Simultaneous Confidence Bands for Linear Regression Models
Author(s): David C. Bowden
Source: *Journal of the American Statistical Association*, Vol. 65, No. 329 (Mar., 1970), pp. 413-421
Published by: Taylor & Francis, Ltd. on behalf of the American Statistical Association
Stable URL: http://www.jstor.org/stable/2283605

© Journal of the American Statistical Association
March 1970, Volume 65, Number 329
Theory and Methods Section

# Simultaneous Confidence Bands for Linear Regression Models

DAVID C. BOWDEN*

In this article a procedure is given for constructing confidence bands of various forms for linear regression models. Application of the procedure yields, as special cases, hyperbolic, straight line segment, uniform width and trapezoidal confidence bands.

## 1. INTRODUCTION

There have been a number of papers which have given procedures for obtaining confidence bands for the simple linear model. Some of the procedures have been extended to the general linear regression model. Working and Hotelling [13] developed hyperbolic bands for the simple linear model with the variance known. Hoel [10] gave an extension of these bands to the general linear model. In some recent developments Graybill and Bowden [8] presented straight line segment bands; Gafarian [7] and also Bowden and Graybill [2] gave uniform width bands for a finite interval; and Bowden and Graybill [2] presented trapezoidal bands for a finite interval. In this article extension of the uniform width and straight line segment bands are made to the general linear regression model. The procedure which generates this result also yields as a special case the bands of Working and Hotelling. Other bands of related interest are found in [1, 3, 5, 9].

The development given here stems from a paper by Dwass [4]. Dwass presented a theorem on confidence interval construction for linear contrasts in the one-way analysis of variance setting. The confidence intervals given by Scheffé and Tukey for linear contrasts and other new results were obtained as special cases of this theorem. Frank [6] extended Dwass's result to obtain simultaneous confidence intervals for all linear combinations of the mean of a $p$-variate normal distribution with known (except possibly for a multiplying constant) covariance matrix where the vector of constants of the linear combination is constrained in a subspace of $p$-dimensional reals.

The general procedure for confidence band construction is stated in Section 2. In Sections 3, 4 and 5 the technique is applied to obtain the aforementioned confidence bands. In the rest of this section some notation and distributional assumptions are stated.

The distributional assumptions are stated as a model. The model is defined as

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{e},$$

where

$$\boldsymbol{X} = \begin{bmatrix} 1 \; X_{11} - \overline{X}_1 \cdots X_{1,m-1} - \overline{X}_{m-1} \\ \cdots \\ 1 \; X_{n1} - \overline{X}_1 \cdots X_{n,m-1} - \overline{X}_{m-1} \end{bmatrix},$$

* David C. Bowden is assistant professor of mathematics and statistics, Colora search was supported in part under National Institutes of Health Training Grant #5 T author's doctoral dissertation.

$X$ is of rank $m$; $\overline{X}_j = (\sum_i X_{ij})/n \; j=1, 2, \cdots m-1$.

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_{m-1} \end{pmatrix}$$

and

$$e \sim \mathrm{MVN}[\mathbf{0}, \sigma^2 \boldsymbol{I}_n].$$

In the above, $\sim$ means "is distributed as," MVN denotes a multivariate normal distribution, and $\boldsymbol{I}_n$ is a $n \times n$ identity matrix. In the following $\hat{\boldsymbol{\beta}}$ will denote the least squares estimate of $\boldsymbol{\beta}$. Also

$$\hat{\sigma}^2 = (\boldsymbol{y}'\boldsymbol{y} - \hat{\boldsymbol{\beta}}'\boldsymbol{X}'\boldsymbol{y})/(n - m).$$

Thus the expected value of an observation $y$ at a given $\mathbf{x}$ can be written as

$$E(y) = \boldsymbol{\beta}'\mathbf{x},$$

where

$$= \begin{pmatrix} 1 \\ x_1 - \overline{X}_1 \\ \cdot \\ \cdot \\ \cdot \\ x_{m-1} - \overline{X}_{m-1} \end{pmatrix}$$

Define

$$\|a\|_p = \begin{cases} \left( \sum_{i=1}^{m} |a_i|^p \right)^{1/p} & 1 \leq p < \infty \\ \max_i |a_i| & p = \infty \end{cases}$$

where $a$ denotes any real valued, $m$-dimension vector.

