# NONPARAMETRIC TESTS FOR BOUNDS ON THE DERIVATIVE OF A REGRESSION FUNCTION

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**Abstract.** We consider two tests of the null hypothesis that the k-th derivative of a regression function is uniformly bounded by a specified constant. These tests can be used to study the shape of the regression function. For instance, we can test for convexity of the regression function by setting k = 2 and the constant equal to zero. Our tests are based on k-th order divided difference of the observations. The asymptotic distribution and efficacies of these tests are computed and simulation results presented.

*Key words and phrases*: Derivative of a regression function, convexity, divided differences.

# 1. Introduction

In some regression analyses, determining certain characteristics of the regression function is more important than obtaining an accurate estimate of the function. For instance, in evolutionary ecology, it is important to determine if the dependence of the probability of survival upon some physical trait is monotone, convex, or concave. The shape of the function determines how the physical trait evolves in the population (see, e.g. Schluter (1988)). Another example of research involving the shape of a regression function is in the analysis of human growth data. The "pubertal spurt" is a rapid period of growth typically occurring at twelve years of age in girls and fourteen years of age in boys. Determining the age span of this spurt involves studying the convexity of height as a function of age. (See, e.g. Gasser *et al.* (1984), for analyses of these types of data.) Here, we study testing that the k-th derivative of the regression function is bounded by a specified number.

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Suppose that the regression function f has k continuous derivatives on a compact interval, which we take to be [0, 1]. We wish to test the hypothesis

(1.1) 
$$H_0: f^{(k)}(t) \le \gamma \quad \text{for all} \quad t \in [0, 1].$$

The test is based on observations

(1.2) 
$$X_i = f(t_i) + \epsilon_i, \quad 1 \le i \le n,$$

where the  $\epsilon_i$ 's are independent and identically distributed with mean zero and  $t_i = i/(n+1)$ . (If one wishes to test  $f^{(k)}(t) \geq \gamma$  instead of (1.1), one uses the proposed statistics with  $X_i$  replaced by  $-X_i$ . If one wishes to test that  $f^{(k)}(t) \leq g(t)$  for all t, for some specified g, one uses the proposed statistics, but with  $X_i$  replaced by  $X_i - G(t_i)$ , where G is any function with  $G^{(k)}(t) \equiv g(t)$ .) Two test statistics, T and S, are defined in Section 2. Both statistics count the number of divided differences of the  $X_i$ 's which are greater than or equal to a specified threshold, and  $H_0$  is rejected if this number is too large. If k = 1 and the specified threshold is chosen appropriately, S is the Mann T-test (Mann (1945)) which is used to test the hypothesis that f is constant, versus the alternative that f is non-decreasing. The Mann test rejects the null hypothesis if the number of times that  $X_i - X_j > 0$ , i > j, is too large. The statistic T is equivalent to a test proposed by Sen (1965) in a time series setting. Sen studied T's null distribution, but not its efficacy, as we do here.

In Section 2 we give the asymptotic distributions of S and T assuming f is on the "boundary" of the null hypothesis,  $f^{(k)}(t) \equiv \gamma$ , and assuming that  $f = f_n$ , a sequence of regression functions local to the null hypothesis. These results can be used to calculate the asymptotic significance levels of the tests and the efficacies. The efficacies are discussed in Section 4. Unfortunately, when  $k \neq 1$ , the asymptotic variances of the statistics depend upon unknown parameters. In Section 3, we present estimates of these parameters. Section 5 contains simulation results. The simulation results and the efficacy calculations indicate that the test statistic S is a good one, particularly if the data contain outliers.

It is possible to construct statistics to test  $H_0: \gamma_1 \leq f^{(k)}(t) \leq \gamma_2$  for all  $t \in [0, 1]$  by counting the number of divided differences of the  $X_i$ 's that fall within a specified interval. For a sequence of functions  $\{f_n\}$  approaching a fixed function, the asymptotic distributions of the test statistics are easily derived by the methods of this paper. However, it is very difficult, if not impossible, to determine the significance levels of the tests, that is, to calculate the supremum, over  $H_0$ , of the probability of rejecting  $H_0$ . Therefore, we do not analyse these tests here.

