < Y(x) < U(x;\mathcal{E})|\mathcal{E}, x\} \geq p \text{ for all } x \in (a,b)\} \geq 1-\alpha,$$

where $Y(x)$ denotes a future Y-value corresponding to x and $Y(x)$ is independent of the training data $\mathcal{E}$. The probability $P_{Y(x)}$ is with respect to $Y(x)$ and conditional on $\mathcal{E}$, and the probability $P_{\mathcal{E}}$ is with respect to $\mathcal{E}$. Then for each future Y the confidence set $C(Y)$ for the corresponding x is defined as

$$C(Y) = \{x \in (a,b) : L(x;\mathcal{E}) < Y < U(x;\mathcal{E})\}.$$

It is shown in Scheffé (1973, Appendix B) that for an infinite sequence of future Y-values, at least p proportion of confidence sets $C(Y)$ contain the true x-values with confidence level $1-\alpha$.

Construction of $(p, 1-\alpha)$-simultaneous tolerance bands is first addressed by Lieberman and Miller (1963), and there are three construction methods in the literature so far. The first is the probability set method by Wilson (1967) and Limam and Thomas (1988). These bands are conservative and two-sided. The second is the construction of central p-proportion simultaneous confidence bands by Lieberman and Miller (1963), Lieberman et al. (1967) and Scheffé (1973). These bands are also conservative and two-sided.

The third is an exact method by Mee et al. (1991) for two-sided bands and

Odeh and Mee (1990) for one-sided bands. Since the first two methods are conservative while Mee et al. (1991) method is exact, the two-sided bands of Mee et al. (1991) are usually narrower and so better than the conservative bands, as demonstrated numerically in Mee et al. (1991). The focus of this chapter is the construction of exact two-sided $(p, 1-\alpha)$-simultaneous tolerance bands. One example is demonstrated in Section 5.3.6.

5.3 Simultaneous tolerance bands

Let $Y(x) = \boldsymbol{x}'\boldsymbol{\beta} + e_x$ denote a future observation at x with $e_x \sim N(0, \sigma^2)$. Assume $Y(x)$ is independent of $\boldsymbol{Y}$ in (1.3). For a given x value, a $(p, 1-\alpha)$-tolerance interval for $Y(x)$ contains at least $100p\%$ proportion of the $Y(x)$ distribution with $1-\alpha$ confidence level. In some practical problems, one may be interested in infinite future observations corresponding to x values in a prespecified covariate interval (a, b) based on the same training data set $\mathcal{E} := \{(x_j, y_j), j = 1, \cdots, n\}$, or equivalently $(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\sigma}})$. This is the motivation of constructing simultaneous tolerance bands over a constrained covariate interval. Based on the same training data set, a $(p, 1-\alpha)$-simultaneous tolerance band for infinite future observations $Y(x)$ over $x \in (a, b)$ contains at least $100p\%$ proportion of the $Y(x)$ distribution for any $x \in (a, b)$ simultaneously with confidence level $1-\alpha$.

Denote the coverage probability at x by

$$C(\boldsymbol{x}, \hat{\boldsymbol{\beta}}, \hat{\sigma}) = P_{Y(x)}\{\boldsymbol{x}'\hat{\boldsymbol{\beta}} - k(x)\hat{\sigma} \leq Y(x) \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + k(x)\hat{\sigma}\}, \tag{5.9}$$

where the tolerance factor $k(x)$ is a positive function of x and sought to satisfy the condition

$$P_{\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\sigma}}}\{C(x, \hat{\boldsymbol{\beta}}, \hat{\sigma}) \geq p \text{ for all } x \in (a, b)\} \geq 1-\alpha. \tag{5.10}$$

Then $\left[\boldsymbol{x}'\hat{\boldsymbol{\beta}} - k(x)\hat{\sigma}, \boldsymbol{x}'\hat{\boldsymbol{\beta}} + k(x)\hat{\sigma}\right]$ is called a simultaneous tolerance band for $Y(x)$ over $x \in (a, b)$, which contains at least p proportion of $Y(x)$ distribution simultaneously for all $x \in (a, b)$ with confidence level $1-\alpha$.

Let $\boldsymbol{b} = (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}(\boldsymbol{0}, (\boldsymbol{X}'\boldsymbol{X})^{-1})$ and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$ denote the two pivotal quantities. Then the coverage probability in (5.9) can be expressed in terms of the pivotal quantities as

$$C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) = \Phi\left(\boldsymbol{x}'\boldsymbol{b} + k(x)U\right) - \Phi\left(\boldsymbol{x}'\boldsymbol{b} - k(x)U\right). \tag{5.11}$$

It is clear that (5.11) is a decreasing function of $|\boldsymbol{x}'\boldsymbol{b}|$ and an increasing function of

$k(x)$. Then (5.10) can be rewritten as

$$P\{C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) \geq p \text{ for all } x \in (a,b)\} = 1-\alpha. \tag{5.12}$$

Methods of constructing simultaneous tolerance bands for given p, (a,b) and $1-\alpha$ have been considered by many authors as pointed out in Section 5.2.2 above. In the following sections, different methods will be discussed.

5.3.1 Probability Set Methods

Denote G as a $(1-\alpha)$ level probability set for $(\boldsymbol{b}, U)$, i.e.,

$$P\{(\boldsymbol{b}, U) \in G\} \geq 1-\alpha.$$

Suppose $k(x)$ is the optimal tolerance factor based on G in the sense that

$$k(x) = \min\left\{k : C(\boldsymbol{x}'\boldsymbol{b}, kU) \geq p, \text{ for } (\boldsymbol{b}, U) \in G\right\}. \tag{5.13}$$

Then $(\boldsymbol{b}, U) \in G$ implies that $C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) \geq p$ for all $x \in (-\infty, \infty)$. Therefore

$$P\{C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) \geq p,\ x \in (-\infty,\infty)\} \geq P\{(\boldsymbol{b}, U) \in G\} \geq 1-\alpha.$$

Wilson (1967), Limam and Thomas (1988) and Chvosteková (2013) constructed two-sided simultaneous tolerance bands by using the probability set method over $x \in (-\infty, \infty)$.

5.3.1.1 The method of Wilson (1967)

Wilson (1967) constructed probability set for $(\boldsymbol{b}, U)$ as

$$G_W = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} + 2\nu(U-m)^2 \leq c\}, \tag{5.14}$$

where $\nu = n-2$ and $m = [(2\nu-1)/(2\nu)]^{1/2}$. By noting that $\boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} + 2\nu(U-m)^2$ has the approximate distribution χ^2_3 as $n \to \infty$, Wilson suggested to use $c = \chi^2_3(1-\alpha)$ and so G_W is an approximate $1-\alpha$ probability set for $(\boldsymbol{b}, U)$.

Note that $\boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} \sim \chi^2_2$ and $U \sim \sqrt{\chi^2_\nu/\nu}$. Expression (5.14) implies $(U-m)^2 \leq c/(2\nu)$ and therefore $U \in m \pm \sqrt{c/(2\nu)}$. As a matter of fact, this method can be improved as the exact value of c can be found such that

$$1-\alpha = \int_{m-\sqrt{c/(2\nu)}}^{m+\sqrt{c/(2\nu)}} \chi^2_2\left(c - 2\nu(u-m)^2\right) f_{\frac{\hat{\sigma}}{\sigma}}(u)du,$$

where $\chi_2^2(.)$ denotes the cumulative distribution function of the chi-square distribution with 2 degrees of freedom, and $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ denotes the probability density function of $U = \hat{\sigma}/\sigma$ and given in (1.4).

For given $\boldsymbol{x}$ and k, define the following sets in R^2

$$H(\boldsymbol{x}, k) = \{(y, r) : y = \boldsymbol{x}'\boldsymbol{b},\ r = kU,\ (\boldsymbol{b}, U) \in G_W\} \tag{5.15}$$

and

$$S_p = \{(y, r) : C(y, r) \geq p\}.$$

From (5.11), $C(y, r) = \Phi(y + r) - \Phi(y - r)$ and therefore $S_p = \{(y, r) : \Phi(y + r) - \Phi(y - r) \geq p\}$. The optimal tolerance factor in (5.13) becomes

$$k(x) = \min\{k : H(\boldsymbol{x}, k) \subseteq S_p\}.$$

Let $\boldsymbol{P}$ denote the square root matrix of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$. Then, for each $\boldsymbol{x}$ and $\boldsymbol{b}$, we have

$$\begin{aligned} |\boldsymbol{x}'\boldsymbol{b}| &= |(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}^{-1}\boldsymbol{b})| \\ &\leq |(\boldsymbol{P}\boldsymbol{x})'| \cdot |\boldsymbol{P}^{-1}\boldsymbol{b}| \\ &= \sqrt{\boldsymbol{x}'(\boldsymbol{P}'\boldsymbol{P})\boldsymbol{x}} \cdot \sqrt{\boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b}}. \end{aligned} \tag{5.16}$$

It is clear that

$$\max_{x \in (-\infty, \infty)} \frac{|\boldsymbol{x}'\boldsymbol{b}|}{\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \leq \sqrt{\boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b}}. \tag{5.17}$$

Inequality (5.17) is also known as the Scheffé projection result; see e.g. Miller (1981). Applying (5.17) to (5.14) gives

$$|\boldsymbol{x}'\boldsymbol{b}| \leq A_x(U) \text{ for all } x \in (-\infty, \infty),\quad U \in [m - \sqrt{c/(2\nu)}, m + \sqrt{c/(2\nu)}], \tag{5.18}$$

where

$$A_x(U) = [c - 2\nu(U - m)^2]^{1/2}\delta(x)$$

and

$$\delta(x) = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$$

is the standard error of $\boldsymbol{x}'\boldsymbol{b}$. Then the set $H(\boldsymbol{x}, k)$ is enlarged to

$$H^*(\boldsymbol{x}, k) = \{(y, r) = (\boldsymbol{x}'\boldsymbol{b}, kU) : y^2/\delta(x)^2 + 2\nu(r/k - m)^2 \leq c\},$$

and the tolerance factor $k(x)$ is also enlarged to satisfy

$$k(x) = \min \{k : H^*(\boldsymbol{x}, k) \subseteq S_p\}. \tag{5.19}$$

The shape of $H^*(\boldsymbol{x}, k)$ is an ellipse. $H^*(\boldsymbol{x}, k) \subseteq S_p$ means that $H^*(\boldsymbol{x}, k)$ must be contained in S_p. When k decreases, the ellipse $H^*(\boldsymbol{x}, k)$ has its centre move towards the origin and the r-axis smaller. The k value which makes this ellipse tangent to S_p is the $k(x)$ satisfying (5.19). However Wilson (1967) did not find the exact value of $k(x)$ such that the ellipse is tangent to the (lower) boundary of S_p, neither did the Modified Wilson method in Limam and Thomas (1988) nor Chvosteková (2013). They approximated the boundary of the region S_p and used the $k(x)$ for which the ellipse is tangent to the approximate boundary of S_p instead.

