

LINEAR LEAST SQUARES ESTIMATES AND NONLINEAR MEANS

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Abstract: The consistency and asymptotic normality of a linear least squares estimate of the form $(X'X)^-X'Y$ when the mean is not $X\beta$ is investigated in this paper. The least squares estimate is a consistent estimate of the best linear approximation of the true mean function for the design chosen. The asymptotic normality of the least squares estimate depends on the design and the asymptotic mean may not be the best linear approximation of the true mean function. Choices of designs which allow large sample inferences to be made about the best linear approximation of the true mean function are discussed.

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1. Introduction

In the standard linear models theory, the mean of an observation vector Y is given by $X\beta$ where X is a known matrix of constants and β is an unknown vector of parameters. The estimate $\hat{\beta} = (X'X)^-X'Y$, where $(X'X)^-$ is a generalized inverse of $X'X$, has many well-known and desirable properties. Considering that both regression and analysis of variance problems are part of the linear models theory, estimates like $\hat{\beta}$ are among the most widely used of all parameter estimates.

If the mean Y is not $X\beta$, the properties of $\hat{\beta}$ are not described by the standard linear models theory. Indeed, it may not be clear what (if anything) $\hat{\beta}$ is estimating. The behavior of $\hat{\beta}$ for large samples when the mean is not $X\beta$ is investigated in this

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paper. This behavior is found to depend on the design used in the experiment. But, for a given design, $\hat{\beta}$ is shown to estimate the best linear approximation of the true mean function in a sense to be defined.

In Section 2, the model and notation are defined. In Section 3, $\hat{\beta}$ is shown to be a consistent estimate of the best linear approximation. The asymptotic normality of $\hat{\beta}$ is investigated in Section 4. Section 5 contains some examples. Designs which are appropriate when the variance is unknown are discussed in Section 6.

The question of 'model robustness', what $\hat{\beta}$ is estimating if the mean is not $X\beta$, has been investigated by authors such as Box and Draper (1959). A model similar to the one herein, but with random regressor variables, has been examined by White (1980, 1981). The results for the fixed regressor case obtained herein are similar to, in some respects, but have important differences with the results of White (1980). Differences between our formulation and that of Burguete, Gallant, and Souza (1982) are discussed in Section 4. Royall and Herson (1973) have described the mean of $\hat{\beta}$ for an arbitrary mean function.

2. Model and notation

Let \mathcal{X} denote a subset of an r -dimensional Euclidean space ($r \geq 1$). \mathcal{X} is the set of possible values of the independent variable x . A *design* for a sample of size n is a specification of n points, $x_{1,n}, \dots, x_{n,n}$, from \mathcal{X} where the n points specify the values of the independent variable at which observations are to be taken. The $x_{i,n}$ need not be all distinct. If a point x is repeated p times then p observations are taken at x . A design can be completely described by a discrete probability measure ξ_n on \mathcal{X} where the probability ξ_n assigns to a point x is the proportion of the n observations to be taken at x . ξ_n will also be called the design.

The observation vector is $Y_n = (Y_{1,n}, \dots, Y_{n,n})'$. It is assumed that for each n

$$Y_{i,n} = m(x_{i,n}) + \varepsilon_{i,n}, \quad i = 1, \dots, n,$$

where m , the unknown mean function, is a real-valued bounded and continuous function on \mathcal{X} and $\varepsilon_{i,n}$, $n = 1, 2, \dots$; $i = 1, \dots, n$, are identically distributed random variables with mean zero and variance σ^2 . It is also assumed that $\varepsilon_{1,n}, \dots, \varepsilon_{n,n}$ are independent for each $n = 1, 2, \dots$. Thus $Y_{1,n}, \dots, Y_{n,n}$ are independent random variables with $EY_{i,n} = m(x_{i,n})$ and variance σ^2 .

Let $f(x) = (f_1(x), \dots, f_p(x))'$ denote a $p \times 1$ vector of real-valued, bounded and continuous functions on \mathcal{X} . For a given design, $x_{1,n}, \dots, x_{n,n}$, let X_n be the $n \times p$ matrix with (i, j) th element $f_j(x_{i,n})$. The asymptotic behavior of the estimate $\hat{\beta}_n = (X_n' X_n)^{-1} X_n' Y_n$ will be investigated in this paper. $\hat{\beta}_n$ will be called a *linear least squares estimate* since, for a given observation $y_n = (y_{1,n}, \dots, y_{n,n})'$, $\hat{\beta}_n$ is the vector β which minimizes $\sum_{i=1}^n (y_{i,n} - \beta' f(x_{i,n}))^2$. Conditions under which $X_n' X_n$ is non-singular and $\hat{\beta}_n$ is uniquely defined are given in Lemmas 3.1 and 3.4.