# 2. Definitions and main results

Suppose that (1.2) holds. We test the null hypothesis  $H_0: f \in \mathcal{F}_{\gamma,k}$ , where

$$\mathcal{F}_{\gamma,k} \equiv \mathcal{F} = \{f : [0,1] \to \mathcal{R} : f \text{ has } k \text{ continuous derivatives and}$$

$$f^{(\kappa)}(t) \leq \gamma \text{ for all } t \in [0,1] \}$$

Our test statistics count the number of k-th order divided differences of the  $X_i$ 's that are larger than a specified value. For instance, when k = 1 and the specified value is c, S is equal to the number of times that  $(X_i - X_j)/(t_i - t_j) \ge c$  for i > j. The statistic T depends on an integer m, chosen by the user. When, say, k = 1 and m = 3, T is equal to the number of times that  $(X_i - X_{i-3})/(t_i - t_{i-3}) \ge c$ . When c = 0 and k = 1, S is equivalent to the statistic studied by Mann (1945). When c = 0, the statistic T is equivalent to one proposed by Sen (1965).

To define S and T for general k, we recursively define  $(\Delta^{m,k} \mathbf{X})_i$ , the k-th order divided difference with spacing m evaluated at i of the n-vector  $\mathbf{X} = (X_1, \ldots, X_n)^t$ as follows. (The dependence upon n is suppressed in the notation.) For k = 0 and  $1 \le i \le n$ 

$$(\Delta^{m,0}\boldsymbol{X})_i = X_i.$$

For k = 1 and  $m + 1 \le i \le n$ 

$$(\Delta^{m,1} \boldsymbol{X})_i = \frac{n+1}{m} (X_i - X_{i-m}) = \frac{n+1}{m} ((\Delta^{m,0} \boldsymbol{X})_i - (\Delta^{m,0} \boldsymbol{X})_{i-m}).$$

For general k and  $km + 1 \le i \le n$ 

$$(\Delta^{m,k}\boldsymbol{X})_i = \frac{n+1}{m} ((\Delta^{m,k-1}\boldsymbol{X})_i - (\Delta^{m,k-1}\boldsymbol{X})_{i-m})$$

To count the number of times that a k-th order divided difference exceeds the specified value c let

$$W_i^m = W_i^{m,k}(c) = I\{(\Delta^{m,k} \boldsymbol{X})_i \ge c\}$$

for  $km + 1 \leq i \leq n$ . Then our two test statistics are

$$T_c^n = T_c^n(m,k) = \sum_{i=km+1}^n W_i^m$$

and

$$S_c^n = S_c^n(k) = \sum_{m=1}^{[(n-1)/k]} \sum_{i=km+1}^n W_i^m = \sum_{m=1}^{[(n-1)/k]} T_c^n(m,k)$$

We will reject  $H_0$  if either  $T_c^n$  or  $S_c^n$  is too large.

The asymptotic significance levels and the efficacies of the test statistics are given in Theorems 2.1 to 2.3 below. We assume that the distribution of  $\epsilon_1$  is continuous. The Appendix contains the proofs of these theorems, in addition to proofs of the asymptotic normality of the test statistics under more general conditions.

First consider the statistic  $S_c^n$ . To define its asymptotic mean and variance, we introduce random variables  $U, U_1(l, l')$ , and  $U_2(l, l'), l, l' = 0, \ldots, k$ . Let

