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Slope modified confidence bands for a simple linear regression model

A.J. Hayter[a,*], H.P. Wynn[b], W. Liu[c]

[a] Industrial and Systems Engineering, Georgia Tech, Atlanta, USA
[b] Department of Statistics, London School of Economics, London, UK
[c] School of Mathematics, University of Southampton, Southampton, UK

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Abstract

Considerable attention has been directed in the statistical literature towards the construction of confidence bands for a simple linear regression model. These confidence bands allow the experimenter to make inferences about the model over a particular region of interest. However, in practice an experimenter will usually first check the significance of the regression line before proceeding with any further inferences such as those provided by the confidence bands. From a theoretical point of view, this raises the question of what the conditional confidence level of the confidence bands might be, and from a practical point of view it is unsatisfactory if the confidence bands contain lines that are inconsistent with the directional decision on the slope. In this paper it is shown how confidence bands can be modified to alleviate these two problems.

Keywords: Simple linear regression; Confidence bands; Acceptance sets; Directional decisions

1. Introduction

Consider the standard simple linear regression model based on data (x_i, y_i), $1 \le i \le n$, so that

$$\sqrt{n}((\hat{\beta}_0 + \hat{\beta}_1\bar{x}) - (\beta_0 + \beta_1\bar{x}))/\sigma \qquad \text{and} \qquad \sqrt{S_{xx}}(\hat{\beta}_1 - \beta_1)/\sigma$$

are independently distributed as standard normal random variables, independently of $\hat{\sigma}^2 = SSE/(n-2) \sim \chi^2_{n-2}/(n-2)$, where $S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2$ and $SSE = \sum_{i=1}^n (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$.

* Corresponding author.
E-mail addresses: ajh@isye.gatech.edu (A.J. Hayter), h.wynn@lse.ac.uk (H.P. Wynn), w.liu@maths.soton.ac.uk (W. Liu).

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There has been a long history of the development of confidence bands for this regression model, dating all the way back to the hyperbolic bands of Working and Hotelling [9]

$$\beta_0 + \beta_1 x \in \hat{\beta}_0 + \hat{\beta}_1 x \pm \hat{\sigma}\sqrt{2F^{\alpha}_{2,n-2}}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{S_{xx}}} \tag{1}$$

for all $x \in \Re$ which may still be the most frequently employed bands. Wynn and Bloomfield [10] showed how to construct confidence bands of this type that guaranteed the confidence level over a restricted region, and Bohrer and Francis [1] showed how to construct just an upper bound of this type. Also, Graybill and Bowden [4] discussed confidence bands where the upper and lower bounds each consist of two straight line segments, and Gafarian [3] pioneered the work on confidence bands with a constant width over a restricted region. A common aspect of this work is that the confidence bands have been designed to achieve a stated confidence level over the region of interest. Liu et al. [7] contains a summary of recent work in this area.

However, in practice it is likely that the first analysis performed by an experimenter will be a test of the significance of the regression model. For a one-sided analysis the regression will be found to be significant when $\hat{\beta}_1 > t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$, say, and for a two-sided analysis the condition will be $|\hat{\beta}_1| > t^{\alpha/2}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$. Furthermore, if the regression is found not to be significant, then it is likely that the experimenter will not be interested in conducting any further analysis of the model. In particular, this implies that in practice the confidence bands will only be constructed and applied in situations where the regression has been found to be significant.

This *modus operandi* has two implications for the confidence bands. Firstly, from a theoretical point of view the nominal confidence level of the bands should be questioned because the probabilistic calculations should be made conditional on the regression having been found to be significant. Secondly, from a practical point of view there may be an unsatisfactory aspect to the confidence bands if, for example, they contain regression models with a negative slope while the significance test has determined that the slope is strictly positive.