## 2. GENERAL PROCEDURE

The use of Hölder's inequality as an intermediate step in obtaining simultaneous confidence intervals was pointed out by Dwass [4]. In the notation of Section 1 Hölder's inequality can be written as

$$|a'z| \leq \|a\|_q \|z\|_p,$$

where $z$ is an arbitrary $(m \times 1)$ vector of real valued numbers and $1/p + 1/q = 1$, $1 \leq p \leq \infty$. The equality holds if $a_i = (\operatorname{sgn} z_i)|z_i|^{p/q}$, $i = 1, 2, \cdots, m$ for $p < \infty$ and if $a_i$ equals one for index $i$ giving max $|z_i|$ and 0 otherwise when $p = \infty$. Thus the following lemma, as given by Frank [6], can be stated.

*Lemma.* $\max \{ |a'z| / \|a\|_q : a \neq 0 \} = \|z\|_p$ for $1 \leq p \leq \infty$ and $1/p + 1/q = 1$ where the maximum is over all non-null vectors $a$.

A general procedure for confidence band construction can now be illustrated.

Set $z=(\hat{\beta}-\beta)/\hat{\sigma}$ and $a=x$. By the lemma

$$|\hat{\beta}'x-\beta'x| \leq \hat{\sigma}||x||_q||(\hat{\beta}-\beta)/\hat{\sigma}||_p.$$

Hence if $z_p^\alpha$ is the 100 $(1-\alpha)$ percentage point of the distribution of

$$||(\hat{\beta}-\beta)/\hat{\sigma}||_p,$$

then

$$P[|\hat{\beta}'x-\beta'x| \leq \hat{\sigma}||x||_q z_p^\alpha, \ \forall x] = 1-\alpha.$$

Thus 100 $(1-\alpha)$ percent confidence bands for $\beta'x$ over all x are

$$\hat{\beta}'x \pm \hat{\sigma}||x||_q z_p^\alpha.$$

The different confidence bands (hyperbolic, straight line segment, uniform and trapezoidal) can be obtained by the right choice of $p$, $a$ and $z$. The hyperbolic bands are given as a special case in Section 3. The straight line segment bands are given as a special case in Section 4 and the uniform width bands in Section 5.

## 3. HYPERBOLIC CONFIDENCE BANDS

In this section the procedure of Section 2 is applied with $p=2$.

### 3.1 Application 1 (p=2)

Given the model stated in Section 1, then

$$P[|\hat{\beta}'x-\beta'x| \leq \hat{\sigma}z_2^\alpha[x'Ux]^{1/2}, \ \forall x] = 1-\alpha,$$

where $z_2^\alpha$ is the 100 $(1-\alpha)$ percentage point of distribution of $||z||_2$,

$$z = \frac{1}{\hat{\sigma}}Q'R'(\hat{\beta}-\beta),$$

$$U = R'^{-1}Q'^{-1}Q^{-1}R^{-1},$$

$Q$ is any non-singular symmetric $m\times m$ matrix, and $R_{m\times m}$ is such that $RR'=X'X$.

*Proof:* Set

$$a = Q^{-1}R^{-1}x$$

and

$$z = \frac{1}{\hat{\sigma}}Q'R'(\hat{\beta}-\beta).$$

Thus

$$|x'(\hat{\beta}-\beta)| = \hat{\sigma}|a'z|,$$

but

$$||a||_2 = [x'R'^{-1}Q'^{-1}Q^{-1}R^{-1}x]^{1/2}$$

and

$$\|z\|_2 = \frac{1}{\hat{\sigma}} [(\hat{\beta} - \beta)' RQQ'R'(\hat{\beta} - \beta)]^{1/2}.$$

Thus, if

$$P[\|z\|_2 \leq z_2^\alpha] = 1 - \alpha,$$

then

$$P[|\mathrm{x}'(\hat{\beta} - \beta)| \leq \hat{\sigma}\|a\|_2 z_2^\alpha, \ \forall \mathrm{x}] = 1 - \alpha.$$

An infinite series expansion for $z_2^\alpha$ can be obtained by the use of a result by Pachares [11]. If $Q=I$, one obtains the hyperbolic confidence bands for the simple linear model and their extension for the general linear regression model, and $z_2^\alpha$ can be found by using the standard $F$ tables.