Let ξ be a probability measure on \mathcal{X} . A $p \times 1$ vector $\beta(m, \xi)$ will be called a *best*

linear approximation of $m(x)$ if

$$\int (m(x) - \beta'(m, \xi)f(x))^2 d\xi(x) = \inf_{\beta} \int (m(x) - \beta'f(x))^2 d\xi(x). \quad (2.1)$$

Since $\beta(m, \xi)$ depends on the unknown mean function m , $\beta(m, \xi)$ is a parameter.

The experimenter chooses ξ so that the definition of best linear approximation in (2.1) accurately reflects how the experimenter wishes to measure the closeness of $\beta'f(x)$ to $m(x)$. If the support of ξ consists only of a finite number of points, $\beta'f(x)$ will be compared to $m(x)$ only at these points in determining $\beta(m, \xi)$. If the aim is to estimate a β so that $\beta'f(x)$ is close to $m(x)$ for all x in \mathcal{X} , a choice of a ξ whose support is all of \mathcal{X} , e.g., uniform on \mathcal{X} , seems more appropriate. In optimal design theory (see, e.g., Kiefer (1959) or Karlin and Studden (1966)) the optimal design often has a support with a finite number of points. These designs may not be very appropriate if the mean $m(x)$ is not of the form $\beta'f(x)$. The fact that what $\hat{\beta}_n$ is estimating depends on the design if $m(x) \neq \beta'f(x)$ has been recognized previously. See, for example, Draper and Smith (1966, Chapter 2, Section 12) or Royall and Herson (1973).

Let $M(\xi)$ denote the $p \times p$ matrix with (i, j) th element $\int f_i(x)f_j(x) d\xi(x)$ and let $c(\xi)$ denote the $p \times 1$ vector with (i) th coordinate $\int f_i(x)m(x) d\xi(x)$. In optimal design theory (see, e.g., Kiefer (1962)) a multiple of $M(\xi)$ is called the information matrix of ξ . If $M(\xi_n)$ is non-singular, $\sigma^2 n^{-1} M^{-1}(\xi_n)$ is the covariance matrix of $\hat{\beta}_n$. By equating the partial derivatives $\partial \int (m(x) - \beta'f(x))^2 d\xi(x) / \partial \beta_j$, $j = 1, \dots, p$, to zero it is easily verified that if $M(\xi)$ is non-singular then $\beta(m, \xi)$ is unique and equals $M^{-1}(\xi)c(\xi)$. Under conditions relating a sequence of designs ξ_n to ξ , it will be shown that $\hat{\beta}_n$ is a consistent estimate of $\beta(m, \xi)$ and $\hat{\beta}_n$ is asymptotically normal with mean $\beta(m, \xi)$. In this sense, the best linear approximation $\beta(m, \xi)$ is the parameter being estimated by the linear least squares estimate $\hat{\beta}_n$ when the mean $m(x)$ is not necessarily linear. The major focus of the latter part of this paper is on the construction of designs ξ_n which ensure that $\hat{\beta}_n$ can be used to make large sample inferences about $\beta(m, \xi)$.

3. Consistency

Let ξ_n be a fixed sequence of designs for sample sizes $n = 1, 2, \dots$. Throughout it will be assumed that ξ_n converges weakly to a probability measure ξ where weak convergence is defined in Billingsley (1968). The main result in this section, the proof of which is deferred until the end of the section, is the following theorem.

Theorem 3.1. *If $M(\xi)$ is non-singular, then $\hat{\beta}_n$ is a consistent estimate of $\beta(m, \xi)$ in that the random vectors $\hat{\beta}_n$ converge in probability to the real-valued vector $\beta(m, \xi) = M^{-1}(\xi)c(\xi)$.*

No assumptions have been made relating the errors, $\varepsilon_{i,n}$, $i = 1, \dots, n$, for a sample of size n to the errors, $\varepsilon_{i,n+1}$, $i = 1, \dots, n+1$, for a sample of size $n+1$. Thus, only weak consistency (convergence in probability) is obtained in Theorem 3.1. If a relationship such as $\varepsilon_{i,n} = \varepsilon_i^*$ for all $n \geq i$, where $\varepsilon_1^*, \varepsilon_2^*, \dots$ is an independent identically distributed sequence of errors, is assumed then $\hat{\beta}_n$ is a strongly consistent (almost sure convergence) estimate of $\beta(m, \xi)$. This is the type of assumption and result found in White (1980) for the random regressor problem. In the random regressor problem the measure ξ in (2.1) is the unknown probability measure for the random regressors $X_{i,n}$. The measure $\xi(x)$, in the formation herein, is chosen by the experimenter to reflect his comparison of $m(x)$ and $\beta'f(x)$.