More precisely, they all used the upper branch of the hyperbola $(r - r_0) - y^2 = h^2$ as the approximation of the (lower) boundary of S_p, where $r_0 = \Phi^{-1}(p)$ and h^2 is chosen to give a good approximation; see the following table given by Wilson.

Table 5.1: Table of h

p	r_0	h^2
0.50	0	0.455
0.75	0.674	0.250
0.80	0.842	0.107
0.90	1.28	0.0657
0.95	1.65	0.0438
0.99	2.33	0.0244

The optimal tolerance factor is chosen such that the ellipsoidal set $H^*(\boldsymbol{x}, k)$ is on and above the hyperbola. Substituting $y^2 = (r - r_0)^2 - h^2$ into the boundary equation of $H^*(\boldsymbol{x}, k)$ gives a quadratic function of r

$$(r - r_0)^2 - h^2 - h^2 - [c - 2\nu(r/k - m)^2]\delta(x)^2 = 0.$$

Setting the discriminant of this the quadratic equation in r equal to 0 and solving the quadratic equation in k gives two solutions. The largest one is used as Wilson's tolerance factor. This method is not only conservative but also approximate, and so not recommended.

5.3.1.2 The method of Limam and Thomas (1988)

Limam and Thomas (1988) constructed $1 - \alpha$ probability set G_{LT} for the pivotal quantities $(\boldsymbol{b}, U)$ as

$$G_{LT} = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} \le U^2 c_1^2 \text{ and } U \ge c_2\}, \tag{5.20}$$

where $c_2 = \sqrt{\chi^2_\nu(\alpha/2)/\nu}$ and $c_1^2 = 2F_{2,\nu}(1-\alpha/2)$ with $F_{2,\nu}(1-\alpha/2)$ being $(1-\alpha/2)$ point of the F distribution with 2 and ν degrees of freedom.

Since $\hat{\boldsymbol{\beta}} \sim \boldsymbol{N}(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1})$ and $\hat{\sigma}^2 \sim \sigma^2\chi^2_\nu/\nu$, we know that event $A = \{(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})'(\boldsymbol{X}'\boldsymbol{X})(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \leq \sigma^2 c_1^2\}$ satisfies $P(A) \geq 1-\alpha/2$ and event $B = \{0 < \sigma < \hat{\sigma}/c_2\}$ satisfies $P(B) \geq 1-\alpha/2$. Applying the Bonferroni inequality to the events A and B gives $P\{(\boldsymbol{b}, u) \in G_{LT}\} > 1-\alpha$. Actually we can find the exact values of c_1 and c_2 in (5.20) such that $P\{(\boldsymbol{b}, u) \in G_{LT}\} = 1-\alpha$.

Similar to Wilson's method, Limam and Thomas (1988) then tried to find the optimal tolerance factor satisfying (5.13) with $G = G_{LT}$. Applying Scheffé projection result (5.17) again to G_{LT} gives

$$|\boldsymbol{x}'\boldsymbol{b}| \leq Uc_1\delta(x) \quad \text{for all } x \text{ and } (\boldsymbol{b}, U) \in G_{LT},$$

where $\delta(x) = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Hence we have

$$C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) \geq C(Uc_1\delta(x), k(x)U) \quad \text{for all} \quad (\boldsymbol{b}, U) \in G_{LT},$$

since $C(y,r) = \Phi(y+r) - \Phi(y-r)$ is decreasing in $|y|$. Also, note that the function $C(Uc_1\delta(x), k(x)U) = \Phi\left[U\left(c_1\delta(x) + k(x)\right)\right] - \Phi[U(c_1\delta(x) - k(x))]$ is increasing in U when $C \geq 1/2$. Therefore

$$C(Uc_1\delta(x), k(x)U) \geq C(c_2c_1\delta(x), c_2k(x)) \quad \text{for all } U \geq c_2.$$

The optimal tolerance factor k can be solved from the equation

$$\begin{aligned} p &= C(c_2c_1\delta(x), c_2k(x)) \\ &= \Phi(c_2c_1\delta(x) + c_2k(x)) - \Phi(c_2c_1\delta(x) - c_2k(x)). \end{aligned}$$

This method is conservative but not approximate.

5.3.1.3 The modified Wilson Method in Limam and Thomas (1988)

Based on the method of Wilson (1967), Limam and Thomas (1988) proposed a modified method. This method is still approximately conservative. They enlarged G_W, the probability set for $(\boldsymbol{b}, U)$, to G_{MW} to give a smaller c in (5.14) and consequently a smaller tolerance factor $k(x)$. From (5.18) and $C(\boldsymbol{x}'\boldsymbol{b}, kU) = \Phi(\boldsymbol{x}'\boldsymbol{b}+kU) - \Phi(\boldsymbol{x}'\boldsymbol{b}-kU)$ is decreasing function in $|\boldsymbol{x}'\boldsymbol{b}|$, we know

$$C(\boldsymbol{x}'\boldsymbol{b}, kU) \geq C(A_x(u), kU) \text{ for } (\boldsymbol{b}, u) \in G_W,$$

where $A_x(U) = [c - 2\nu(U-m)^2]^{1/2}\delta(x)$. Since $A_x(U)$ decreases and kU increases in U, the coverage $C(A_x(U), kU) = \Phi(A_x(U)+kU) - \Phi(A_x(U)-kU)$ is increasing in U over $U \in [m, m+\sqrt{c/(2\nu)}]$, then $C(A_x(U), kU)$ is minimized at $U = m$. Therefore, only the subset of G_W on $U \in [m - \sqrt{c/(2\nu)}, m]$,is needed for determining the tolerance factor $k(x)$.

The set G_{MW} in Limam and Thomas (1988) is defined as $G_{MW} = G_{M1} \cup G_{M2}$, where

$$G_{M1} = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} + 2\nu(U-m)^2 \leq c_m \text{ for } m - \sqrt{c/(2\nu)} \leq U \leq m\}$$

and

$$G_{M2} = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} \leq U^2 c_m/m^2 \text{ for } U \geq m\}.$$

For $c = c_m$, we have $G_{MW} \subset G_W$ and therefore $P\{G_{MW}\} < P\{G_W\}$. Likewise, $P\{G_{MW}\} = P\{G_W\}$ implies $c_m < c$. It is clear that the set G_{M2} intersects with G_{M1} at $U = k$. The value of c_m can be computed such that

$$1 - \alpha = \int_{m-\sqrt{c/(2\nu)}}^{m} \chi_2^2\left(c_m - 2\nu(u-m)^2\right) f_{\frac{\hat{\sigma}}{\sigma}}(u)du + \int_m^\infty \chi_2^2\left(c_m u^2/m^2\right) f_{\frac{\hat{\sigma}}{\sigma}}(u)du.$$

For a given c_m, the tolerance factor $k(x)$ can be computed by using the Wilson's method.

As a matter of fact, this method can be improved further. One can construct $G_{M2^*} = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} \leq \varsigma U^2 c^*/m^2 \text{ for } U \geq m\}$ with $\varsigma > 1$ to make the probability set G_{MW} larger and consequently the value of c^* smaller. But this conservative method is still based on the Wilson's method which evolves approximation and so not recommended.

5.3.1.4 The Method of Chvosteková

Chvosteková (2013) constructed the $(1-\alpha)$ probability set for $(\boldsymbol{b}, U)$ as

$$G_C = \{(\boldsymbol{b}, U) : \boldsymbol{b}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{b} - n\ln[U^2(n-2)] \leq c_C\}, \tag{5.21}$$

where c_C satisfies

$$\begin{aligned} & P(\chi_2^2 \leq c_C + n\ln[u^2(n-2)]) \\ = & \int_0^\infty P\left(\chi_2^2 \leq c_C + n\ln[u^2(n-2)]\right) f_{\frac{\hat{\sigma}}{\sigma}}(u)du = 1 - \alpha. \end{aligned}$$

Chvosteková (2013) considered the tolerance factor $k(x)$ in (5.13) as a function of $d = \delta(x) = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Similar to the modified Wilson Method, for a given c_C, the tolerance factor $k(d)$ can be computed by using the Wilson's method such that

$$P\{C(\boldsymbol{x}'\boldsymbol{b}, k(x)U) \geq p, x \in (-\infty, \infty)\} \geq P\{(\boldsymbol{b}, U) \in G_C\} \geq 1 - \alpha.$$

Again, this method is approximately conservative and so not recommended.