## 4. STRAIGHT LINE SEGMENT CONFIDENCE BANDS

In this section the procedure of Section 2 is applied with $p=\infty$.

### 4.1 Application 2($p=\infty$)

Given the model stated in Section 1, then

$$P\left[ |\hat{\beta}'\mathrm{x} - \beta'\mathrm{x}| \leq \hat{\sigma}\left[ |\ell_1| + \sum_{i=1}^{m-1} |(x_i - \overline{X}_i)\ell_{i+1}| \right] z_\infty^\alpha, \ \forall \mathrm{x} \right] = 1 - \alpha,$$

where $\ell_i \neq 0$, $i=1, 2, \cdots, m$ and $z_\infty^\alpha$ is the 100 $(1-\alpha)$ percentage point of $\max_i |z_i|$ with $z$ defined below.

*Proof:* Let $D$ denote a $(m \times m)$ diagonal matrix with $\ell_i$ as the $i$th diagonal element. Define

$$z = \frac{1}{\hat{\sigma}} D^{-1}(\hat{\beta} - \beta)$$

and

$$a = D\mathrm{x}.$$

Since $p=\infty$ and $q=1$, the lemma gives $|\hat{\beta}'\mathrm{x} - \beta'\mathrm{x}| \leq \|D\mathrm{x}\|_1 \max_i |z_i|$. But

$$\|D\mathrm{x}\|_1 = |\ell_1| + \sum_{i=1}^{m-1} |(x_i - \overline{X}_i)\ell_{i+1}|.$$

The result follows immediately.

If $m=2$, $\ell_1 = 1/\sqrt{n}$ and $\ell_2 = 1/((\sum X_{i1} - \overline{X}_1)^2)^{1/2}$, then the result of Graybill and Bowden [8] is obtained. It can be shown for the model of Section 1 with $m=2$ that

$$z_\infty^\alpha = d/|\ell_1|\sqrt{n},$$

where

$$P[|t_1| \leq d, \ |t_2| \leq Ad] = 1 - \alpha,$$

and $t_1$ and $t_2$ are distributed as a bivariate $t$ distribution, $n-2$ degrees of freedom with zero correlation and

$$A = \frac{|\ell_2|}{|\ell_1|} \quad \frac{(\sum(X_{i1} - \overline{X}_1)^2)^{1/2}}{\sqrt{n}}.$$

The proof is straightforward and is omitted.

Table III of [2] can be used to find the $d$ value for $\alpha=.1$ and .05. Their $D$ is the same as $d$ here. If $\ell_i$ is the square root of variance of $\hat{\beta}_{i-1}$ divided by $\sigma$ then the inequality by Sidák [12] can easily be used to find an approximation of $z_\infty{}^\alpha$.

## 5. CONFIDENCE BANDS OF UNIFORM OR TRAPEZOIDAL WIDTH

In this section the procedure of Section 2 is applied with $p=1$.

### 5.1 Application 3 ($p=1$)

Given the model stated in Section 1, then

$$P\left\{ |\hat{\beta}'\mathrm{x} - \beta'\mathrm{x}| \leq \hat{\sigma} z_1{}^\alpha \max\left[1, \max_i \frac{|2x_i - (c_i + b_i)|}{(b_i - c_i)}\right], \forall \mathrm{x}\right\} = 1 - \alpha,$$

where $z_1{}^\alpha$ is the 100 $(1-\alpha)$ percentage point of the distribution of $\sum^m{}_{i=1} |z_i|$ with the $z_i$ defined below and $c_i$, $b_i(c_i<b_i)$, $i=1, 2, \cdots, m-1$ are arbitrary real constants.