The following lemma gives a condition under which $M(\xi)$ will be non-singular. The functions $f_1(x), \dots, f_p(x)$ are called *linearly independent*- ξ if, for a $p \times 1$ real-valued vector α , $\alpha'f(x) = 0$ a.s. ξ implies $\alpha = 0$.

Lemma 3.1. *If $f_1(x), \dots, f_p(x)$ are linear independent- ξ then $M(\xi)$ is non-singular.*

Proof. Let α be a $p \times 1$ real-valued vector. Assume $M(\xi)\alpha = 0$. To show $M(\xi)$ is non-singular it suffices to show $\alpha = 0$. $M(\xi)\alpha = 0$ implies $0 = \alpha'M(\xi)\alpha = \int (\alpha'f(x))^2 d\xi(x)$. This implies $\alpha'f(x) = 0$ a.s. ξ . Since $f_1(x), \dots, f_p(x)$ are linearly independent- ξ , $\alpha = 0$. \square

To study the asymptotic behavior of $\hat{\beta}_n$, it is useful to note that

$$\begin{aligned} \hat{\beta} &= (X_n'X_n)^{-1}X_n'Y_n \\ &= (n^{-1}X_n'X_n)^{-1}(n^{-1}X_n'\varepsilon_n) + (n^{-1}X_n'X_n)^{-1}(n^{-1}X_n'm_n) \end{aligned} \tag{3.1}$$

where $\varepsilon_n = (\varepsilon_{1,n}, \dots, \varepsilon_{n,n})'$ and $m_n = (m(x_{1,n}), \dots, m(x_{n,n}))'$. The asymptotic behavior of $n^{-1}X_n'\varepsilon_n$, $n^{-1}X_n'm_n$ and $n^{-1}X_n'X_n$ is described in the following three lemmas.

Lemma 3.2. *Under the model the random vectors $n^{-1}X_n'\varepsilon_n$ converge in probability to 0.*

Proof. It suffices to show that for any $\delta > 0$,

$$\lim_{n \rightarrow \infty} P\left(\left|\sum_{i=1}^n f_r(x_{i,n})\varepsilon_{i,n}\right| > n\delta\right) = 0 \quad \text{for } r = 1, \dots, p. \tag{3.2}$$

Let $a = \max_{1 \leq r \leq p} \sup_x f_r^2(x)$. Since the f_r are bounded, $a < \infty$. Fix $\delta > 0$. By Chebyshev's Inequality and the fact that $\varepsilon_{1,n}, \dots, \varepsilon_{n,n}$ are uncorrelated with mean zero,

$$\begin{aligned} P\left(\left|\sum_{i=1}^n f_r(x_{i,n})\varepsilon_{i,n}\right| > n\delta\right) &\leq E\left(\sum_{i=1}^n f_r(x_{i,n})\varepsilon_{i,n}\right)^2 / n^2\delta^2 \\ &= \sigma^2 \sum_{i=1}^n f_r^2(x_{i,n}) / n^2\delta^2 \leq \sigma^2 a / n\delta^2. \end{aligned}$$

Thus Equation (3.2) is true. \square

For the sake of completeness it should be noted that the result of Lemma 3.2 and hence the consistency result of Theorem 3.1 holds under the condition that for each n , $\varepsilon_{1,n}, \dots, \varepsilon_{n,n}$ are uncorrelated with means all zero and variances all bounded above by σ^2 . The stronger condition that $\varepsilon_{1,n}, \dots, \varepsilon_{n,n}$ are i.i.d. is not necessary.

Lemma 3.3. *Under the assumptions of the model, $\lim_{n \rightarrow \infty} n^{-1} X_n' m_n = c(\xi)$.*

Proof. Coordinatewise, this result is

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n f_r(x_{i,n}) m(x_{i,n}) = \int f_r(x) m(x) d\xi(x), \quad r = 1, \dots, p. \quad (3.3)$$

Note that

$$n^{-1} \sum_{i=1}^n f_r(x_{i,n}) m(x_{i,n}) = \int f_r(x) m(x) d\xi_n(x).$$

Since f_r and m are bounded and continuous and ξ_n converges weakly to ξ , Equation (3.3) is true. \square

Lemma 3.4. *If $M(\xi)$ is non-singular then:*

- (i) $\lim_{n \rightarrow \infty} n^{-1} X_n' X_n = M(\xi)$,
- (ii) $n^{-1} X_n' X_n$ is non-singular for all sufficiently large n , and
- (iii) $\lim_{n \rightarrow \infty} (n^{-1} X_n' X_n)^- = M^{-1}(\xi)$.