5.3.2 Simultaneous tolerance bands for central p proportion

Lieberman and Miller (1963) and Scheffé (1973) considered tolerance bands for the central p proportion. The central p proportion of the standard normal distribution centered at $\boldsymbol{x}'\boldsymbol{\beta}$ is given by

$$I_x(p) = (\boldsymbol{x}'\boldsymbol{\beta} - z_{(1+p)/2}\sigma, \boldsymbol{x}'\boldsymbol{\beta} + z_{(1+p)/2}\sigma) \text{ for all } x \in (a, b) \tag{5.22}$$

where $z_{(1+p)/2}$ is the two-sided p-percentile point of the normal distribution, that is,

$$p = \frac{1}{\sqrt{2\pi}} \int_{-z_{(1+p)/2}}^{z_{(1+p)/2}} \exp(-y^2/2)dy.$$

Simultaneous tolerance bands which contain the central p-proportion over $x \in (a, b)$ have the general form as

$$P\{I_x(p) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm k(x)\hat{\sigma} \text{ for all } x \in (a, b)\} = 1 - \alpha. \tag{5.23}$$

Since $Y(x) = \boldsymbol{x}'\boldsymbol{\beta} + e$ with $e \sim N(0, \sigma^2)$, then $P\{Y(x) \in I_x(p)\} = p$ and the band in (5.23) satisfies

$$P\left\{P_{Y(x)}\left[\boldsymbol{x}'\hat{\boldsymbol{\beta}} - k(x)\hat{\sigma} \leq Y(x) \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + k(x)\hat{\sigma}\right] \geq p \text{ for all } x \in (a, b)\right\} \geq 1 - \alpha.$$

Lieberman and Miller (1963) proposed a method of constructing tolerance bands for a fixed p and all values of $x \in (-\infty, \infty)$. They also considered methods for different p and all $x \in (-\infty, \infty)$. Scheffé (1973) considered the construction of conservative tolerance bands for a fixed p central proportion over a finite covariate interval $x \in (a, b)$.

5.3.2.1 The method of Lieberman (1963) for central p proportion

Lieberman and Miller (1963) constructed tolerance bands for a fixed p central proportion in regression. For the simple linear regression case, they considered the tolerance bands over the whole range $x \in (-\infty, \infty)$ such that, at the specified confidence level $1 - \alpha$, simultaneously for all $x \in (-\infty, \infty)$, at least the central p proportion of the $Y(x)$ distribution is contained in the tolerance bands. The tolerance band constructed by Lieberman and Miller (1963) is of the form

$$1-\alpha = P\left\{ I_x(p) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm c_L\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} \text{ for all } x \in (-\infty,\infty) \right\}. \tag{5.24}$$

Here the constant c_L satisfies

$$1-\alpha = P\left\{ \frac{(Z_1 \pm \sqrt{n} z_{(1+p)/2})^2 + Z_2^2}{\chi_\nu^2/\nu} \le (c_L)^2 \right\}, \tag{5.25}$$

where $Z_1 \sim N(0,1)$, $Z_2 \sim N(0,1)$ and χ_ν^2 are independent random variables.

Lemma 5.3.1. *For $C > 0$,*

$$\sum_{i=1}^n a_i^2 \le C^2,$$

if and only if

$$\left| \sum_{i=1}^n a_i b_i \right| \le C \left(\sum_{i=1}^n b_i^2 \right)^{-1/2} \quad \text{for all } \mathrm{b_1, \cdots, b_n},$$

provided $a_1 b_1 \neq 0$.

Lemma 5.3.1 can be easily proved by using Cauchy-Schwarz inequality; see Lieberman and Miller (1963). Notice that (5.24) is equivalent to

$$P\left\{ \left| \frac{1}{\sqrt{n}} \frac{\sqrt{n}(\beta_0 - \hat{\beta}_0)}{\sigma} + \frac{x}{\sqrt{S_{xx}}} \frac{\sqrt{S_{xx}}(\beta_1 - \hat{\beta}_1)}{\sigma} \pm z_{(1+p)/2} \right| \le \right. \\ \left. \frac{c_L\hat{\sigma}\sqrt{1/n + x^2/S_{xx}}}{\sigma} \text{ for all } x \in (-\infty,\infty) \right\}. \tag{5.26}$$

Since $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1) \sim \boldsymbol{N}(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1})$ and $(\boldsymbol{X}'\boldsymbol{X})^{-1} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & 1/\sqrt{S_{xx}} \end{pmatrix}$, then we have $\frac{\sqrt{n}(\beta_0 - \hat{\beta}_0)}{\sigma} \sim N(0,1)$ and $\frac{\sqrt{S_{xx}}(\beta_1 - \hat{\beta}_1)}{\sigma} \sim N(0,1)$. Therefore, (5.26) can be written as

$$P\left\{ \left| \frac{1}{\sqrt{n}} \left(Z_1 \pm \sqrt{n} z_{(1+p)/2} \right) + \frac{x}{\sqrt{S_{xx}}} Z_2 \right| \le \right. \\ \left. \frac{c_L\hat{\sigma}\sqrt{1/n + x^2/S_{xx}}}{\sigma} \text{ for all } x \in (-\infty,\infty) \right\}. \tag{5.27}$$

Applying Lemma 5.3.1 to (5.27) gives (5.25). The critical constant c_L in (5.25) can be solved by numerical quadrature method. For a given c_L, note that the probability in

(5.25) can be expressed as

$$h(c_L) = \int_{-\infty}^{\infty}\int_0^{\infty}\Big[\Phi(\sqrt{c_L{}^2u^2-y^2}-\sqrt{n}z_{(1+p)/2})- \Phi(-\sqrt{c_L{}^2u^2-y^2}+\sqrt{n}z_{(1+p)/2})\Big] f_{\frac{\hat{\sigma}}{\sigma}}(u)\varphi(y)dudy.$$

where $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of $\sqrt{\chi^2_\nu/\nu}$ and $\varphi(y)=\frac{1}{\sqrt{2\pi}}e^{-y^2/2}$ is the probability density function of the standard normal distribution. We can search for the value of c_L such that $h(c_l)=1-\alpha$.

5.3.2.2 The method of Scheffé (1973)

Scheffé (1973) also considered tolerance bands for central p proportion in regression. For the simple linear regression case, the tolerance band is of the form

$$I_x(p)\subset \boldsymbol{x}'\hat{\boldsymbol{\beta}}\pm\hat{\sigma}\left[c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] \text{ for all } x\in[a,b],$$

where $I_x(p)$ is the central p proportion of the standard normal distribution centered at $\boldsymbol{x}'\boldsymbol{\beta}$ given in (5.22), and the critical constants c_1 and c_2 are determined such that

$$P\left\{I_x(p)\subset \boldsymbol{x}'\hat{\boldsymbol{\beta}}\pm\hat{\sigma}\left[c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] \text{ for all } x\in[a,b]\right\}=1-\alpha. \quad (5.28)$$

It is clear that the band in (5.28) satisfies

$$P\Big\{P_{Y(x)}\Big[\boldsymbol{x}'\hat{\boldsymbol{\beta}}-\hat{\sigma}\left(c_1+c_1\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)\le Y(x)\le \boldsymbol{x}'\hat{\boldsymbol{\beta}}+ \hat{\sigma}\left(c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)\Big]\ge p \text{ for all } x\in[a,b]\Big\}\ge 1-\alpha. \quad (5.29)$$

The fact that the probability of the event in (5.28) is $1-\alpha$ implies that the probability in (5.29) is at least $1-\alpha$. Using the pivotal quantities $\boldsymbol{b}=(\hat{\boldsymbol{\beta}}-\boldsymbol{\beta})/\sigma\sim \boldsymbol{N}\left(\boldsymbol{0},(\boldsymbol{X}'\boldsymbol{X})^{-1}\right)$ and $U=\hat{\sigma}/\sigma\sim\sqrt{\chi^2_\nu/\nu}$ in (5.29) gives the following probability statement

$$P\Big\{P_N\Big[\boldsymbol{x}'\hat{\boldsymbol{b}}-U\left(c_1+c_1\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)\le N\le \boldsymbol{x}'\hat{\boldsymbol{b}}+ U\left(c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)\Big]\ge p \text{ for all } x\in[a,b]\Big\}\ge 1-\alpha, \quad (5.30)$$

where $N\sim N(0,1)$. It is worth noting that sufficient conditions for (5.30) are that

$$\boldsymbol{x}'\hat{\boldsymbol{b}}-U\left[c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right]\le -z_{(1+p)/2} \text{ and}$$

$$\boldsymbol{x}'\hat{\boldsymbol{b}}+U\left[c_1+c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right]\ge z_{(1+p)/2} \text{ for all } x\in[a,b]$$

or

$$\left|\boldsymbol{x}'\hat{\boldsymbol{b}}\right| \leq U\left[c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] - z_{(1+p)/2} \text{ for all } x \in [a,b]. \tag{5.31}$$

The probability of the event in (5.31) is equivalent to the probability in (5.28). Note that the probability space of $(\hat{\boldsymbol{b}}, U)$ is 3-dimensional. In order to calculate c_1 and c_2 in a reduced 2-dimensional space, they used Cauchy-Schwarz inequality to enlarge $|\boldsymbol{x}'\boldsymbol{b}|$ in (5.31):

$$\begin{aligned} & |\boldsymbol{x}'\boldsymbol{b}| = |(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}^{-1}\boldsymbol{b})| \\ \leq \ & \|(\boldsymbol{P}\boldsymbol{x})'\|\|\boldsymbol{P}^{-1}\boldsymbol{b}\| \\ = \ & \chi_2\|(\boldsymbol{P}\boldsymbol{x})'\| \\ = \ & \chi_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}, \quad \text{for all } x \in [a,b], \end{aligned}$$

where $\boldsymbol{P}$ is the square root matrix of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$. Thus, the condition (5.31) can be satisfied if

$$\chi_2 \leq \frac{U\left[c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] - z_{(1+p)/2}}{\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \quad \text{for all } x \in [a,b],$$

in another word,

$$\chi_2 \leq \inf_{x\in[a,b]} \frac{U\left[c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] - z_{(1+p)/2}}{\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}}.$$

Let

$$I(U, c_1, c_2, p) = \inf_{x\in[a,b]} \frac{U\left[c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right] - z_{(1+p)/2}}{\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}}$$

and G_S be the set in the 2-dimensional (χ_2, U)-space where

$$\chi_2 \leq I(U, c_1, c_2, p). \tag{5.32}$$

The next question is how to choose c_1 and c_2 such that

$$P\{(\chi_2, U) \in G_S\} = 1 - \alpha.$$

Denote

$$S(x) = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}},$$

$$S_1 = \inf_{x\in[a,b]} S(x) \quad \text{and} \quad S_2 = \sup_{x\in[a,b]} S(x).$$