*Proof:* Define $a_1=1$,

$$a_{i+1} = \frac{2x_i - (c_i + b_i)}{(b_i - c_i)}, \qquad i = 1, 2, \cdots, m - 1$$

$$z_1 = (\hat{\beta}_0 - \beta_0)/\hat{\sigma} + \sum_{i=1}^{m-1} \left(\frac{c_i + b_i}{2} - \overline{X}_i\right)(\hat{\beta}_i - \beta_i)/\hat{\sigma}$$

and

$$z_{i+1} = (b_i - c_i)(\hat{\beta}_i - \beta_i)/2\hat{\sigma}, \qquad i = 1, 2, \cdots, m - 1.$$

Then

$$|\boldsymbol{a}'\boldsymbol{z}| = |\mathrm{x}'(\hat{\beta} - \beta)|/\hat{\sigma}.$$

But by the lemma with $p=1$

$$|\boldsymbol{a}'\boldsymbol{z}| \leq \max_i a_i\left(\sum_{i=1}^m |z_i|\right).$$

The bands given by Application 3 are of uniform width in the region of the $x_i$ values for which

$$\max\left[1, \max_i \left|\frac{2x_i - (c_i + b_i)}{b_i - c_i}\right|\right] = 1.$$

The maximum is equal to one when $c_i \leq x_i \leq b_i$, $i=1, 2, \cdots, m-1$. The uniform segment of the bands for $m=2$ has been presented by Gafarian [7] and also by Bowden and Graybill [2]. One can see, however, that their results can be extended to the entire regression line. Graphically this amounts to placing straight lines through the opposite ends of the uniform width bands. The bands beyond the closed interval $[c_1, b_1]$ are those two lines.

If one changes the model into a polynomial in $x_1$, then uniform width bands can be obtained for $x_1 \in [c_1, b_1]$. This result is stated next.

### 5.2 Application 4 ($p=1$)

Given the model in Section 1 with

$$\boldsymbol{X} = \begin{bmatrix} 1 & X_{11} - \overline{X}_1 \cdots X_{11}{}^{m-1} - (\overline{X_1{}^{m-1}}) \\ & \cdots \\ 1 & X_{n1} - \overline{X}_1 \cdots X_{n1}{}^{m-1} - (\overline{X_1{}^{m-1}}) \end{bmatrix},$$

$$(\overline{X_1^j}) = \frac{1}{n}\sum_{i=1}^{n} X^j{}_{i1}; \quad j = 1, 2, \cdots, m-1$$

and

$$\mathbf{x} = \begin{bmatrix} 1 \\ x_1 - \overline{X}_1 \\ \cdot \\ \cdot \\ \cdot \\ x_1{}^{m-1} - (\overline{X_1{}^{m-1}}) \end{bmatrix},$$

then

$$P\left\{ \left| \hat{\boldsymbol{\beta}}'\mathbf{x} - \boldsymbol{\beta}'\mathbf{x} \right| \leq \hat{\sigma}(z_1')^\alpha \max \left[ 1, \left[ \frac{2x_1 - (c_1 + b_1)}{b_1 - c_1} \right]^{m-1}, \ \forall \mathbf{x} \right] \right\} \geq 1 - \alpha$$

where $c_1$ and $b_1$ are real numbers and $(z_1')^\alpha$ is the 100 $(1-\alpha)$ percentage point of the distribution of $\sum |z_i|$ with $z_i$ defined below.

*Proof:* Define

$$\begin{aligned} \boldsymbol{a}' &= [1, (2x_1 - (c_1 + b_1))/(b_1 - c_1), [(2x_1 - (c_1 + b_1))/(b_1 - c_1)]^2, \cdots, \\ &\quad [(2x_1 - (c_1 + b_1))/(b_1 - c_1)]^{m-1}], \\ z_1 &= (\hat{\beta}_0 - \beta_0)/\hat{\sigma} + \sum_{i=1}^{m-1} \left[ \left( \frac{c_1 + b_1}{2} \right)^i - (\overline{X_1{}^i}) \right] (\hat{\beta}_i - \beta_i)/\hat{\sigma}, \\ z_{k+1} &= \left( \frac{b_1 - c_1}{2} \right)^k \left[ (\hat{\beta}_k - \beta_k)/\hat{\sigma} + \sum_{j=1}^{m-k-1} \left( \frac{c_1 + b_1}{2} \right)^j \binom{k+j}{j} \right. \\ &\quad \left. \cdot (\hat{\beta}_{k+j} - \beta_{k+j})/\hat{\sigma} \right], \\ k &= 1, \cdots, m-2 \end{aligned}$$

and

$$z_m = \left(\frac{b_1 - c_1}{2}\right)^{m-1} (\hat{\beta}_{m-1} - \beta_{m-1})/\hat{\sigma}.$$