Proof. Elementwise, statement (i) is

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n f_r(x_{i,n}) f_s(x_{i,n}) = \int f_r(x) f_s(x) d\xi(x), \quad r, s = 1, \dots, p. \quad (3.4)$$

Note that

$$n^{-1} \sum_{i=1}^n f_r(x_{i,n}) f_s(x_{i,n}) = \int f_r(x) f_s(x) d\xi_n(x).$$

Since f_r and f_s are bounded and continuous and ξ_n converges weakly to ξ , Equation (3.4) is true.

Since the determinant is a continuous function, by (i),

$$\lim_{n \rightarrow \infty} |n^{-1} X_n' X_n| = |M(\xi)| \neq 0.$$

If A_n and A are non-singular matrices and $\lim_{n \rightarrow \infty} A_n = A$, then $\lim_{n \rightarrow \infty} A_n^{-1} = A^{-1}$. By (i) and (ii), $n^{-1} X_n' X_n$ is non-singular for all large n and (iii) is true. \square

Proof of Theorem 3.1. This theorem follows from Equation (3.1) and Lemmas 3.2, 3.3 and 3.4. \square

4. Asymptotic normality

In this section, the asymptotic normality of $n^{-1/2}(\hat{\beta}_n - \beta(m, \xi))$ is investigated. As in Section 3, it is assumed that ξ_n is a fixed sequence of designs for sample sizes $n = 1, 2, \dots$ which converges weakly to a probability measure ξ . The asymptotic normality result is given in Theorem 4.1.

Theorem 4.1. *Assume $M(\xi)$ is non-singular. Let $m_n = (m(x_{1,n}), \dots, m(x_{n,n}))$. Assume that*

$$\lim_{n \rightarrow \infty} n^{1/2}((X'_n X_n)^- X'_n m_n - \beta(m, \xi))$$

exists and equals the $p \times 1$ vector b . Then $n^{1/2}(\hat{\beta}_n - \beta(m, \xi))$ converges weakly to a multivariate normal random vector with mean b and covariance matrix $\sigma^2 M^{-1}(\xi)$.

Proof. Let $T_n = n^{-1/2} X'_n \epsilon_n$. Note that

$$n^{1/2}(\hat{\beta}_n - \beta(m, \xi)) = (n^{-1} X'_n X_n)^- T_n + n^{1/2}((X'_n X_n)^- X'_n m_n - \beta(m, \xi)). \tag{4.1}$$

By assumption, the last term converges to b . By Lemma 3.4, $\lim_{n \rightarrow \infty} (n^{-1} X'_n X_n)^- = M^{-1}(\xi)$. So to prove the desired result it suffices, by an extension of Slutsky's Theorem (Billingsley (1968), Theorem 5.5), to show that the random vectors T_n converge weakly to U where U is a p -dimensional multivariate normal random vector with mean 0 and covariance matrix $\sigma^2 M(\xi)$.

To prove the convergence of T_n to U , it suffices, by the Cramér-Wold device (Billingsley (1968), p. 48), to show that $\alpha' T_n$ converges weakly to $\alpha' U$ for all p -dimensional vectors α . Fix $\alpha \neq 0$. Let $W_{j,n} = n^{-1/2}(\alpha' f(x_{j,n})) \epsilon_{j,n}$. Then $\alpha' T_n = \sum_{j=1}^n W_{j,n}$ so it suffices to show that $\sum_{j=1}^n W_{j,n}$ converges weakly to $\alpha' U$. By the definition of $\epsilon_{j,n}$, $W_{1,n}, \dots, W_{n,n}$ are independent random variables with zero means and variances respectively equal to $n^{-1}(\alpha' f(x_{j,n}))^2 \sigma^2$. Thus it suffices, by the Normal Central Limit Theorem (Loève (1963), p. 288), to show that

$$\lim_{n \rightarrow \infty} \sum_{j=1}^n E W_{j,n}^2 = \sigma^2 \alpha' M(\xi) \alpha \tag{4.2}$$

and that

$$\lim_{n \rightarrow \infty} \sum_{j=1}^n E(W_{j,n} I(|W_{j,n}| > \delta))^2 = 0 \quad \text{for all } \delta > 0 \tag{4.3}$$

where I is the indicator function.

To verify Equation (4.2) note that $\sum_{j=1}^n E W_{j,n}^2 = \sigma^2 \alpha' (n^{-1} X'_n X_n) \alpha$. By Lemma 3.4, $\lim_{n \rightarrow \infty} (n^{-1} X'_n X_n) = M(\xi)$ so Equation (4.2) is true.