(2.1) 
$$U = \left(\frac{m}{n+1}\right)^k (\Delta^{m,k} \boldsymbol{\epsilon})_i,$$

where  $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_n)^t$ . Notice that the distribution of U depends only upon k and the distribution of  $\epsilon_1$ . For fixed l, l', m, m', i, and i' with  $\{i - km, \ldots, i - m, i\} \cap \{i' - km', \ldots, i' - m', i'\} = \{i - lm\} = \{i' - l'm'\}, (\Delta^{m,k}\boldsymbol{\epsilon})_i \text{ and } (\Delta^{m',k}\boldsymbol{\epsilon})_{i'} \text{ involve}$ exactly one common  $\boldsymbol{\epsilon}$ , namely  $\boldsymbol{\epsilon}_{i-lm} = \boldsymbol{\epsilon}_{i'-l'm'}$ . Thus the joint distribution of  $(m/(n+1))^k (\Delta^{m,k}\boldsymbol{\epsilon})_i$  and  $(m'/(n+1))^k (\Delta^{m',k}\boldsymbol{\epsilon})_{i'}$  does not depend upon n, m, m', i, or i': it depends only upon the position of the "overlap" determined by l, l', and k and upon the distribution of  $\boldsymbol{\epsilon}_1$ . Therefore, we can define

$$(U_1(l,l'),U_2(l,l')) = \left( \left(\frac{m}{n+1}\right)^k (\Delta^{m,k} \boldsymbol{\epsilon})_i, \left(\frac{m'}{n+1}\right)^k (\Delta^{m',k} \boldsymbol{\epsilon})_{i'} \right).$$

The dependence of the distributions of U and  $(U_1(l, l'), U_2(l, l'))$  on k and the distribution of  $\epsilon_1$  is suppressed.

Let

$$\mu_S^* = \mu_S^*(c,\gamma) = \int_{\alpha=0}^{1/k} (1-k\alpha) P\{U \ge \alpha^k (c-\gamma)\} d\alpha,$$

and

$$\sigma_{S}^{*2} = \sigma_{S}^{*2}(c,\gamma) = \sum_{l,l'=0}^{k} \int_{\alpha,\alpha'=0}^{1/k} [1 - \max\{l\alpha, l'\alpha'\} - \max\{(k-l)\alpha, (k-l')\alpha'\}]_{+} \\ \times \operatorname{cov}(I\{U_{1}(l,l') \ge \alpha^{k}(c-\gamma)\}, I\{U_{2}(l,l') \ge \alpha'^{k}(c-\gamma)\})d\alpha d\alpha'.$$

Here  $u_+$  is the positive part of u.

Let  $f_{\gamma}^{*}(t) \equiv f^{*}(t) = \gamma t^{k}/k!$  (so  $f^{*(k)} \equiv \gamma$ ) and let  $P_{f}$  be the probability assuming that f is the true regression function.

THEOREM 2.1. If  $\sigma_S^* > 0$ , then

$$\sup_{f\in\mathcal{F}} P_f\left\{\frac{S_c^n - n^2\mu_S^*}{n^{3/2}\sigma_S^*} \ge z_\beta\right\} = P_{f^*}\left\{\frac{S_c^n - n^2\mu_S^*}{n^{3/2}\sigma_S^*} \ge z_\beta\right\} \to \beta,$$

where  $z_{\beta}$  is the  $1-\beta$  quantile of the standard normal distribution. If  $c = \gamma$  and the distribution of  $\epsilon_1$  is symmetric, then  $n^2 \mu_S^*$  can be replaced by the exact expectation of  $S_c^n$ 

$$E_0(S_c^n) = \frac{n^*}{2} \left( n - \frac{k}{2}(n^* + 1) \right)$$

where  $n^*$  is the largest integer in (n-1)/k.

To study the asymptotic distribution of  $T_c^n$ , define new random variables  $V_1(l)$ and  $V_2(l)$ , l = 0, ..., k - 1:

$$(V_1(l), V_2(l)) = \left(\frac{m}{n+1}\right)^k ((\Delta^{1,k}\boldsymbol{\epsilon})_{i+k-l}, (\Delta^{1,k}\boldsymbol{\epsilon})_i).$$