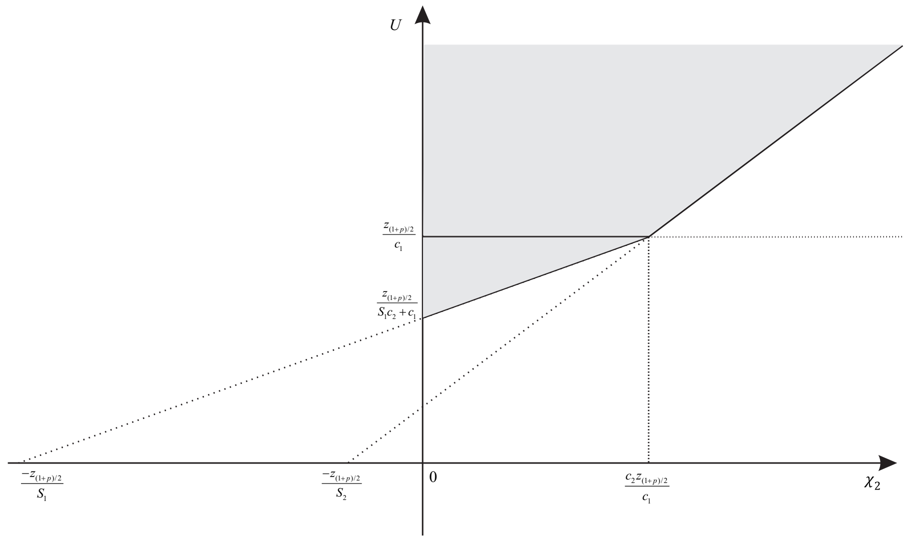


Figure 5.1: *The shaded set is G_S*

It is straightforward that

$$\begin{aligned}
I(U, c_1, c_2, p) &= c_2 U + \inf_{x\in[a,b]} \frac{c_1 U - z_{(1+p)/2}}{S(x)} \\
&= \begin{cases} c_2 U + \dfrac{c_1 U - z_{(1+p)/2}}{S_1} & \text{if } U \le z_{(1+p)/2}/c_1, \\ c_2 U + \dfrac{c_1 U - z_{(1+p)/2}}{S_2} & \text{if } U \ge z_{(1+p)/2}/c_1. \end{cases}
\end{aligned}$$

Substituting this into (5.32) gives

$$\chi_2 \le \begin{cases} \left(c_2 + S_1^{-1} c_1\right) U - S_1^{-1} z_{(1+p)/2} & \text{if } U \le z_{(1+p)/2}/c_1, \\ \left(c_2 + S_2^{-1} c_1\right) U - S_2^{-1} z_{(1+p)/2} & \text{if } U \ge z_{(1+p)/2}/c_1. \end{cases} \tag{5.33}$$

To simplify the calculation of c_1 and c_2, Scheffé (1973) defined

$$c_1 = c z_{(1+p)/2} A, \quad \text{where } A = \nu^{1/2}/\chi_{2,\alpha}(\nu)$$

with $\chi_{2,\alpha}(\nu)$ being the lower α-point of $\chi_2(\nu)$, and

$$c_2 = cB, \quad \text{where } B = \sqrt{2F_{1-\alpha}(2,\nu)}$$

with $F_{1-\alpha}(2,\nu)$ being the upper α-point of the $F(2,\nu)$ distribution. Using this in (5.33) gives

$$\chi_2 \le \begin{cases} c\left(B + S_1^{-1} z_{(1+p)/2} A\right) U - S_1^{-1} z_{(1+p)/2} & \text{if } U \le 1/(cA), \\ c\left(B + S_2^{-1} z_{(1+p)/2} A\right) U - S_2^{-1} z_{(1+p)/2} & \text{if } U \ge 1/(cA). \end{cases} \tag{5.34}$$

The constant c can be determined so that the probability of the event in (5.34) is $1-\alpha$. Denote the probability by $P(c)$. It is clear that the point $\frac{z_{(1+p)/2}}{S_1 c_2 + c_1}$ in the figure (5.21) can be written as $\frac{z_{(1+p)/2}}{c(S_1 B + z_{(1+p)/2} A)}$. Then

$$P(c) = \int_{\frac{z_{(1+p)/2}}{c(S_1 B+z_{(1+p)/2}A)}}^{\frac{1}{cA}} f_{\frac{\hat{\sigma}}{\sigma}}(u) \left\{ \int_0^{L_1(u)} f_{\chi_2}(y) dy \right\} du + \int_{\frac{1}{cA}}^{\infty} f_{\frac{\hat{\sigma}}{\sigma}}(u) \left\{ \int_0^{L_2(u)} f_{\chi_2}(y) dy \right\} du, \qquad (5.35)$$

where

$$L_1(u) = c \left(B + S_1^{-1} z_{(1+p)/2} A \right) u - S_1^{-1} z_{(1+p)/2}$$

and

$$L_2(u) = c \left(B + S_2^{-1} z_{(1+p)/2} A \right) u - S_2^{-1} z_{(1+p)/2}.$$

Recall that $f_{\frac{\hat{\sigma}}{\sigma}}(u)$ is the probability density function of U which is given in (1.4). The probability density function of χ_2 is

$$f_{\chi_2}(y) = y \exp(-y^2/2).$$

The critical constant c can be solved so that the probability $P(c)$ in (5.35) is $1-\alpha$. Scheffé's method is doubly conservative since the tolerance bands are only for central p proportion, and also involves Cauchy-Schwarz inequality. This method can be easily generalised to polynomial regression.

In fact, this method can be improved. Note that the probability of event (5.34) is

$$P(c_1, c_2) = \int_{\frac{z_{(1+p)/2}}{c_2 S_1 + c_1}}^{\frac{z_{(1+p)/2}}{c_1}} f_{\frac{\hat{\sigma}}{\sigma}}(u) \left\{ \int_0^{L_1(u)} f_{\chi_2}(y) dy \right\} du + \int_{\frac{z_{(1+p)/2}}{c_1}}^{\infty} f_{\frac{\hat{\sigma}}{\sigma}}(u) \left\{ \int_0^{L_2(u)} f_{\chi_2}(y) dy \right\} du, \qquad (5.36)$$

where

$$L_1^*(u) = \left(c_2 + S_1^{-1} c_1 \right) u - S_1^{-1} z_{(1+p)/2}$$

and

$$L_2^*(u) = \left(c_2 + S_2^{-1} c_1 \right) u - S_2^{-1} z_{(1+p)/2}.$$

Then we can search for the one pair of c_1 and c_2 directly from (5.36) such that $P(c_1, c_2) = 1 - \alpha$ and also the average width of the band is smallest.

5.3.2.3 Exact simultaneous tolerance bands for central p proportion

The focus of this section is the construction of exact two-sided $(p, 1-\alpha)$-simultaneous tolerance bands. This topic is new. The tolerance band is of the form

$$I_x(p) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \hat{\sigma}\left(z_{(1+p)/2}/\theta + c\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right) \quad \text{for all } x \in (a,b),$$

where $\theta = \sqrt{\frac{2}{\nu}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = \frac{\nu}{2}\left(\frac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$. The critical constant c can be chosen such that

$$P\left\{I_x(p) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \hat{\sigma}\left(z_{(1+p)/2}/\theta + c\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right) \text{ for all } x \in (a,b)\right\} = 1-\alpha. \tag{5.37}$$

This particular form of simultaneous tolerance bands is used because the two-sided confidence bands for the $100p$-percentile line of a similar form studied in Chapter 2 and 3 work well in comparison with several other forms and the critical constant c can be computed as shown below.

To find the critical constant c, the probability in (5.37) is written as

$$\begin{aligned} & P\left\{I_x(p) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \hat{\sigma}\left(z_{(1+p)/2}/\theta + c\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right) \text{ for all } x \in (a,b)\right\} \\ = \; & P\left\{Q* \le c\right\}, \end{aligned}$$

where

$$\begin{aligned} Q^* &= \max\left\{Q_1,\ Q_2\right\} \\ Q_1 &= \max_{x\in(a,b)} \frac{\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_{(1+p)/2}(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_{(1+p)/2})^2\xi}} \\ Q_2 &= \max_{x\in(a,b)} \frac{-\boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) + z_{(1+p)/2}(\hat{\sigma}/\theta - \sigma)}{\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + (z_{(1+p)/2})^2\xi}}. \end{aligned}$$

Note that

$$\begin{aligned} Q_1 &= \max_{x\in(a,b)} \frac{(\boldsymbol{Px})'\boldsymbol{N}/U + z_{(1+p)/2}(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_{(1+p)/2})^2\xi}} \\ Q_2 &= \max_{x\in(a,b)} \frac{-(\boldsymbol{Px})'\boldsymbol{N}/U + z_{(1+p)/2}(1/\theta - 1/U)}{\sqrt{(\boldsymbol{Px})'(\boldsymbol{Px}) + (z_{(1+p)/2})^2\xi}}, \end{aligned}$$

where $\boldsymbol{P}$ is the square root matrix of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$, $\boldsymbol{N} = \boldsymbol{P}^{-1}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}(\boldsymbol{0}, \boldsymbol{I})$ and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$ and is independent of $\boldsymbol{N}$.

Similar to Section 2.2.2, the following simple simulation-based method for finding c fast and accurately is used. A large number R of independent replicates of Q_1 : $Q_{11}, \cdots, Q_{1R}$ and Q_2 : $Q_{21}, \cdots, Q_{2R}$ are simulated. Then we get a sequence of Q^* : $Q_1^*, \cdots, Q_R^*$ satisfying $Q_j^* = \max\{Q_{1j}, Q_{2j}\},\ j = 1 \cdots, R$. The $1-\alpha$-quantile $Q_1^*, \cdots, Q_R^*$ is used as c. It is well known that this approximation approaches c almost surely as R approaches infinity, see Serfling (1980). This approach of using sample quantile to approximate the population quantile has been used successfully in solving many problems; see for example, Edwards and Berry (1987), Liu et al. (2004) and Liu et al. (2005).

In each simulation, independent $\boldsymbol{N}$ and U are simulated first and then Q_1, Q_2 and so Q^* can be computed by using projection method, turning point method or quadratic programming method as discussed in Section 2.2.2.