Finally to verify Equation (4.3), let $B = \sup_x |\alpha' f(x)|$. Since the f_j are bounded, $B < \infty$. Fix $\delta > 0$. Since $\epsilon_{1,n}, \dots, \epsilon_{n,n}$ are i.i.d. random variables,

$$\overline{\lim} \sum_{j=1}^n E W_{j,n}^2 I(|W_{j,n}| > \delta) \leq B^2 \overline{\lim} n^{-1} \sum_{j=1}^n E \epsilon_{j,n}^2 I(|\epsilon_{j,n}| > \delta n^{1/2} B^{-1})$$

$$\begin{aligned}
 &= B^2 \overline{\lim} E \varepsilon_{1,1}^2 I(|\varepsilon_{1,1}| > \delta n^{1/2} B^{-1}) \\
 &= 0. \quad \square
 \end{aligned}$$

White’s (1980) results on asymptotic normality for the random regressor problem differ from those of Theorem 4.1 in two respects. If the $X_{i,j}$ are a random sample from ξ then the asymptotic mean is always zero. But the asymptotic covariance matrix depends on the mean $m(x)$. In Theorem 4.1 the mean may not be zero but the covariance matrix does not depend on $m(x)$.

Burguete, Gallant, and Souza (1982) have also considered a model similar to the one considered herein. Their asymptotic normality results differ from those in Theorem 4.1 in an important way. Although $\hat{\beta}_n$ is a consistent estimate of $\beta(m, \xi)$, they do not consider $\hat{\beta}_n$ to be estimating $\beta(m, \xi)$ but rather β_n^0 , a parameter which depends on the sample size n . Indeed, they assume the data generating model changes as n changes. Their results can not be used to make large sample inferences about $\beta(m, \xi)$. In this paper the focus is on inference about $\beta(m, \xi)$, a parameter which may be of interest to the experimenter regardless of the sample size.

In Theorem 4.1, the asymptotic mean b depends on the unknown function $m(x)$. In order for Theorem 4.1 to be useful for making large sample inferences about $\beta(m, \xi)$, say to construct confidence sets for $\beta(m, \xi)$, b must be zero for all bounded, continuous functions $m(x)$. Lemmas 3.3 and 3.4 show that $(X_n' X_n)^{-1} X_n' m_n$ converges to $\beta(m, \xi)$ for all bounded, continuous $m(x)$. It is reasonable to expect that $b=0$ if ξ_n converges to ξ fast enough in some sense. Conditions under which this is true are examined in the remainder of this section. A useful result in this regard is given in Corollary 4.1. It should be noted that one important situation in which $b=0$ is if $m(x) = \beta' f(x)$ for some β . In this case $(X_n' X_n)^{-1} X_n' m_n = \beta = \beta(m, \xi)$ for all large n .

To simplify notation, for the remainder of this section assume that $\mathcal{X} = (u, v)$ an interval on the real line. Similar results hold if x is a r -dimensional vector. Let $\xi_n(x)$ and $\xi(x)$ also denote the distribution functions of the probability measures ξ_n and ξ . Assume there is a function $h(x)$ such that $\lim_{n \rightarrow \infty} n^{1/2} (\xi_n(x) - \xi(x)) = h(x)$ almost everywhere with respect to Lebesgue measure on (u, v) . Assume that

$$\int_u^v \sup_n n^{1/2} |\xi_n(x) - \xi(x)| \, dx < \infty.$$

Assume the functions m, f_1, \dots, f_p are differentiable on (u, v) . Let g' denote the derivative of a function g . The mean vector b in Theorem 3.1 can be written in terms of the function h . To obtain this result, the following lemma will be used.

Lemma 4.1. *Let $\phi(x)$ be a real-valued function defined on (u, v) with a derivative ϕ' and let $G(x)$ be a distribution function with support contained in (u, v) . Then*

$$\int_u^v \phi(x) \, dG(x) = \int_u^v \phi'(x)(1 - G(x)) \, dx + \phi(u). \tag{4.4}$$

Proof. As

$$\int_u^v \phi(x) dG(x) = \int_u^v \int_u^x \phi'(u) du dG(x) + \phi(u),$$

Equation (4.4) follows from Fubini's Theorem (Loève (1963), p. 135) by interchanging the integration order. \square

The next theorem gives an expression for the mean b of Theorem 4.1 in terms of matrices which depend on the function h . Let d denote the $p \times 1$ vector with (i) th coordinate $-\int_u^v (f_i(x)m(x))'h(x) dx$. Let D denote the $p \times p$ matrix with (i, j) th element $\int_u^v (f_i(x)f_j(x))'h(x) dx$.