Since  $(\Delta^{1,k}\boldsymbol{\epsilon})_i$  and  $(\Delta^{1,k}\boldsymbol{\epsilon})_{i+k-l}$  involve the l+1 common errors,  $\epsilon_{i-l}, \ldots, \epsilon_i$ , the joint distribution of  $V_1(l)$  and  $V_2(l)$  depends only upon l, k, and the distribution of  $\epsilon_1$ . For  $\alpha_0 \in (0, 1/k)$ , let

$$\mu_T^* = \mu_T^*(c, \gamma, \alpha_0) = (1 - k\alpha_0) P\{U \ge \alpha_0^k(c - \gamma)\}$$

and

$$\begin{split} \sigma_T^{*2} &= \sigma_T^{*2}(c,\gamma,\alpha_0) \\ &= 2\sum_{l=0}^{k-1} (1 - (2k - l)\alpha_0)_+ \operatorname{cov}(I\{V_1(l) \ge \alpha_0^k(c - \gamma)\}, I\{V_2(l) \ge \alpha_0^k(c - \gamma)\}) \\ &+ (1 - k\alpha_0) \operatorname{var}(I\{U \ge \alpha_0^k(c - \gamma)\}). \end{split}$$

THEOREM 2.2. Suppose that

(2.2) 
$$m = m_n = [n\alpha_0] \quad \text{with} \quad \alpha_0 \in (0, 1/k)$$

and [x] the greatest integer less than or equal to x. Suppose that  $\sigma_T^* > 0$ . Then

$$\sup_{f \in \mathcal{F}} P_f\left\{\frac{T_c^n - n\mu_T^*}{n^{1/2}\sigma_T^*} \ge z_\beta\right\} = P_{f^*}\left\{\frac{T_c^n - n\mu_T^*}{n^{1/2}\sigma_T^*} \ge z_\beta\right\} \to \beta$$

If  $c = \gamma$  and the distribution of  $\epsilon_1$  is symmetric, then  $n\mu_T^*$  can be replaced by the exact expectation of  $T_c^n$ 

$$E_0(T_c^n) = (n - km)/2.$$

We now consider the efficacies of the test statistics under local alternatives. Although results for general local alternatives are given in the Appendix, we present results here only for alternatives local to  $f^*$ , the "worst case" function in  $\mathcal{F}$ . We assume that  $X_i^n = f_n(i/(n+1)) + \epsilon_i$  with  $f_n(t) = f^*(t) + \delta_n n^{-1/2}g(t)$ , where g has k continuous derivatives. To define the efficacies, we need to define a functional which is similar to  $\Delta^{m,k}$ , the divided difference vector. We call this new functional,  $\Delta_g^{\alpha,k}$ , the k-th order divided difference functional with spacing  $\alpha$ of a function g. It is defined for g a function from the unit interval to the reals, k integer, and  $\alpha$  in (0, 1/k).  $\Delta_g^{\alpha,k}$  is defined recursively:

$$\begin{split} &\Delta_{g}^{\alpha,0}(t) = g(t) \quad t \in [0,1] \\ &\Delta_{g}^{\alpha,1}(t) = \frac{1}{\alpha} [g(t) - g(t-\alpha)] = \frac{1}{\alpha} [\Delta_{g}^{\alpha,0}(t) - \Delta_{g}^{\alpha,0}(t-\alpha)] \quad t \in [\alpha,1] \\ &\Delta_{g}^{\alpha,k}(t) = \frac{1}{\alpha} [\Delta_{g}^{\alpha,k-1}(t) - \Delta_{g}^{\alpha,k-1}(t-\alpha)] \quad t \in [k\alpha,1]. \end{split}$$

We define

$$\Delta_g^{0,k}(t) = g^{(k)}(t).$$

Note that, for  $g = (g(1/(n+1)), \dots, g(n/(n+1)))^t$ ,  $\Delta_g^{m/(n+1),k}(i/(n+1)) = (\Delta^{m,k}g)_i$ .