The purpose of this paper is to show how these two concerns can be addressed by simple modifications to the confidence bands. When the significance of the model is assessed with a one-sided analysis, it is appropriate to take any existing confidence band methodology and to modify it by removing lines with non-positive slopes. The modified confidence bands satisfy the required confidence level with the single caveat that they should only be used when the regression model has been found to be significant. When the significance of the model is assessed with a two-sided analysis, it will be seen that similar modifications can also usually be made to the confidence bands.

The two-sided case has connections with the work of Finner [2], who showed how to construct a confidence set for a mean that contains only positive values if a two-sided test that the mean is zero is rejected with a positive estimate, and a confidence set that contains only negative values if a two-sided test that the mean is zero is rejected with a negative estimate. In a similar fashion, the objective of this paper is to provide confidence bands that only contain lines with positive slopes when the regression is found to be significant with a two-sided test and the slope estimate is positive, and to provide confidence bands that only contain lines with negative slopes when the regression is found to be significant with a two-sided test and the slope estimate is negative. Hayter and Hsu [5] also use the acceptance set approach used in this paper to produce confidence sets consistent with the decisions of stepwise testing procedures.

This paper is also related to earlier work by Olshen [8] and Kiefer [6] regarding the conditional level of confidence statements and tests. However, it is important to note that the approach used in this paper is not concerned with conditional confidence levels. Instead, the objective is to develop procedures that provide confidence bands with a required confidence level regardless of whether the regression is significant or not. Further, the procedures are developed so that the confidence bands provided in the cases where the regression is significant have desirable properties.

To clarify this point, it is useful to distinguish between a "structural" condition on the model in which the experimenter is interested (in this case whether or not the regression can be shown to be significant) and the generation of the confidence bands. In practice, these are considered sequentially so that the experimenter implements a simple decision tree. If the structural condition is not met (so that the regression is not significant) then the experimenter stops and does not proceed to the second step of confidence band construction. On the other hand, if the structural condition is met (so that the regression is significant) then the experimenter proceeds to the second step and constructs the confidence bands.

The approach taken in this paper is that the confidence level of the bands produced in step 2 will not be conditioned on the outcome of the structural event in step 1. Instead, the confidence bands are developed to have the required confidence level taken by themselves for all possible values of the model. The key point, though, is that the shape of the confidence bands can be developed with the knowledge that they will only be used when the initial structural condition is satisfied, and this allows them to be fine-tuned to meet the experimenter's requirements in this case.

Section 2 of this paper discusses the relationship between confidence bands and acceptance sets, which provides the basis for the theoretical discussion of one-sided problems in Section 3 and two-sided problems in Section 4.

2. Generating confidence bands from acceptance sets

Suppose that, for each $(\beta_0, \beta_1) \in \Re^2$, an acceptance set $A(\beta_0, \beta_1) \subseteq \Re^2$ is defined with the property that

$$P_{\beta_0,\beta_1}((\hat{\beta}_0, \hat{\beta}_1) \in A(\beta_0, \beta_1)) \geq 1 - \alpha. \quad (2)$$

Then, for a given observed value of $(\hat{\beta}_0, \hat{\beta}_1)$, these acceptance sets generate a confidence set for (β_0, β_1) with a confidence level of at least $1 - \alpha$. A particular value (β_0, β_1) is contained within the confidence set if and only if the observed value of $(\hat{\beta}_0, \hat{\beta}_1)$ is contained within the acceptance set $A(\beta_0, \beta_1)$.

Furthermore, a confidence set for (β_0, β_1) can be used to provide confidence bands for the regression line. The band at a particular x value can be constructed as the smallest interval that contains all values of $\beta_0 + \beta_1 x$ for (β_0, β_1) values within the confidence set. Consequently, it can be seen that a $1 - \alpha$ level confidence band can be generated from acceptance sets satisfying the property (2).