This method can be easily generated to polynomial regression and multiple regression.

5.3.3 The method of Mee et al. (1991)

Mee et al. (1991) proposed a method of constructing tolerance bands over a constrained region which is symmetric about the mean of the observations of the covariate variable. This method is conservative for both simple and multiple linear regression. For the simple linear regression case, Mee et al. (1991) considered the tolerance factor $k(x)$ in (5.13) as a function of $d = \delta(x) = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Suppose d belongs to a finite interval $(d_{\min}, d_{\max})$. Without loss of generality, assume the covariate is mean-centered, i.e., $\bar{x} = 0$, we have

$$d^2 = \boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} = \frac{1}{n} + \frac{(x-\bar{x})^2}{\sum(x_i-\bar{x})^2} = \frac{1}{n} + \frac{x^2}{S_{xx}},$$

where $S_{xx} = \sum x_i^2$. Then $d \in (d_{\min}, d_{\max})$ implies $x \in \mathcal{X}$, where

$$\mathcal{X} = \left(-\frac{(nd_{\max}^2-1)S_{xx}}{n}, -\frac{(nd_{\min}^2-1)S_{xx}}{n}\right) \cup \left(\frac{(nd_{\min}^2-1)S_{xx}}{n}, \frac{(nd_{\max}^2-1)S_{xx}}{n}\right).$$

It is clear that $\mathcal{X}$ is the union of two intervals symmetric about the origin 0 unless $nd_{\min}^2 - 1 = 0$. When $d_{\min}^2 = 1/n$, then $\mathcal{X} = \left(-\frac{(nd_{\max}^2-1)S_{xx}}{n}, \frac{(nd_{\max}^2-1)S_{xx}}{n}\right)$.

They constructed tolerance bands over $x \in \mathcal{X}$ as

$$P\left\{C(\boldsymbol{x'b}, k(d)U) \geq p \text{ for all } x \in \mathcal{X}\right\} > 1-\alpha. \tag{5.38}$$

Particularly they chose

$$k(d) = \lambda(z_{(1+p)/2} + 2d) \tag{5.39}$$

for the simple linear regression where $z_{(1+p)/2}$ is the $100(1+p)/2$ percentile of the standard normal distribution and λ is a constant which depends on n, p, $1-\alpha$ and $(d_{\min}, d_{\max})$.

Using Cauchy-Schwarz inequality gives

$$\begin{aligned} & \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} |\boldsymbol{x}'\boldsymbol{b}| \\ = & \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} |(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}^{-1}\boldsymbol{b})| \\ \le & \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \|(\boldsymbol{P}\boldsymbol{x})'\|\|\boldsymbol{P}^{-1}\boldsymbol{b}\| \\ = & d\|\boldsymbol{P}^{-1}\boldsymbol{b}\| \\ \sim & d\chi_2, \end{aligned} \tag{5.40}$$

where $\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & 1/\sqrt{S_{xx}} \end{pmatrix}$. It is noteworthy that the inequality in (5.40) is strict with probability 1. The constant λ in $k(d)$ was chosen by Mee et al. (1991) such that

$$\begin{aligned} & P\left\{\Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \ge p \text{ for all } d \in (d_{\min}, d_{\max})\right\} \\ = & P\left\{\min_{d_{\min}\le d\le d_{\max}} \Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \ge p\right\} \\ = & 1-\alpha. \end{aligned} \tag{5.41}$$

Note that the tolerance factor $k(d)$ determined in this way guarantees (5.38). Therefore, the table of λ values given in the paper Mee et al. (1991) are conservative. A computer program is given in Mee and Reeve (1989) for computing the constant λ such that the probability in (5.41) is $1-\alpha$. In next section, we introduce another method for the computation of λ.

5.3.3.1 A new computation method for finding $k(d)$

The simultaneous tolerance bands given in Mee et al. (1991) were recommended in the literature as they were constructed over a finite region and had no approximation involved. In this section, we give a method of computing the constant λ which satisfies

$$P\{\min_{d_{\min}\le d\le d_{\max}} \Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \ge p\} = 1-\alpha,$$

where $k(d) = \lambda(z_{(1+p)/2} + 2d)$. Denote

$$\begin{aligned} g(d) &= \Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \\ &= \Phi[d\chi_2 + \lambda(z_{(1+p)/2} + 2d)U] - \Phi[d\chi_2 - \lambda(z_{(1+p)/2} + 2d)U], \end{aligned}$$

and

$$G = \min_{d_{\min} < d < d_{\max}} g(d).$$

We have

$$g'(d) = (\chi_2 + 2\lambda U)\varphi[d\chi_2 + \lambda(z_{(1+p)/2} + 2d)U] - (\chi_2 - 2\lambda U)\varphi[d\chi_2 - \lambda(z_{(1+p)/2} + 2d)U],$$

where $\varphi(y) = \frac{1}{\sqrt{2\pi}} e^{-y^2/2}$.

For each given d value, when $\chi_2 - 2\lambda U \leq 0$, it is clear that $g'(d) > 0$ and so $G = g(d_{\min})$. When $\chi_2 - 2\lambda U > 0$, in order to find G, we need to solve the equation $g'(d) = 0$, i.e.,

$$(\chi_2 + 2\lambda U)\varphi[d\chi_2 + \lambda(z_{(1+p)/2} + 2d)U] = (\chi_2 - 2\lambda U)\varphi[d\chi_2 - \lambda(z_{(1+p)/2} + 2d)U].$$

Taking log function on both sides gives

$$\begin{aligned} & -\frac{1}{2}[(\chi_2 + 2\lambda U)d + \lambda U z_{(1+p)/2}]^2 + \log[(\chi_2 + 2\lambda U)/\sqrt{2\pi}] \\ = & -\frac{1}{2}[(\chi_2 - 2\lambda U)d + \lambda U z_{(1+p)/2}]^2 + \log[(\chi_2 - 2\lambda U)/\sqrt{2\pi}]. \end{aligned}$$

Then we have a quadratic equation in d

$$4\chi_2\lambda U d^2 + 2\chi_2\lambda U z_{(1+p)/2} d - \log\frac{\chi_2 + 2\lambda U}{\chi_2 - 2\lambda U} = 0. \tag{5.42}$$

Let the discriminant of the quadratic equation (5.42) denote by

$$\Delta = 4(\chi_2\lambda U z_{(1+p)/2})^2 + 16\chi_2\lambda U \log\frac{\chi_2 + 2\lambda U}{\chi_2 - 2\lambda U}.$$

Since $\frac{\chi_2+2\lambda U}{\chi_2-2\lambda U} > 1$, then $\log\frac{\chi_2+2\lambda U}{\chi_2-2\lambda U} > 0$. It is clear that $\Delta > 0$ and so the equation (5.42) has two roots

$$d_1 = \frac{-2\chi_2\lambda U z_{(1+p)/2} d - \sqrt{\Delta}}{8(\chi_2\lambda U z_{(1+p)/2})} \quad \text{and} \quad d_2 = \frac{-2\chi_2\lambda U z_{(1+p)/2} d + \sqrt{\Delta}}{8(\chi_2\lambda U z_{(1+p)/2})}.$$

Then

$$G = \begin{cases} \min[g(d_{\min}),\ g(d_{\max})] & \text{if } d_2 < d_{\min}, \\ \min[g(d_{\min}),\ g(d_2),\ g(d_{\max})] & \text{if } d_1 < d_{\min} < d_2 < d_{\max}, \\ \min[g(d_{\min}),\ g(d_1)\ g(d_2),\ g(d_{\max})] & \text{if } d_{\min} < d_1 < d_2 < d_{\max}, \\ \min[g(d_{\min}),\ g(d_1),\ g(d_{\max})] & \text{if } d_{\min} < d_1 < d_{\max} < d_1, \\ \min[g(d_{\min}),\ g(d_{\max})] & \text{if } d_{\max} < d_1; \end{cases}$$

The critical constant λ can be found by using the simulation method. We first generate independent variables $\chi_{2,i}$ and U_i, $i = 1, 2, \cdots, R$. Denote

$$\begin{aligned} g_i(d) &= \Phi[d\chi_{2,i} + k_i(d)U_i] - \Phi[d\chi_{2,i} - k_i(d)U] \\ &= \Phi[d\chi_{2,i} + \lambda_i(z_{(1+p)/2} + 2d)U] - \Phi[d\chi_{2,i} - \lambda_i(z_{(1+p)/2} + 2d)U_i] \end{aligned}$$

and $G_i = \min_{d_{\min}<d<d_{\max}} g_i(d)$. We can find λ_i such that the corresponding $G_i = p$, $i = 1, 2, \cdots, R$. Then λ can be approximated by the $\langle(1-\alpha)R\rangle$th largest of the R replicates of λ_i, $i = 1, 2, \cdots, R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$. We can also use numerical quadrature method to find λ. Then the probability in (5.41) becomes

$$h(\lambda) = \int_0^\infty \int_0^\infty f_{\chi_2}(x) f_{\frac{\hat\sigma}{\sigma}}(u) \boldsymbol{I}_{\left\{\min_{d_{\min}<d<d_{\max}} f(d) \geq p\right\}} dx du, \tag{5.43}$$

where $f_{\chi_2}(x)$ is the probability density function of χ_2 and $f_{\frac{\hat\sigma}{\sigma}}(u)$ is the probability density function of U. We can search the value of λ such that $h(\lambda) = 1 - \alpha$.

5.3.3.2 The choice of the constant κ

To improve the method of Mee et al. (1991), we can search for the best κ such that the band below has the smallest average band width. Denote $d = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}} = \sqrt{1/n + x^2/S_{xx}}$ and $k(d) = \lambda(z_{(1+p)/2} + \kappa d)$, where $z_{(1+p)/2}$ is the $100(1+p)/2$ percentile of the standard normal distribution and λ. This new type of simultaneous tolerance bands has the general form

$$Y(x) \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm k(d)\hat\sigma \quad \text{for all } d \in (d_{\min}, d_{\max}), \tag{5.44}$$

where $Y(x) = \boldsymbol{x}'\boldsymbol{\beta} + e$ with $e \sim N(0, 1)$. Throughout this section, we choose $d_{\min} = 1/\sqrt{n}$, then

$$x \in \left(-(nd_{\max}^2 - 1)S_{xx}/n, (nd_{\max}^2 - 1)S_{xx}/n\right).$$

Mee et al. (1991) chose $\kappa = (q + 2)^{-1/2}$ where $q - 1$ is the number of covariates. Particularly, for the simple linear regression case with $q = 2$, they used $\kappa = 2$.