Theorem 4.2. Assume $M(\xi)$ is non-singular. Then $b = M^{-1}(\xi)(d + DM^{-1}(\xi)c(\xi))$.

Proof. Let $A_n = n^{-1}X_n'X_n$. By Lemma 3.4, A_n is non-singular for all large n so we shall write A_n^{-1} for A_n^-

$$\begin{aligned} b &= \lim_{n \rightarrow \infty} n^{1/2}(A_n^{-1}(n^{-1}X_n'm_n) - M^{-1}(\xi)c(\xi)) \\ &= \lim_{n \rightarrow \infty} n^{1/2}(A_n^{-1}(n^{-1}X_n'm_n - c(\xi)) + (A_n^{-1} - M^{-1}(\xi))c(\xi)). \end{aligned}$$

To prove the desired result it suffices to prove that

$$\lim_{n \rightarrow \infty} n^{1/2}A_n^{-1}(n^{-1}X_n'm_n - c(\xi)) = M^{-1}(\xi)d \tag{4.5}$$

and

$$\lim_{n \rightarrow \infty} n^{1/2}(A_n^{-1} - M^{-1}(\xi))c(\xi) = M^{-1}(\xi)DM^{-1}(\xi)c(\xi). \tag{4.6}$$

By Lemma 3.4, $\lim_{n \rightarrow \infty} A_n^{-1} = M^{-1}(\xi)$. Thus to prove Equation (4.5) it suffices to show that

$$\begin{aligned} &\lim_{n \rightarrow \infty} n^{1/2} \left(\int_u^v f_r(x)m(x) d\xi_n(x) - \int_u^v f_r(x)m(x) d\xi(x) \right) \\ &= -\lim_{n \rightarrow \infty} \int_u^v (f_r(x)m(x))' n^{1/2}(\xi_n(x) - \xi(x)) dx \\ &= -\int_u^v (f_r(x)m(x))' h(x) dx, \quad r = 1, \dots, n. \end{aligned} \tag{4.7}$$

The first equality is true by Lemma 4.1 and the second equality is true by the assumptions made about $n^{1/2}(\xi_n(x) - \xi(x))$ and the Dominated Convergence Theorem (Loève (1963), p. 125).

Note that $A_n^{-1} - M(\xi) = A_n^{-1}(M(\xi) - A_n)M^{-1}(\xi)$. By Lemma 3.4, $\lim_{n \rightarrow \infty} A_n^{-1} = M^{-1}(\xi)$. Thus to prove Equation (4.6) it suffices to show that

$$\begin{aligned}
 & \lim_{n \rightarrow \infty} n^{1/2} \left(\int_u^v f_r(x) f_s(x) d\xi(x) - \int_u^v f_r(x) f_s(x) d\xi_n(x) \right) \\
 &= \lim_{n \rightarrow \infty} \int_u^v (f_r(x) f_s(x))' n^{1/2} (\xi_n(x) - \xi(x)) dx \\
 &= \int_u^v (f_r(x) f_s(x)) h(x) dx, \quad r = 1, \dots, p; s = 1, \dots, p.
 \end{aligned}
 \tag{4.8}$$

The first equality is true by Lemma 4.1 and the second equality is true by the assumptions made about $n^{1/2}(\xi_n(x) - \xi(x))$ and the Dominated Convergence Theorem. \square

Corollary 4.1. *Assume $M(\xi)$ is non-singular. If $\lim_{n \rightarrow \infty} n^{1/2}(\xi_n(x) - \xi(x)) = 0$ almost everywhere with respect to Lebesgue measure on (u, v) then $n^{1/2}(\hat{\beta}_n - \beta(m, \xi))$ converges weakly to a multivariate normal random vector with mean 0 and covariance matrix $\sigma^2 M^{-1}(\xi)$.*

Proof. $h(x) = \lim_{n \rightarrow \infty} n^{1/2}(\xi_n(x) - \xi(x)) = 0$ a.e. implies $d = 0$ and $D = 0$. Thus by Theorem 4.2, the mean b in Theorem 4.1 is 0. \square

5. Examples

In this section two examples are considered. In the first example a fairly general method of constructing designs which satisfy the conditions of Corollary 4.1 is given. The second example gives a sequence of designs for which the function $h(x)$ is non-zero.