While the shapes of the acceptance sets are often not explicitly stated in the theoretical justification of a confidence band methodology, any confidence band can be described in this way. For example, the hyperbolic bands given in (1) are generated from acceptance sets $A(\beta_0, \beta_1)$ containing all $(\hat{\beta}_0, \hat{\beta}_1)$ values satisfying

$$n((\hat{\beta}_0 + \hat{\beta}_1\bar{x}) - (\beta_0 + \beta_1\bar{x}))^2 + S_{xx}(\hat{\beta}_1 - \beta_1)^2 \leq 2\hat{\sigma}^2 F^{\alpha}_{2,n-2} \quad (3)$$

which each have an exact coverage probability of $1 - \alpha$ (for a given value of $(\hat{\beta}_0, \hat{\beta}_1)$ the confidence set for (β_0, β_1) is also given by this inequality). In this case the acceptance sets all have the same shape, but in general there is no reason for the shapes to be identical as long as (2) is satisfied.

It is useful to consider the acceptance sets that underlie the confidence band methodologies for the theoretical discussions in Sections 3 and 4, where modifications are proposed to address the issues raised by the significance tests of the regression models. It will be seen that the trick is to find acceptance sets that automatically generate confidence bands from which the significance of the regression can be inferred, so that a separate test of the significance of the regression becomes redundant.

3. One-sided significance tests

In this case it is desirable to have a confidence band methodology for which the bands only contain lines of positive slope when $\hat{\beta}_1 > t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$ and which guarantees the required confidence level $1-\alpha$. This can be achieved by any choice of acceptance sets that satisfy (2) together with the condition

$$\beta_1 \le 0 \Rightarrow A(\beta_0, \beta_1) \cap \left\{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 > t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}\right\} = \emptyset. \tag{4}$$

Notice that if such a procedure is employed then a separate significance test of the regression is redundant because it is performed automatically by this confidence band procedure and the result of the significance test can be inferred from the confidence bands. Thus, such a procedure assuages the two concerns raised in the introduction, because firstly the probabilistic properties of the bands do not need to be conditioned on the result of a prior significance test, and secondly the bands only contain lines of positive slope when $\hat{\beta}_1 > t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$.

Any collection of acceptance sets satisfying (2) can be modified to satisfy (4). For example, an acceptance set with $\beta_1 \le 0$ that violates (4) can be changed to $\{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 \le \beta_1 + t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}\}$ and this will satisfy (2). This will modify the confidence band generated when $\hat{\beta}_1 > t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$ by removing from it those lines with a non-positive slope. The confidence sets generated for situations where $\hat{\beta}_1 \le t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}}$ will also change and may become wider, but in this case the regression is not significant and the confidence bands will not be used.

In summary, any valid $1-\alpha$ confidence band procedure can be modified in this way, whether it guarantees a confidence level over the whole real line or just over a restricted region, whether it provides upper and lower bounds or just one bound, and regardless of the shape of the confidence bands. If the experimenter only uses the confidence bands once the regression has been found to be significant, then the confidence bands can be used with the lines removed that have a non-positive slope (if there are any of them). The resulting modified bands satisfy the specified confidence level and are consistent with the slope parameter having been found to be positive.

The modified confidence bands can be illustrated with reference to the hyperbolic bands given in (1). If $\hat{\beta}_1 > \hat{\sigma}\sqrt{2F^{\alpha}_{2,n-2}}/\sqrt{S_{xx}}$, then both the upper and lower bands have strictly positive slopes over the whole real line. In this case the regression is significant and the confidence bands only contain lines with strictly positive slopes, so that they do not need to be modified. Notice that in this case the observed value $(\hat{\beta}_0, \hat{\beta}_1)$ is not contained within any of the acceptance sets (3) for $\beta_1 \le 0$, so that the confidence set for (β_0, β_1) only contains elements with $\beta_1 > 0$.