By use of the binomial expansion it can be verified that

$$|\mathbf{a}'\mathbf{z}| = |\mathbf{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})|/\hat{\sigma}.$$

The following argument shows that the inequality in Application $4(p=1)$ is appropriate. For $p=1$, as stated in general in Section 2,

$$\max_{\mathbf{a}\neq 0} \frac{|\mathbf{a}'\mathbf{z}|}{\max_i a_i} = \sum_{i=1}^{m} |z_i|.$$

However $\mathbf{a}'$ is restricted to be of the form $[1, a_*, a_*^2, \cdots, a_*^{m-1}]$. Thus if the probability is to be exactly $1-\alpha$, the following equation must hold for all subspaces in $\mathbf{z}$ space which have positive probability.

$$|z_1 + a_* z_2 + \cdots + a_*^{m-1} z_m| = \begin{cases} \displaystyle\sum_{i=1}^{m} |z_i|, & |a_*| \leq 1 \\ a_*^{m-1} \displaystyle\sum_{i=1}^{m} |z_i|, & |a_*| > 1. \end{cases}$$

For $m=3$, this can be written as

$$\frac{z_1}{\sum_{i=1}^{m} |z_i|} + \frac{z_2 a_*}{\sum_{i=1}^{m} |z_i|} + \frac{z_3 a_*^2}{\sum_{i=1}^{m} |z_i|} = \begin{cases} \pm 1, & |a_*| \leq 1 \\ \pm a_*^2, & |a_*| > 1. \end{cases}$$

Hence given the $z_i$ the problem is to solve a quadratic equation.

Straight forward calculations show that there exists a set of $\mathbf{z}$ with positive probability with no real solution to the above equation. Hence inequality is appropriate.

The last result of this section will yield Bowden and Graybill trapezoidal bands as a special case.

### 5.3 Application 5 ($p=1$)

Given the model in Section 1, with $m=2$, then

$$P\left\{ |\hat{\boldsymbol{\beta}}'\mathbf{x} - \boldsymbol{\beta}'\mathbf{x}| \leq \hat{\sigma}(z_1'')^\alpha \max\left[ \left|\frac{k+1}{b_1-c_1}\left(x_1 - \frac{c_1 k + b_1}{k+1}\right)\right|, \left|\frac{k-1}{b_1-c_1}\left(x_1 - \frac{kc_1 - b}{k-1}\right)\right| \right] \right\}, \quad \forall \mathbf{x} = 1 - \alpha,$$

where $k$ is the ratio of the width of the bands at $b_1$ to the width of the bands at $c_1$ and $(z_1'')^\alpha$ is the 100 $(1-\alpha)$ percentage point of the distribution of $\sum |z_i|$ with $\mathbf{z}$ defined below.

*Proof:* Define

$$\boldsymbol{a} = \begin{bmatrix} \dfrac{k+1}{b_1 - c_1} & \left(x_1 - \dfrac{c_1 k + b_1}{k+1}\right) \\ \dfrac{k-1}{b_1 - c_1} & \left(x_1 - \dfrac{kc_1 - b_1}{k-1}\right) \end{bmatrix}$$

and

$$\hat{\sigma}\boldsymbol{z} = \begin{bmatrix} \dfrac{1}{2k}\left\{[(c_1 k - b_1) - (k-1)\overline{X}_1](\hat{\beta}_1 - \beta_1) + (k-1)(\hat{\beta}_0 - \beta_0)\right\} \\ \dfrac{1}{2k}\left\{[(c_1 k + b_1) - (k+1)\overline{X}_1](\hat{\beta}_1 - \beta_1) + (k+1)(\hat{\beta}_0 - \beta_0)\right\} \end{bmatrix}.$$

Thus

$$\hat{\sigma}\,|\,\boldsymbol{a}'\boldsymbol{z}\,| = |\mathbf{x}'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})|\,.$$