Define the coverage $C(x)$ for $\boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \hat\sigma\lambda(z_{(1+p)/2} + \kappa d)$ by

$$\begin{aligned} C(x) &= P\left\{Y(x) \in \left[\boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \hat\sigma\lambda(z_{(1+p)/2} + \kappa d)\right]\right\} \\ &= \Phi\left[\boldsymbol{x}'\boldsymbol{b} + \lambda(z_{(1+p)/2} + \kappa d)U\right] - \Phi\left[\boldsymbol{x}'\boldsymbol{b} - \lambda(z_{(1+p)/2} + \kappa d)U\right], \end{aligned}$$

where $\boldsymbol{b} = (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma$ and $U = \hat\sigma/\sigma$.

Similar to (5.41), the critical constant λ in (5.44) can be determined such that

$$\begin{aligned} & P\{\Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \geq p \text{ for all } d \in (d_{\min}, d_{\max})\} \\ = \; & P\{\min_{d_{\min} \leq d \leq d_{\max}} \Phi[d\chi_2 + k(d)U] - \Phi[d\chi_2 - k(d)U] \geq p\} \\ = \; & 1 - \alpha, \end{aligned} \tag{5.45}$$

where $k(d) = \lambda(z_{(1+p)/2} + \kappa d)$. Using Cauchy-Schwarz inequality, one can easily prove that the tolerance factor $k(d)$ determined in this way can guarantee

$$P\{\Phi(\boldsymbol{x}'\boldsymbol{b} + k(d)U) - \Phi(\boldsymbol{x}'\boldsymbol{b} - k(d)U) \geq p \text{ for all } d \in (d_{\min}, d_{\max})\} > 1 - \alpha. \tag{5.46}$$

Denote $d = \sqrt{(1+\tau^2)/n}$ and $\delta = \sqrt{S_{xx}/n}$ then $x \in (-\tau\delta, \tau\delta)$. The average width of the band in (5.44) over $x \in (-\tau\delta, \tau\delta)$ is given by

$$AW_\kappa = \int_{-\tau\delta}^{\tau\delta} 2k(d)\hat{\sigma}dx/(2\tau\delta). \tag{5.47}$$

$$\begin{aligned} AW_\kappa/\hat{\sigma} &= \int_{-\tau\delta}^{\tau\delta} 2\left[\lambda(z_{(1+p)/2} + \kappa\sqrt{1/n + x^2/S_{xx}})\right] dx/(2\tau\delta) \\ &= 2z_{(1+p)/2}\lambda + \frac{\kappa\lambda}{\tau\sqrt{n}}\left[\frac{1}{2}\ln\frac{\tau + \sqrt{1+\tau^2}}{-\tau + \sqrt{1+\tau^2}} + \tau\sqrt{1+\tau^2}\right]. \end{aligned}$$

The value of κ depends on n, τ, p and $1-\alpha$. We provide the optimal values of κ in Table 5.2 for the pre-specified $p = 0.95$ and $1 - \alpha = 0.95$. The value AW_κ means the average width of a band with a specific coefficient κ, while AW_M means the average width of the band given in Mee et al. (1991). The value κ is chosen as 2 in Mee et al. (1991). In the table, for example, when $n = 100$ and $\tau = 2$, from our investigation, the 'best' $\kappa = 1$ results in the narrowest band with the average band width $4.6530\hat{\sigma}$. Comparing AW_κ with the 'best' κ to AW_M, the difference is small. From the table, we can conclude that κ does not contribute to the average band width much and so can be stuck to $\kappa = 2$ in the following construction of bands.

Table 5.2: Table of κ when $p = 0.95$ and $1 - \alpha = 0.95$

n	τ	κ	$AW_\kappa/\hat{\sigma}$	$AW_M/\hat{\sigma}$
10	0.5	1.80	7.4501	7.4508
10	1	1.80	7.6824	7.6839
10	2	1.80	8.3908	8.3944
10	3	1.80	9.2401	9.2482
10	4	1.80	10.1459	10.1595
20	0.5	1.50	5.7630	5.7657
20	1	1.50	5.8920	5.8991
20	2	1.70	6.3151	6.3219
20	3	1.80	6.8345	6.8406
20	4	1.90	7.3952	7.3986
30	0.5	1.10	5.2562	5.2615
30	1	1.20	5.3477	5.3597
30	2	1.60	5.6650	5.6794
30	3	1.70	6.0688	6.0793
30	4	1.80	6.5043	6.5134
40	0.5	1.00	5.0006	5.0067
40	1	1.10	5.0712	5.0873
40	2	1.50	5.3285	5.3500
40	3	1.70	5.6668	5.6835
40	4	1.80	6.0358	6.0482
50	0.5	1.00	4.8434	4.8499
50	1	1.00	4.9003	4.9195
50	2	1.30	5.1171	5.1453
50	3	1.60	5.4115	5.4346
50	4	1.70	5.7362	5.7536
100	0.5	0.60	4.5040	4.5117
100	1	0.70	4.5327	4.5573
100	2	1.00	4.6530	4.7020
100	3	1.10	4.8418	4.8879
100	4	1.50	5.0543	5.0967

5.3.3.3 A computation method of constructing exact bands based on Mee et al. (1991)

In fact, we can improve the method of Mee et al. (1991) by finding the exact maximum value of $|\boldsymbol{x}'\boldsymbol{b}|$ for a given $d = \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$. Since $|\boldsymbol{x}'\boldsymbol{b}| = |(\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}^{-1}\boldsymbol{b})|$, $\boldsymbol{P}^{-1}\boldsymbol{b} \sim$

$\boldsymbol{N}_2(\mathbf{0}, \boldsymbol{I}) = (N_1, N_2)'$ and $d^2 = 1/n + x^2/S_{xx}$, then

$$\begin{aligned}
& \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} |\boldsymbol{x}'\boldsymbol{b}| \\
= & \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \left| \left(\frac{1}{\sqrt{n}}, \frac{x}{\sqrt{S_{xx}}} \right) \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} \right| \\
= & \max_{d=\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}} \left| \left(\frac{N_1}{\sqrt{n}}, \frac{xN_2}{\sqrt{S_{xx}}} \right) \right| \\
= & \frac{|N_1|}{\sqrt{n}} + |N_2|\sqrt{d^2 - \frac{1}{n}}
\end{aligned}$$

The modified $k(d)$ can be calculated such that

$$\begin{aligned}
1-\alpha = P\Bigg\{ \min_{d_{\min} \le d \le d_{\max}} & \Phi\left[\frac{|N_1|}{\sqrt{n}} + |N_2|\sqrt{d^2 - \frac{1}{n}} + k(d)U \right] - \\
& \Phi\left[\frac{|N_1|}{\sqrt{n}} + |N_2|\sqrt{d^2 - \frac{1}{n}} - k(d)U \right] \ge p \Bigg\}.
\end{aligned}$$

Denote

$$\begin{aligned}
g(d) &= \Phi\left[\frac{\chi_{11}}{\sqrt{n}} + \chi_{12}\sqrt{d^2 - \frac{1}{n}} + k(d)U \right] - \Phi\left[\frac{\chi_{11}}{\sqrt{n}} + \chi_{12}\sqrt{d^2 - \frac{1}{n}} - k(d)U \right] \\
&= \Phi\left[\frac{\chi_{11}}{\sqrt{n}} + \chi_{12}\sqrt{d^2 - \frac{1}{n}} + \lambda(z_{(1+p)/2} + 2d)U \right] - \\
& \quad \Phi\left[\frac{\chi_{11}}{\sqrt{n}} + \chi_{12}\sqrt{d^2 - \frac{1}{n}} - \lambda(z_{(1+p)/2} + 2d)U \right],
\end{aligned}$$

where χ_{11} and χ_{12} are independent and $\sqrt{\chi_1^2}$ distributed. The constant λ can be found by using the simulation method. We generate independent variables $\chi_{11,i}$, $\chi_{12,i}$ and U_i, $i = 1, 2, \cdots, R$. Denote

$$\begin{aligned}
g_i(d) &= \Phi\left[\frac{\chi_{11,i}}{\sqrt{n}} + \chi_{12,i}\sqrt{d^2 - \frac{1}{n}} + \lambda(z_{(1+p)/2} + 2d)U_i \right] - \\
& \quad \Phi\left[\frac{\chi_{11,i}}{\sqrt{n}} + \chi_{12,i}\sqrt{d^2 - \frac{1}{n}} - \lambda(z_{(1+p)/2} + 2d)U_i \right]
\end{aligned}$$

Since for a given value λ, MATLAB built-in function `fmin` can be used to calculate $G_i = \min_{d_{\min} < d < d_{\max}} g_i(d)$, then we can search the values of λ_i such that the corresponding $G_i = p$, $i = 1, 2, \cdots, R$. The value of λ can be approximated by the $\langle(1-\alpha)R\rangle$ th largest of the R replicates of λ_i, $i = 1, 2, \cdots, R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$.

5.3.4 Exact simultaneous tolerance bands over any given finite interval

In this section, we present methods of constructing exact simultaneous tolerance bands over any given finite covariate interval, which includes symmetric intervals and the whole range $(-\infty, \infty)$ as special cases.