Example 1. Let $\xi(x)$ be a fixed continuous and strictly increasing distribution function on the real line. Let $\xi^{-1}(x)$ denote the inverse of $\xi(x)$. Let n_1, n_2, \dots and m_1, m_2, \dots be sequences of positive integers such that n_i/m_i is an integer for each i and $\lim_{i \rightarrow \infty} m_i/n_i^{1/2} = 0$. For $k = 1, \dots, n_i/m_i$, let $I_{k,i}$ denote the interval $(\xi^{-1}((k-1)m_i/n_i), \xi^{-1}(km_i/n_i))$. Let ξ_{n_i} denote any design with m_i observations in each of the intervals $I_{k,i}$. Then ξ_{n_i} converges weakly to ξ . Furthermore, $\sup_{\mathcal{X}} |\xi_{n_i}(x) - \xi(x)| \leq m_i/n_i$. So since $\lim_{i \rightarrow \infty} m_i/n_i^{1/2} = 0$, $\lim_{i \rightarrow \infty} n_i^{1/2}(\xi_{n_i}(x) - \xi(x)) = 0$. By Corollary 4.1, the mean vector in Theorem 4.1 is zero for a sequence of designs constructed in this way. A special case of interest is the case of $m_i = N$ for some fixed N and $n_i = Ni$.

Example 2. Here is an example of a sequence of designs for which the $h(x)$ function is non-zero and, by Theorem 4.2, the mean vector b in Theorem 4.1 is not zero for all mean functions $m(x)$. Let $[u, v] = [0, 1]$ and let ξ be the uniform distribution on $[0, 1]$. Let $n_i = i^2$ for $i = 1, 2, \dots$. Let ξ_{n_i} be the design which takes one observation

at each of the $i^2 - i$ points $1/i + k/i^2$, $k = 0, 1, \dots, i^2 - i - 1$, and i observations at 1. For each i , $x - 1/i < \xi_{n_i}(x) \leq x$ for all $x \in [0, 1]$ so $\xi_{n_i}(x)$ converges to $\xi(x)$. But for any i and any $x \in (1/i, 1)$,

$$-1/i < \xi_{n_i}(x) - \xi(x) \leq -1/i + 1/i^2.$$

Thus for all $x \in (0, 1)$,

$$\begin{aligned} h(x) &= \lim_{i \rightarrow \infty} n_i^{1/2}(\xi_{n_i}(x) - \xi(x)) \\ &= \lim_{i \rightarrow \infty} i(\xi_{n_i}(x) - \xi(x)) = -1. \end{aligned}$$

Suppose $f_1(x) = 1$ and $f_2(x) = x$. Suppose $m(x) = x^2$. Then using the result of Theorem 4.2, the mean vector b can be calculated to be $b = (-1, 2)'$.

6. Inferences when σ^2 is unknown

Corollary 4.1 states that if

$$\lim_{n \rightarrow \infty} n^{1/2}(\xi_n(x) - \xi(x)) = 0 \tag{6.1}$$

a.e. on \mathcal{X} , then $n^{1/2}(\hat{\beta}_n - \beta(m, \xi))$ has an asymptotic multivariate normal distribution with mean 0 and covariance matrix $\sigma^2 M^{-1}(\xi)$. This asymptotic distribution can be used to make large sample inferences about $\beta(m, \xi)$ if σ^2 is known. Typically the parameter σ^2 is unknown. But if a consistent estimate s^2 of σ^2 is available, then the asymptotic distribution can still be used to make large sample inferences about $\beta(m, \xi)$.

The usual estimate of σ^2 , $(Y_n - X_n \hat{\beta}_n)'(Y_n - X_n \hat{\beta}_n)/(n - p)$ is a positively biased estimate of σ^2 if $m(x) \neq \beta'f(x)$. This is discussed for the simple linear regression case in Draper and Smith (1966, Section 1.5). If this estimate is used, the resulting inference procedures will be conservative. But if ξ_n is a sequence of designs satisfying (6.1), then there exists a sequence of designs ξ_n^* which also satisfies (6.1) and admits a consistent, 'pure error' estimate of σ^2 . This fact is explained in this section.

If s^2 is a consistent estimate of σ^2 , $M(\xi)$ is nonsingular, and (6.1) is satisfied, then, by Corollary 4.1, $n(\hat{\beta}_n - \beta(m, \xi))'M(\xi)(\hat{\beta}_n - \beta(m, \xi))/s^2$ converges weakly to a chi-squared random variable with p degrees of freedom. Let $\chi_p^2(\alpha)$ denote the α th percentile of a chi-squared distribution with p degrees of freedom. Then an approximate $100(1 - \alpha)\%$ confidence region for $\beta(m, \xi)$ is given by

$$\{\beta: n(\hat{\beta}_n - \beta)'M(\xi)(\hat{\beta}_n - \beta)/s^2 \leq \chi_p^2(1 - \alpha)\}. \tag{6.2}$$

The test which rejects $H_0: \beta(m, \xi) = \beta_0$ if

$$n(\hat{\beta}_n - \beta_0)'M(\xi)(\hat{\beta}_n - \beta_0)/s^2 > \chi_p^2(1 - \alpha) \tag{6.3}$$

is an approximate size α test of H_0 .