THEOREM 2.3. Suppose that U, as defined in (2.1), has a continuous density  $f_U$  and that  $\delta_n \to \delta < \infty$ . Suppose  $\sigma_S^* > 0$  and let

$$e_S = e_S(g) = \frac{1}{\sigma_S^*} \int_{\alpha=0}^{1/k} \int_{t=\alpha k}^1 \alpha^k f_U(\alpha^k(c-\gamma)) \Delta_g^{\alpha,k}(t) dt d\alpha$$

Then, under  $f_n$ ,

$$\frac{S_c^n - n^2 \mu_S^*}{n^{3/2} \sigma_S^*} - \delta e_S \Longrightarrow N(0, 1).$$

Suppose that  $\sigma_T^* > 0$  and let

$$e_T = e_T(g, \alpha_0) = \frac{\alpha_0^k f_U(\alpha_0^k(c-\gamma))}{\sigma_T^*} \int_{t=\alpha_0 k}^1 \Delta_g^{\alpha_0, k}(t) dt.$$

If  $m = m_n$  satisfies (2.2), then under  $f_n$ ,

$$\frac{T_c^n - n\mu_T^*}{n^{1/2}\sigma_T^*} - \delta e_T \Longrightarrow N(0, 1).$$

3. Estimation of  $\sigma_S^*$  and  $\sigma_T^*$ 

The results of Theorems 2.1 and 2.2 indicate how we would use the statistics  $S_c^n$  and  $T_c^n$  to construct asymptotic level  $\alpha$  tests of  $H_0: f^{(k)}(t) \leq \gamma$ . If we assume that the regression error distribution is symmetric about zero and set  $c = \gamma$  then the asymptotically level  $\alpha$  tests reject  $H_0$  if  $S_c^n \geq E_0(S_c^n) + z_\alpha n^{3/2} \sigma_S^*(c,c)$  or if  $T_c^n \geq E_0(T_c^n) + z_\alpha n^{1/2} \sigma_T^*(c,c,\alpha_0)$ . However, the parameters  $\sigma_S^*$  and  $\sigma_T^*$  are typically unknown. In this section we consider two types of estimates of  $\sigma_S^*$  and  $\sigma_T^*$  (or equivalently, of the standard errors of  $S_c^n$  and  $T_c^n$ ). One estimate is based on the asymptotics of Theorems 2.1 and 2.2. The other estimate uses bootstrapped samples. In simulation studies, we found that the asymptotic-based estimate of  $\sigma_S^{*2}$  performed poorly, often taking on negative values. The asymptotic-based estimate of  $\sigma_T^*$ .

We present an estimate of  $\sigma_T^*$  that satisfies

$$\lim_{n \to \infty} \sup_{f \in \mathcal{F}_n} P_f\{T_c^n \ge E_0(T_c^n) + z_\alpha n^{1/2} \hat{\sigma}_T^*\} = \alpha$$

where

$$\mathcal{F}_n = \{ f \in \mathcal{F} : -\rho_n n^k \le f^{(k)}(t) \text{ for all } t \},\$$

and  $\rho_n$  is any sequence of positive numbers tending to zero. As usual,  $T_c^n$  is constructed using  $m_n$  as in (2.2). We see that we must estimate

$$\sigma_T^{*2} = \sum_{l=0}^{k-1} 2(1 - (2k - l)\alpha_0) + C(l) + (1 - k\alpha_0)/4$$

where C(l) is the covariance between  $I\{V_1(l) \ge 0\}$  and  $I\{V_2(l) \ge 0\}$ . We estimate  $\sigma_T^{*2}$  by substituting estimates of C(l). Our estimate,  $\hat{C}(l)$ , is the sample covariance between the collection of pairs

$$\begin{aligned} &\{(I\{(\Delta^{1,k}\boldsymbol{X})_i \geq c\}, I\{(\Delta^{1,k}\boldsymbol{X})_{i-k+l} \geq c\}), i = 2k - l + 1, \dots, n\} \\ & \cup \{(I\{(\Delta^{2,k}\boldsymbol{X})_i \geq c\}, I\{(\Delta^{2,k}\boldsymbol{X})_{i-2k+2l} \geq c\}), i = 4k - 2l + 1, \dots, n\}. \end{aligned}$$

Then  $\hat{C}(l)$  converges to C(l) in probability, uniformly on  $\mathcal{F}_n$  and our estimate of  $\sigma_T^{*2}$  converges uniformly to  $\sigma_T^{*2}$ . (It is possible to use only the first set of pairs in the estimation of C(l), but simulations showed that including the second set of pairs greatly increased the finite sample accuracy of the estimate.)