5.3.4.1 Constant-width tolerance bands over a finite interval

The hyperbolic bands proposed by Lieberman and Miller (1963) all have widths at x proportional to $\hat{\sigma}\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}$, the standard error of $\boldsymbol{x}'\hat{\boldsymbol{\beta}}$. The bands by Scheffé (1973) contained central p proportion and have widths at x equal $\hat{\sigma}\left(c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)$ for all $x \in (a, b)$, where c_1 and c_2 are constants. The bands by Mee et al. (1991) also have widths at x equal $\hat{\sigma}\left(c_1 + c_2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}}\right)$, where c_1 and c_2 are constants, but their bands are only for finite intervals which are symmetric about $\bar{x}$, the mean of the observations on the variable x. These three types of bands have a common property that the width of a band is smaller when x is nearer the center of the covariates $\bar{x}$ and becomes larger when x is further away from the center. Sometimes, one may need a band that has the same width for all $x \in (a, b)$. To the author's knowledge, there is little information in literature about two-sided simultaneous tolerance band over any finite interval $x \in (a, b)$. Two-sided constant width band is first addressed by Eberhardt and Mee (1994) and claimed as a good balance between efficiency and simplicity for linear calibration problems. A tolerance band that has the same width over the covariate interval (a, b) is called a constant width tolerance band and of the general form:

$$Y(x) \subset \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm k\hat{\sigma} \quad \text{for all } x \in (a, b),$$

where k is the critical constant determined such that

$$1-\alpha = P\left\{P_{Y(x)}\left[\boldsymbol{x}'\hat{\boldsymbol{\beta}} - k\hat{\sigma} \leq Y(x) \leq \boldsymbol{x}'\hat{\boldsymbol{\beta}} + k\hat{\sigma}\right] \geq p \;\text{ for all } x \in (a, b)\right\}. \quad (5.48)$$

Let $\boldsymbol{b} = (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \sim \boldsymbol{N}\left(\boldsymbol{0}, (\boldsymbol{X}'\boldsymbol{X})^{-1}\right)$ and $U = \hat{\sigma}/\sigma \sim \sqrt{\chi^2_\nu/\nu}$. Then (5.48) can be expressed as

$$1-\alpha = P\left\{P_N\left[\boldsymbol{x}'\boldsymbol{b} - kU \leq N \leq \boldsymbol{x}'\boldsymbol{b} + kU\right] \geq p \;\text{ for all } x \in (a, b)\right\}, \quad (5.49)$$

where $N \sim N(0,1)$. We therefore have that the critical constant k should be chosen satisfying

$$1-\alpha = P\left\{\min_{x\in(a,b)}[\Phi(\boldsymbol{x}'\boldsymbol{b}+kU)-\Phi(\boldsymbol{x}'\boldsymbol{b}-kU)]\ge p\right\}. \tag{5.50}$$

Note that $(\boldsymbol{P}^{-1}\boldsymbol{b}) \sim \boldsymbol{N}(\boldsymbol{0},\boldsymbol{I})$, where $\boldsymbol{P}$ is the square root matrix of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$, and given by

$$\boldsymbol{P} = \begin{pmatrix} 1/\sqrt{n} & 0 \\ 0 & 1/\sqrt{S_{xx}} \end{pmatrix}.$$

Let $(N_1, N_2)' = (\boldsymbol{P}^{-1}\boldsymbol{b}) \sim \boldsymbol{N}_2(\boldsymbol{0},\boldsymbol{I})$. We have

$$\boldsymbol{x}'\boldsymbol{b} = (\boldsymbol{P}\boldsymbol{x})'(\boldsymbol{P}^{-1}\boldsymbol{b}) = \frac{N_1}{\sqrt{n}} + \frac{xN_2}{\sqrt{S_{xx}}}.$$

Denote by

$$C(\boldsymbol{x}'\boldsymbol{b}, kU) = [\Phi(\boldsymbol{x}'\boldsymbol{b}+kU)-\Phi(\boldsymbol{x}'\boldsymbol{b}-kU)]$$

and

$$g(x) = |\boldsymbol{x}'\boldsymbol{b}| = \frac{N_1}{\sqrt{n}} + \frac{xN_2}{\sqrt{S_{xx}}}.$$

Note that $C(\boldsymbol{x}'\boldsymbol{b}, kU)$ is a decreasing function of $|\boldsymbol{x}'\boldsymbol{b}|$. Thus, for a given value of U, in order to find $\min_{x\in(a,b)} C(\boldsymbol{x}'\boldsymbol{b}, kU)$, we only need to find $\max_{x\in(a,b)}|g(x)|$. Since $g(x)$ is a linear function, then

$$\max_{x\in(a,b)}|g(x)| = \begin{cases} |g(a)| & \text{if } \frac{a+b}{2} \le -\frac{N_1\sqrt{S_{xx}/n}}{N_2}, \\ |g(b)| & \text{if } \frac{a+b}{2} \ge -\frac{N_1\sqrt{S_{xx}/n}}{N_2}. \end{cases}$$

Denote by $h(a,b) = \max_{x\in(a,b)}|\boldsymbol{x}'\boldsymbol{b}| = \max_{x\in(a,b)}|g(x)|$. Thus

$$\begin{aligned} h(a,b) &= \max\{|g(a)|, |g(b)|\} \\ &= \frac{|g(a)|+|g(b)|+|(|g(a)|-|g(b)|)|}{2}. \end{aligned}$$

Let $C(k) = \min_{x\in(a,b)} C(\boldsymbol{x}'\boldsymbol{b}, kU)$. Then we have, for a give value of U and a finite interval (a,b),

$$C(k) = \min_{x\in(a,b)} C(\boldsymbol{x}'\boldsymbol{b}, kU) = \Phi(h(a,b)+kU) - \Phi(h(a,b)-kU). \tag{5.51}$$

Simulation method can be used to calculate the critical constant k. Generate $\boldsymbol{N}_i = (N_{1,i}, N_{2,i})' \sim \boldsymbol{N}(\boldsymbol{0},\boldsymbol{I})$ and $U_i \sim \sqrt{\chi^2_\nu/\nu}$, $i = 1, 2, \cdots, R$. For each i and any k, $C_i(k)$ is easily calculated from (5.51), i.e.,

$$C_i(k) = \min_{x\in(a,b)} C(\boldsymbol{x}'\boldsymbol{b}, kU) = \Phi(h_i(a,b)+kU_i) - \Phi(h_i(a,b)-kU_i).$$

Then for each i, we can search for the one k_i such that

$$C_i(k_i) = p.$$

After obtaining all k_i, $i = 1, 2, \cdots, R$, we sort them in ascending order. Since $C(\boldsymbol{x}'\boldsymbol{b}, kU)$ is an increasing function of k, then the $\langle(1-\alpha)R\rangle$th largest simulated value of the R replicates of k_i, can be used as the critical constant k, that satisfies the probability in (5.48) is at least $1 - \alpha$.

We can also use numerical quadrature method since the probability statement in (5.49) can be written as

$$\mu(k) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \varphi(x_1)\varphi(x_2) f_{\frac{\hat{\sigma}}{\sigma}}(u) \boldsymbol{I}_{\{\Phi(h(a,b)+kU)-\Phi(h(a,b)-kU)\geq p\}} du dx_1 dx_2, \quad (5.52)$$

where $\varphi(x_1) = \frac{1}{\sqrt{2\pi}} e^{-x_1^2/2}$ and $\varphi(x_2) = \frac{1}{\sqrt{2\pi}} e^{-x_2^2/2}$ are the probability density function of the independent standard normal variables N_1 and N_2. Then we can search for the value of k such that $\mu(k) = 1 - \alpha$.

5.3.4.2 New exact simultaneous tolerance bands over any given finite interval

In this section, we consider simultaneous tolerance bands of the general form

$$P\left\{P_{Y(x)}\left[Y(x) \in \boldsymbol{x}'\hat{\boldsymbol{\beta}} \pm \lambda k(x)\hat{\sigma}\right] \geq p \text{ for all } x \in (a, b)\right\}, \quad (5.53)$$

where $k(x) = \left(z_{(1+p)/2}/\theta + \sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right)$, $\theta = \sqrt{\dfrac{2}{\nu}}\dfrac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}$ and $\xi = \dfrac{\nu}{2}\left(\dfrac{\Gamma(\frac{\nu}{2})}{\Gamma(\frac{\nu+1}{2})}\right)^2 - 1$. The probability in (5.53) can be written as

$$\begin{aligned} & P\left\{P\left(e/\sigma \in \boldsymbol{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})/\sigma \pm \lambda k(x)\hat{\sigma}/\sigma\right) \geq p \text{ for all } x \in (a, b)\right\} \\ = \; & P\left\{\min_{a\leq x\leq b} \Phi\left[(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N} \pm \lambda U\left(z_{(1+p)/2}/\theta + 2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right)\right] \geq p\right\}. \end{aligned}$$

The critical constant λ can be calculated by using the simulation method. We first generate independent variables $\boldsymbol{N}_i$ and U_i, $i = 1, 2, \cdots, R$. Denote

$$g_i(x) = \Phi\left[(\boldsymbol{P}\boldsymbol{x})'\boldsymbol{N}_i \pm \lambda U_i\left(z_{(1+p)/2}/\theta + 2\sqrt{\boldsymbol{x}'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x} + z^2_{(1+p)/2}\xi}\right)\right]$$

and $G_i = \min_{a<x<b} g_i(x)$. Since for a given value λ, MATLAB built-in function `fmin` can be used to calculate G_i then we can search the values of λ_i such that the corresponding $G_i = p$, $i = 1, 2, \cdots, R$. The value of λ can be approximated by the $\langle(1-\alpha)R\rangle$th

largest of the R replicates of λ_i, $i = 1, 2, \cdots, R$, where $\langle(1-\alpha)R\rangle$ denotes the integer part of $(1-\alpha)R$.