However, if $t^{\alpha}_{n-2}\hat{\sigma}/\sqrt{S_{xx}} < \hat{\beta}_1 \le \hat{\sigma}\sqrt{2F^{\alpha}_{2,n-2}}/\sqrt{S_{xx}}$, then the regression is significant but the upper band in (1) has a strictly negative slope for

$$x < x_1^* = \bar{x} - \frac{\hat{\beta}_1 S_{xx}}{\sqrt{n}\sqrt{2F_{2,n-2}^{\alpha}\hat{\sigma}^2 - S_{xx}\hat{\beta}_1^2}}$$

and the lower band has a strictly negative slope for

$$x > x_2^* = \bar{x} + \frac{\hat{\beta}_1 S_{xx}}{\sqrt{n}\sqrt{2F_{2,n-2}^{\alpha}\hat{\sigma}^2 - S_{xx}\hat{\beta}_1^2}}.$$

These confidence bands can be modified by lowering the upper bound to the value obtained at x_1^* for $x < x_1^*$ and by raising the lower bound to the value obtained at x_2^* for $x > x_2^*$. Notice that in this case some of the acceptance sets (3) with $\beta_1 < 0$ contain the observed value $(\hat{\beta}_0, \hat{\beta}_1)$. The modification alters these acceptance sets so that the confidence bands do not contain any of the negative gradient regression lines. This will affect the confidence bands that would be obtained when $\hat{\beta}_1 \leq t_{n-2}^{\alpha}\hat{\sigma}/\sqrt{S_{xx}}$ and the regression is not significant, but the experimenter will not use the confidence bands in this case.

Finally, from the point of view of desiring the confidence bands obtained when the regression is found to be significant to be as narrow as possible, it is interesting to note that it is sensible to generate confidence bands with acceptance sets for $\beta_1 > 0$ that each contain

$$\left\{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 \leq t_{n-2}^{\alpha}\hat{\sigma}/\sqrt{S_{xx}}\right\}$$

because this will allow the part of the acceptance set in the complement of this region to be as small as possible while maintaining (2). This fine-tuning of a standard confidence band procedure has the potential to eliminate some lines with small positive slopes from the confidence bands when $\hat{\beta}_1$ is just slightly larger than $t_{n-2}^{\alpha}\hat{\sigma}/\sqrt{S_{xx}}$.

4. Two-sided significance tests

If a two-sided significance test is required, then it is desirable to have a confidence band methodology for which the bands only contain lines of positive slope when $\hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$, only contain lines of negative slope when $\hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$, and which guarantees the required confidence level $1 - \alpha$. This can be achieved by any choice of acceptance sets that satisfy (2) together with the two conditions

$$\beta_1 \leq 0 \Rightarrow A(\beta_0, \beta_1) \cap \left\{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}\right\} = \emptyset \quad (5)$$

and

$$\beta_1 \geq 0 \Rightarrow A(\beta_0, \beta_1) \cap \left\{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}\right\} = \emptyset. \quad (6)$$

As before, if such a procedure is employed, then a separate significance test of the regression is redundant because it is performed automatically by this confidence band procedure and the result of the significance test can be inferred from the confidence bands.

Any collection of acceptance sets satisfying (2) can be modified to satisfy (5) and (6), and if $\hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$ this will remove lines with non-positive slopes from the confidence bands, and if $\hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$ this will remove lines with non-negative slopes from the confidence bands. However, for some confidence band procedures it may be necessary to add lines of positive slope to the confidence bands in the first case, and to add lines with negative slopes to the confidence bands in the second case. To see why this may be the case, consider an acceptance set for a strictly negative value of β_1 that violates (5). The part of the acceptance set with $\hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$ needs to be removed, and something may need to be added to the acceptance set in order to maintain a coverage probability of $1-\alpha$, as required by (2). If it is necessary to add values with $\hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$, then this may affect the confidence bands obtained when the significance test provides sufficient evidence to establish that $\beta_1 < 0$.