To estimate the standard error of  $S_c^n$  (or  $T_c^n$ ) from a sample  $(X_i, t_i)$ ,  $i = 1, \ldots, n$ , we draw with replacement a bootstrap sample of size n from  $(X_i, t_i)$ . We then calculate the resulting value of  $S_c^n$  (or  $T_c^n$ ). This process is repeated many times, and the standard deviation of the resulting values of  $S_c^n$  (or  $T_c^n$ ) is used as the estimate of the standard error. The exact theoretical properties of this procedure are unknown but simulation studies, presented in Section 5, indicate that the resulting estimates are good.

## 4. Efficacy

Here we study relative Pitman efficiencies of tests of  $H_0: f^{(k)}(t) \equiv \gamma$  versus  $H_1: f^{(k)}(t) > \gamma$  for some t. Three tests are considered: the two tests introduced in Section 2, which use statistics  $S_c^n$  and  $T_c^n$ , and the least squares regression test. The efficacies are calculated with respect to local alternatives of the form  $f_n(t) = f^*(t) + n^{-1/2}\delta_n g(t)$ , where  $f^*$  is as in Theorem 2.1,  $\delta_n \to \delta$ , finite, and g has k continuous derivatives. Throughout we assume that, in the construction of  $T_c^n, m = m_n$  as in (2.2). No one of the three tests is clearly superior to the others and, for large classes of alternatives, all three have no power (see Theorem 4.1).

From Theorem 2.3, we see that the Pitman efficacy of  $S_c^n$  is  $e_S = e_S(g)$  and the Pitman efficacy of  $T_c^n$  is  $e_T = e_T(g, \alpha_0)$ .

For the least squares regression test, assume that  $f(t) = \beta_0 + \beta_1(t-1/2) + \cdots + \beta_k(t-1/2)^k$ , with the  $\beta_j$ 's unknown. Let M = M(n,k) denote the  $n \times (k+1)$  design matrix with  $M_{ij} = (i/(n+1)-1/2)^{j-1}$ . Then the least squares estimate of  $\beta_k$  is  $\hat{\beta}_k = ((M^t M)^{-1} M^t X)_{k+1}$ , and the least squares regression test rejects  $H_0$  at approximate significance level  $\alpha$  if  $(k!)\hat{\beta}_k \geq \gamma + (k!)z_\alpha \operatorname{var}^{1/2}(\hat{\beta}_k)$ . (We could base our test on the parameterization  $f(t) = \beta_0^* + \beta_1^* t + \cdots + \beta_k^* t^k$ , rejecting  $H_0$  when  $\hat{\beta}_k^*$  is too large. However, these two parameterizations are equivalent—that is,  $\hat{\beta}_k = \hat{\beta}_k^*$ . The  $\beta_k$  parameterization is more convenient for the proof of Theorem 4.1 below.)

To calculate the efficacy of the least squares regression test, assume that the variance of  $\epsilon_i$  is  $\sigma^2$ . Then, under the local alternative hypothesis, the variance of  $\hat{\beta}_k$  is  $\sigma^2((M^tM)^{-1})_{k+1,k+1}$ , the mean is  $\beta_k + n^{-1/2}\delta_n((M^tM)^{-1}M^tg)_{k+1}$ , where  $g = (g(1/(n+1)), \ldots, g(n/(n+1)))^t$ , and so the efficacy is

$$e_{LS} = \lim_{n} n^{-1/2} \frac{((M^t M)^{-1} M^t \boldsymbol{g})_{k+1}}{\sigma((M^t M)^{-1})_{k+1,k+1}^{1/2}}$$

We now show that all three tests have no power against a special class of local alternatives. We assume that  $n \ge k + 1$ , so that our estimators are well-defined.

THEOREM 4.1. If  $g^{(k)}(t) = -g^{(k)}(1-t)$  for all t, then  $e_{LS} = e_S = e_T = 0$ .