5.3.5 Comparison of the two-sided simultaneous tolerance bands under the average width criterion

To compare different simultaneous tolerance bands, we use the average width criterion. For a simultaneous tolerance band

$$\left[\boldsymbol{x}'\hat{\boldsymbol{\beta}} - k(x)\hat{\sigma}, \boldsymbol{x}'\hat{\boldsymbol{\beta}} + k(x)\hat{\sigma}\right] \quad \forall x \in (a, b),$$

the average width is

$$\frac{\int_a^b (\text{width at } x)\ dx}{b-a} = \frac{\int_a^b 2k(x)\hat{\sigma}\ dx}{b-a}$$

The smaller the average width, the better the band. In this section, we only consider five different kind of bands:

- Scheffé - the band of Scheffé (1973) in Section 5.3.2.2
- Mee - the band of Mee et al. (1991) in Section 5.3.3.1
- ExactC - the exact simultaneous tolerance band for central p proportion in Section 5.3.2.3
- Limam - the band of Limam and Thomas (1988) in Section 5.3.1.2
- Exact - the exact simultaneous tolerance bands for p-proportion over any given finite interval in Section 5.3.4.2

Mee et al. (1991) considered an example with $n = 15$, $p = 0.75$, $1 - \alpha = 0.95$. Let $(a, b) = (\tau_1\sqrt{S_{xx}/n}, \tau_2\sqrt{S_{xx}/n})$. In Mee et al. (1991), the values of τ_1 and τ_2 were chosen as -4 and 4 respectively and so the interval (a, b) is symmetric about 0. We study three different cases:

	Case1	Case2	Case3
τ_1	0	3	8
τ_2	4	4	10

The ratios of the average widths of Scheffé, Mee, ExactC, Limam relative to Exact are given in the Table 5.3.5.

Table 5.3: Ratios of the average widths relative to the Exact band

Bands	Case1	Bands	Case2	Bands	Case3
Scheffé	1.283	Scheffé	1.413	Scheffé	1.344
Limam	1.152	Limam	1.387	Limam	1.427
ExactC	1.198	ExactC	1.120	ExactC	1.093
Mee	1.076	Mee	1.199	Mee	1.241
Exact	1	Exact	1	Exact	1

We need to emphasize that none of these three intervals (a, b) considered in this example is symmetric. But in Mee et al. (1991), only conservative bands over a symmetric covarite interval can be constructed. The value 1.283 in the table is larger than 1. It means Scheffé's band under Case1 is 28% wider than our new Exact band. From our investigation, the band Exact performs better than the other bands all the time.

5.3.6 Example

Krishnamoorthy (2001) provide data from a calibration experiment of breathalyzers, which are used to measure blood alcohol concentration, see Table 5.3.6.

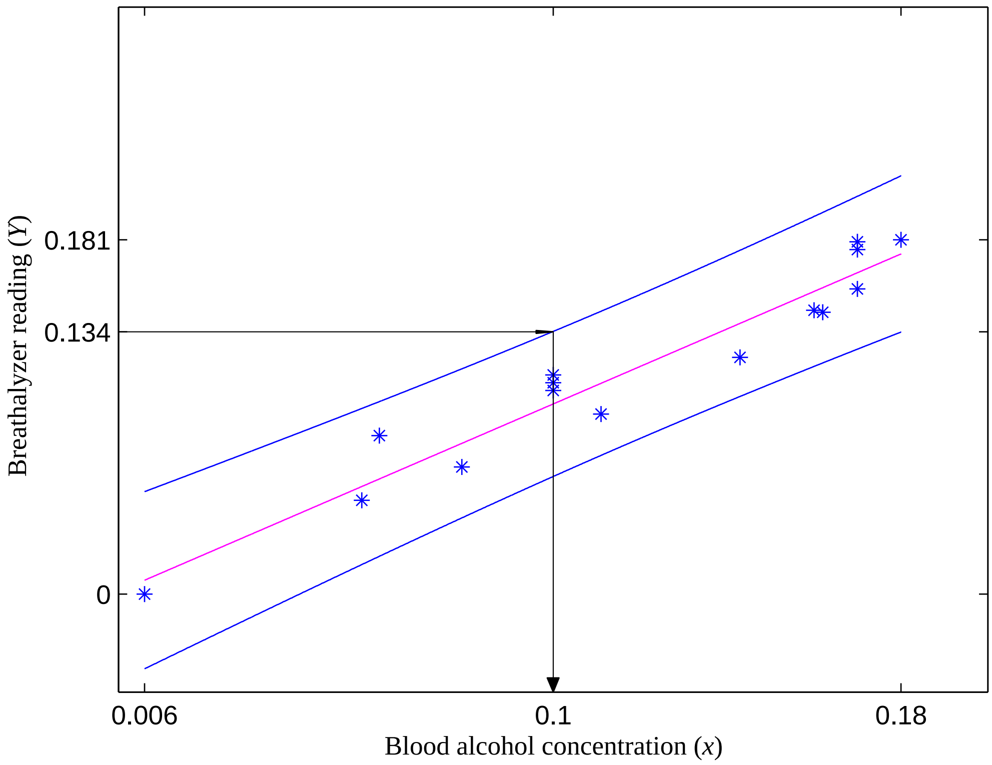
Table 5.4: Data from Krishnamoorthy *et al. (2001)*

Observation (i)	Breathalyzer (Y)	Blood alcohol concentration reading (x)
1	.145	.160
2	.156	.170
3	.181	.180
4	.108	.100
5	.180	.170
6	.112	.100
7	.081	.060
8	.104	.100
9	.176	.170
10	.048	.056
11	.092	.111
12	.144	.162
13	.121	.143
14	.065	.079
15	.000	.006

In the calibration experiment conducted in a laboratory, the percentages of alcohol concentration in blood of a sample of 15 subjects were measured on a breathalyzer

(Y) and by a laboratory test (x). The measure x is assumed to be without measurement error and so exact, as the laboratory test is accurate. A simple linear regression model can be used based on the 15 pairs of observations, with the fitted least squares line $Y = 0.0013 + .958x$, $\hat{\sigma} = 0.0137$, $R^2 = 0.93$, $\nu = 13$, $\min(x_1, \cdots, x_{15}) = .006$, $\max(x_1, \cdots, x_{15}) = .180$, $\bar{x} = .1178$, and $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2 = .0386$. To infer the true x-values corresponding to the future Y-values obtained form drivers is the main purpose of the experiment. From the policemen's point of view, a lower confidence bound on x is desirable in order to determine whether the blood alcohol concentration of a driver is above the legal limit. In many states in the USA, the legal limit is 0.1 percent. For this, one can construct the *Exact* simultaneous tolerance band based on the training data from the calibration experiment. For $p = 0.90$, $1 - \alpha = 0.95$ and $(a, b) = (.006, .180)$, the λ in the simultaneous tolerance band *Exact* is 1.0735 by using the method in the Section 5.3.4.2. When $x = 0.1$,, the upper simultaneous tolerance limit is 0.134. Hence if the breathalyzer reading of a future driver is $Y = 0.134$ or above then the lower confidence bound on the true blood alcohol concentration is at least 0.1, the legal limit. The two-sided *Exact* simultaneous tolerance band is plotted in Figure 5.1.

Figure 5.2: *The two-sided Exact STB with* $(p, 1 - \alpha) = (0.90, 0.95)$



5.4 Conclusions

Statistical calibration using regression is a useful statistical tool with many applications. The key component for inference related to infinitely many future observed Y-values is the construction of $(p, 1-\alpha)$-simultaneous tolerance bands. In this chapter, the construction of two-sided $(p, 1-\alpha)$-simultaneous tolerance bands has been considered. The method of constructing exact bands for central p proportion over any finite interval has been proposed. This method can readily be generalised to multiple regression and polynomial regression. Furthermore, a method of constructing exact simultaneous tolerance bands has been considered. This method is uniformly better than the other methods.

Chapter 6

Conclusions and Future Work

Methods have been given in this thesis to compute the exact symmetric simultaneous confidence bands for the percentile line over a finite interval of the covariate x. The work allows us to compare, in terms of average band width, the exact symmetric bands with the conservative symmetric bands which use the critical values over the entire range $x \in (-\infty, \infty)$ previously given in the literature. It is observed that the exact symmetric bands can be much narrower than the corresponding conservative symmetric bands. Furthermore, we have proposed asymmetric bands which are uniformly and can be very substantially narrower than the corresponding exact symmetric bands when $\gamma \neq 0.5$. So the asymmetric bands should always be used under the average band width criterion. The confidence bands for a percentile line generalize the confidence bands for the mean regression function and can have applications in real problems as demonstrated in the example in Chapter 3.

Turner and Bowden (1979) considered one-sided simultaneous confidence bands for a percentile line but only gave conservative critical constants over the whole range $(-\infty, \infty)$. Exact one-sided simultaneous confidence bands for a percentile line over a finite covariate interval has been studied in this thesis.

For comparison between bands, one can also use the area/volume of a confidence set corresponding to a confidence band, see Liu and Hayter (2007), instead of the average band width. Although only simple linear regression is considered in this thesis, as in several published papers, the methods proposed in this thesis can easily be generalized to multiple linear regression and polynomial regression.

Statistical calibration using regression is a useful statistical tool with many applications. The key component for inference related to infinitely many future observed Y-values is the construction of $(p, 1-\alpha)$-simultaneous tolerance bands. The central p content simultaneous tolerance bands and the bands constructed from a probability set are intrinsically conservative. Mee et al. (1991) proposed a method of constructing two-sided $(p, 1-\alpha)$-simultaneous tolerance bands over a constrained region which is symmetric about the mean of the observations of the covariate variable. This method is conservative for simple linear regression and better than other methods published in the literature.

In this thesis, the construction of exact two-sided $(p, 1-\alpha)$-simultaneous tolerance bands has been considered. The method of constructing exact bands for central p proportion over any finite interval has been proposed. This method can readily be generalised to multiple regression and polynomial regression. Furthermore, a method of constructing exact simultaneous tolerance bands has been considered. This method is uniformly better than the other methods. Simultaneous tolerance bands have applications in real problems as demonstrated in the example in Chapter 5.

6.1 Summary

The contributions of the current work to the body of knowledge may be summarised as:

- Methods given in this work allow the construction of exact symmetric simultaneous confidence bands for a percentile line over a finite covariate interval $x \in (a, b)$;
- The exact symmetric simultaneous confidence bands are uniformly narrower than the corresponding conservative symmetric bands over $x \in (a, b)$;
- Asymmetric simultaneous confidence bands proposed in this work are uniformly narrower than the corresponding exact symmetric bands over $x \in (a, b)$;
- Calibration and the construction of simultaneous tolerance bands has been discussed;
- Methods given in this work allow the construction of exact simultaneous tolerance bands over $x \in (a, b)$;
- Methods proposed in this work can be generalized to multiple regression and polynomial regression.

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