An unbiased, consistent, ‘pure error’ estimate of σ^2 may be obtained in this way. Let $[a]$ denote the greatest integer not greater than a . Let $\varepsilon, 0 < \varepsilon < \frac{1}{2}$, be a fixed number. Suppose ξ_n is a sequence of designs for sample sizes $n = 1, 2, \dots$ which satisfies (6.1). Let x_0 be an arbitrary fixed point in \mathcal{X} and $\delta_{x_0}(x)$ the distribution function of a point mass at x_0 . Consider the sequence of designs ξ_n^* defined by

$$\xi_n^*(x) = ([n^\varepsilon]/n)\delta_{x_0}(x) + ((n - [n^\varepsilon])/n)\xi_{n - [n^\varepsilon]}(x).$$

ξ_n^* is a design for a sample of size n which takes $[n^\varepsilon]$ observations at x_0 and $n - [n^\varepsilon]$ observations distributed according to $\xi_{n - [n^\varepsilon]}$.

Let $Y_1, \dots, Y_{[n^\varepsilon]}$ denote the $[n^\varepsilon]$ observations at x_0 and $\bar{Y}_{[n^\varepsilon]}$ the sample mean of these observations. Then

$$s_n^2 = \sum_{i=1}^{[n^\varepsilon]} (Y_i - \bar{Y}_{[n^\varepsilon]})^2 / ([n^\varepsilon] - 1)$$

is an unbiased, consistent estimate of σ^2 since it is just a usual sample variance. (Here we have assumed that the errors $\varepsilon_{i,n}$ have a finite fourth moment.) This s_n^2 may be used for s^2 in (6.2) or (6.3). Furthermore, the sequence ξ_n^* satisfies (6.1), to see this note that

$$\begin{aligned} n^{1/2} |\xi_n^*(x) - \xi(x)| &\leq \frac{n^{1/2}[n^\varepsilon]}{n} |\delta_{x_0}(x) - \xi_{n - [n^\varepsilon]}(x)| \\ &\quad + \frac{n^{1/2}(n - [n^\varepsilon])^{1/2}}{(n - [n^\varepsilon])^{1/2}} |\xi_{n - [n^\varepsilon]}(x) - \xi(x)|. \end{aligned} \tag{6.4}$$

It suffices to show that the right-hand side converges to zero a.e. on \mathcal{X} . The first term on the right-hand side converges to zero for all x since $(n^{1/2}[n^\varepsilon]/n)$ converges to zero and $0 \leq |\delta_{x_0}(x) - \xi_{n - [n^\varepsilon]}(x)| \leq 1$ for all x . The last term in (6.4) converges to zero a.e. on \mathcal{X} since $(n/(n - [n^\varepsilon]))^{1/2}$ converges to one and $(n - [n^\varepsilon])^{1/2} |\xi_{n - [n^\varepsilon]}(x) - \xi(x)|$ converges to zero a.e. on \mathcal{X} . This last fact is true since $n - [n^\varepsilon]$ converges to infinity and the sequence ξ_n satisfies (6.1). Thus the sequence of designs ξ_n^* and the estimate s_n^2 can be used to make large sample inference about $\beta(m, \xi)$ in (6.2) or (6.3).

The above scheme is only one of many ways in which a consistent estimate of σ^2 can be obtained. As another example, consider the designs in Example 1. Suppose the m_i observations in $I_{k,i}$ are all taken at the same $x_{k,i} \in I_{k,i}$. Let $Y_{j,k,i}, j = 1, \dots, m_i$, denote the observations at $x_{k,i}$ and let $\bar{Y}_{k,i}$ denote their sample mean. Then

$$s_{n_i}^2 = \sum_{k=1}^{n_i/m_i} \sum_{j=1}^{m_i} (Y_{j,k,i} - \bar{Y}_{k,i})^2 / (n - n_i/m_i)$$

is an unbiased, consistent, ‘pure error’ estimate of σ^2 which may be used in (6.2) and (6.3).

Lemma 4.1, Theorem 4.2, and Corollary 4.1 were proved only for \mathcal{X} an interval on the real line. But since similar results hold for x an r -dimensional vector, the

method of constructing designs discussed in this section can be used to obtain an estimate of σ^2 when x is a vector.

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