The result follows directly. It can be shown that under the model of Section 1 if

$$P[\,|\,t_1\,| < d,\ |\,t_2\,| < Ad] = 1 - \alpha,$$

where $t_1$ and $t_2$ are distributed as a bivariate $t$ distribution with correlation $\rho$,

$$\rho = -\left(1 + \frac{(b_1 - \overline{X}_1)}{s^2}(c_1 - \overline{X}_1)\right) \Big/ \left[\left(1 + \frac{(b_1 - \overline{X}_1)^2}{s^2}\right) \cdot \left(1 + \frac{(c_1 - \overline{X}_1)^2}{s^2}\right)\right]^{1/2},$$

$n-2$ degrees of freedom, $s^2 = \sum(X_{i1} - \overline{X}_1)^2/n$ and

$$A = \left\{(1 + (b_1 - \overline{X}_1)^2/s^2)/k^2(1 + (c_1 - \overline{X}_1)^2/s^2\right\}^{1/2},$$

then

$$(z_1'')^\alpha = \frac{1}{k}\left(\frac{1}{n} + \frac{(b_1 - \overline{X}_1)^2}{ns^2}\right)^{1/2} d.$$

The proof is straight forward and is omitted. Table III of [2] can be applied with $A$ given above to obtain the value of $d$.

The trapezoidal bands of Bowden and Graybill can be obtained by setting $k$ such that

$$k^2 = (s^2 + (b_1 - \overline{X}_1)^2)/(s^2 + (c_1 - \overline{X}_1)^2).$$

It should be noted that a relationship exists between the trapezoidal bands ($p=1$) and the straight line segment bands ($p=\infty$). Consider the trapezoidal bands with $c_1 = \overline{X}_1$ and $k = (1 + (b_1 - \overline{X}_1)^2/s^2)^{1/2}$. The straight line segment bands are obtained as the limit of the trapezoidal bands as $b_1$ becomes infinite.

## REFERENCES

[1] Bowden, D. C., *Simultaneous Confidence Bands*, Doctoral dissertation, Colorado State University, Fort Collins, Colorado, 1968.

[2] Bowden, D. C. and Graybill, F. A., "Confidence Bands of Uniform and Proportional Width for Linear Models," *Journal of the American Statistical Association*, 61 (1966), 182–98.

[3] Dunn, O. J., "A Note on Confidence Bands for a Regression Line over a Finite Range," *Journal of the American Statistical Association*, 63 (1968), 1028–33.

[4] Dwass, M., "Multiple Confidence Procedures," *Annals of the Institute of Statistical Mathematics*, 10 (1959), 277–82.

[5] Folks, J. L. and Antle, C. E., "Straight Line Confidence Regions for Linear Models," *Journal of the American Statistical Association*, 62 (1967), 1365–74.

[6] Frank, O., "Simultaneous Confidence Intervals," *Skandivavisk Aktuarietidskrift*, 49 (1966), 78–84.

[7] Gafarian, A. V., "Confidence Bands in Straight Line Regression," *Journal of the American Statistical Association*, 59 (1964), 182–213.

[8] Graybill, F. A. and Bowden, D. C., "Linear Segment Confidence Bands for Simple Linear Models," *Journal of the American Statistical Association*, 62 (1967), 403–8.

[9] Halperin, M. and Gurian, J., "Confidence Bands in Linear Regression with Constraints on the Independent Variables," *Journal of the American Statistical Association*, 63 (1968), 1020–7.

[10] Hoel, P. G., "Confidence Regions for Linear Regressions," *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability*, Berkeley: University of California Press, 1951, 75–81.

[11] Pachares, J., "Note on the Distribution of a Definite Quadratic Form," *Annals of Mathematical Statistics*, 26 (1955), 128–31.

[12] Sidak, Z., "Rectangular Confidence Regions for the Means of Multivariate Normal Distributions," *Journal of the American Statistical Association*, 62 (1967), 627–33.

[13] Working, H. and Hotelling, H., "Application of the Theory of Error to the Interpretation of Trends," *Journal of the American Statistical Association*, 24 (1929), 73–85.