**PROOF.** If  $g^{(k)}(t) + g^{(k)}(1-t) = 0$  for all t, then  $g(t) + (-1)^k g(1-t)$  is a polynomial of degree k-1. This fact will be used in calculating all three efficacies.

First consider  $e_{LS}$ . Let  $\hat{\boldsymbol{b}} = (M^t M)^{-1} M^t \boldsymbol{g} = (\hat{b}_0, \ldots, \hat{b}_k)^t$ . We will show that  $\hat{b}_k = 0$ . Let  $\boldsymbol{g}^* = (g(n/(n+1)), g((n-1)/(n+1)), \ldots, g(1/(n+1)))^t$ . Since  $g(t) + (-1)^k g(1-t)$  is a polynomial of degree k-1, for  $n \ge k+1$ ,  $\boldsymbol{g} + (-1)^k \boldsymbol{g}^*$ can be fit perfectly via least squares by a polynomial of degree k-1,

$$[(M^{t}M)^{-1}M^{t}(\boldsymbol{g}+(-1)^{k}\boldsymbol{g}^{*})]_{k+1}=0.$$

Let  $\hat{\boldsymbol{b}}^* = (M^t M)^{-1} M^t \boldsymbol{g}^*$ . Thus  $\hat{b}_k + (-1)^k \hat{b}_k^* = 0$ . But, as argued below,  $\hat{b}_j^* = (-1)^j \hat{b}_j$ ,  $j = 0, \dots, k$ , and so  $0 = \hat{b}_k + (-1)^{2k} \hat{b}_k = 2\hat{b}_k$ .

The fact that  $\hat{b}_j^* = (-1)^j \hat{b}_j, \ j = 0, \dots, k$ , follows directly from the fact that  $\hat{b}$  minimizes

$$\sum_{i} \left[ g\left(\frac{i}{n+1}\right) - \sum_{j} b_{j} \left(\frac{i}{n+1} - \frac{1}{2}\right)^{j} \right]^{2}$$

and  $\hat{\boldsymbol{b}}^{*}$  minimizes

$$\sum_{i} \left[ g\left(\frac{n+1-i}{n+1}\right) - \sum_{j} b_j \left(\frac{i}{n+1} - \frac{1}{2}\right)^j \right]^2$$
$$= \sum_{l} \left[ g\left(\frac{l}{n+1}\right) - \sum_{j} b_j (-1)^j \left(\frac{l}{n+1} - \frac{1}{2}\right)^j \right]^2$$

To show that  $e_S = e_T = 0$ , we show that  $\int_{t=\alpha k}^{1} \Delta_g^{\alpha,k}(t) dt = 0$  for all  $\alpha$ . Let  $g^*(t) = g(1-t)$ . Then, by induction on k,  $\Delta_{g^*}^{\alpha,k}(t) = (-1)^k \Delta_g^{\alpha,k}(1+k\alpha-t)$  for  $k\alpha \leq t \leq 1$ . Since  $g(t) + (-1)^k g(1-t) = g(t) + (-1)^k g^*(t)$  is a polynomial of degree k-1,

$$0 = \Delta_g^{\alpha,k}(t) + (-1)^k \Delta_{g^*}^{\alpha,k}(t) = \Delta_g^{\alpha,k}(t) + \Delta_g^{\alpha,k}(1+k\alpha-t).$$

Therefore

$$\int_{t=k\alpha}^{1} \Delta_{g}^{\alpha,k}(t)dt = -\int_{t=k\alpha}^{1} \Delta_{g}^{\alpha,k}(1+k\alpha-t)dt = -\int_{x=k\alpha}^{1} \Delta_{g}^{\alpha,k}(x)dx.$$