This problem does not arise with the modification of the hyperbolic confidence bands (1). The acceptance sets (3) violate (5) for

$$\left(t_{n-2}^{\alpha/2} - \sqrt{2F_{2,n-2}^{\alpha}}\right)\hat{\sigma}/\sqrt{S_{xx}} < \beta_1 \le 0$$

and violate (6) for

$$0 \le \beta_1 < \left(\sqrt{2F_{2,n-2}^{\alpha}} - t_{n-2}^{\alpha/2}\right)\hat{\sigma}/\sqrt{S_{xx}}.$$

Modified acceptance sets can be chosen to be

$$A(\beta_0, 0) = \left\{(\hat{\beta}_0, \hat{\beta}_1) : |\hat{\beta}_1| \le t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}\right\}$$

and

$$\begin{aligned} A(\beta_0, \beta_1) = &\left\{(\hat{\beta}_0, \hat{\beta}_1) : \beta_1 \le \hat{\beta}_1 \le \beta_1 + t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}\right\} \\ &\cup \{(\hat{\beta}_0, \hat{\beta}_1) : \hat{\beta}_1 \le \beta_1, n((\hat{\beta}_0 + \hat{\beta}_1\bar{x}) - (\beta_0 + \beta_1\bar{x}))^2 + S_{xx}(\hat{\beta}_1 - \beta_1)^2 \le 2\hat{\sigma}^2 F_{2,n-2}^{\alpha}\} \end{aligned}$$

for $(t_{n-2}^{\alpha/2} - \sqrt{2F_{2,n-2}^{\alpha}})\hat{\sigma}/\sqrt{S_{xx}} < \beta_1 \le 0$ with the symmetric version of this for $0 \le \beta_1 < (\sqrt{2F_{2,n-2}^{\alpha}} - t_{n-2}^{\alpha/2})\hat{\sigma}/\sqrt{S_{xx}}$. Notice that these modified acceptance sets all have coverage probabilities of exactly $1-\alpha$, with both components of the acceptance sets for $\beta_1 \neq 0$ each having coverage probabilities of $(1-\alpha)/2$, and that they satisfy conditions (5) and (6). Furthermore, the modified acceptances sets with $\beta_1 < 0$ do not include any additional elements with $\hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$, and the modified acceptances sets with $\beta_1 > 0$ do not include any additional elements with $\hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$.

In summary, the modified confidence bands are simply obtained by deleting lines from (1) that are inconsistent with the slope of the regression line when it has been found to be significant although, as before, if the regression is not significant then the confidence bands should not be used. Specifically, if $|\hat{\beta}_1| > \hat{\sigma}\sqrt{2F_{2,n-2}^{\alpha}}/\sqrt{S_{xx}}$, then the confidence bands (1) can be used without any modification. However, if $t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}} < |\hat{\beta}_1| \le \hat{\sigma}\sqrt{2F_{2,n-2}^{\alpha}}/\sqrt{S_{xx}}$, then the confidence bands (1) can be modified as explained at the end of Section 3. If $\hat{\beta}_1$ is positive then the confidence bands can be modified by lowering the upper bound to the value obtained at x_1^* for $x < x_1^*$ and by raising the lower bound to the value obtained at x_2^* for $x > x_2^*$. If $\hat{\beta}_1$ is negative then the confidence bands can be modified by lowering the upper bound to the value obtained at x_1^* for $x > x_1^*$ and by raising the lower bound to the value obtained at x_2^* for $x < x_2^*$.

Finally, as in the one-sided case, some fine-tuning of the acceptance sets can allow shorter confidence bands when $|\hat{\beta}_1|$ is only just large enough for the regression to be determined to be significant. In this case it is sensible to define all acceptance sets with $\beta_1 \neq 0$ to contain

$$\left\{(\hat{\beta}_0, \hat{\beta}_1) : |\hat{\beta}_1| \le t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}\right\}$$

so that for $\beta_1 > 0$ the part of the acceptance set with $\hat{\beta}_1 > t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$ is as small as possible, and for $\beta_1 < 0$ the part of the acceptance set with $\hat{\beta}_1 < -t_{n-2}^{\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}$ is as small as possible.

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