We now consider the case of testing for convexity, that is, with k = 2, and we set  $c = \gamma$ . We assume that the density of  $\epsilon_i$  is symmetric about 0. Then we easily calculate that

$$\begin{split} e_{LS} &= \frac{\sqrt{5}}{\sigma} \int_{0}^{1} g(t)(6t^{2} - 6t + 1)dt, \\ e_{S} &= \frac{f_{U}(0)}{\sigma_{S}^{*}} \int_{\alpha=0}^{1/2} \int_{t=2\alpha}^{1} (g(t) - 2g(t - \alpha) + g(t - 2\alpha))dtd\alpha, \\ e_{T} &= \frac{f_{U}(0)}{\sigma_{T}^{*}} \int_{t=2\alpha_{0}}^{1} (g(t) - 2g(t - \alpha_{0}) + g(t - 2\alpha_{0}))dt, \\ \sigma_{S}^{*2} &= \frac{1}{4} \left( P\{\epsilon_{3} - 2\epsilon_{2} + \epsilon_{1} \ge 0, \epsilon_{5} - 2\epsilon_{4} + \epsilon_{3} \ge 0\} - \frac{1}{4} \right) \\ &+ \frac{1}{4} \left( P\{\epsilon_{5} - 2\epsilon_{4} + \epsilon_{3} \ge 0, \epsilon_{4} - 2\epsilon_{2} + \epsilon_{1} \ge 0\} - \frac{1}{4} \right) \\ &+ \frac{1}{12} \left( P\{\epsilon_{5} - 2\epsilon_{4} + \epsilon_{3} \ge 0, \epsilon_{6} - 2\epsilon_{4} + \epsilon_{2} \ge 0\} - \frac{1}{4} \right), \end{split}$$

and

$$\sigma_T^{*2} = 2(1 - 4\alpha_0)_+ \left( P\{\epsilon_3 - 2\epsilon_2 + \epsilon_1 \ge 0, \epsilon_5 - 2\epsilon_4 + \epsilon_3 \ge 0\} - \frac{1}{4} \right) + 2(1 - 3\alpha_0)_+ \left( P\{\epsilon_4 - 2\epsilon_3 + \epsilon_2 \ge 0, \epsilon_3 - 2\epsilon_2 + \epsilon_1 \ge 0\} - \frac{1}{4} \right) + (1 - 2\alpha_0)/4.$$

The test based on T with  $\alpha_0$  close to a half should do very well when g(1) - g(1/2) is much bigger than g(1/2) - g(0). For the special case  $g(t) = \rho(t - 1/2)^r$ ,  $r \ge 2$ ,

$$e_{LS} = \frac{\sqrt{5}\rho}{\sigma} \frac{1}{2^{r+1}} [1 + (-1)^r] \frac{r}{(r+1)(r+3)},$$
  
$$e_S = \frac{f_U(0)\rho}{\sigma_S^*} \frac{1}{2^{r+2}} [1 + (-1)^r] \frac{r}{(r+1)(r+2)},$$

and

$$e_T(g,\alpha_0) = \frac{f_U(0)\rho}{\sigma_T^*} \frac{1}{r+1} [1+(-1)^r] \\ \cdot \left(\frac{1}{2^{r+1}} - 2\left(\frac{1}{2} - \alpha_0\right)^{r+1} + \left(\frac{1}{2} - 2\alpha_0\right)^{r+1}\right).$$

Since  $\sigma_T^* \to 0$  as  $\alpha_0 \to 1/2$ , we easily see that

$$\lim_{\alpha_0 \to 1/2} \lim_{r \to \infty} e_T(g, \alpha_0) / e_S = \infty,$$

and

$$\lim_{\alpha_0 \to 1/2} \lim_{r \to \infty} e_T(g, \alpha_0) / e_{LS} = \infty$$

for r not an odd integer. However we do not recommend using the statistic T, since its efficacy is highly dependent upon the choice of  $\alpha_0$ . Our recommendation is also supported by the simulation results of Section 5.

We now compare  $e_{LS}$  and  $e_S$  for general g in the case that the  $\epsilon_i$ 's are normally distributed with mean zero and variance  $\sigma^2$ . In this case,

$$\frac{e_S}{e_{LS}} = \frac{1}{\sqrt{60\pi}\sigma_S^*} \frac{\int_{\alpha=0}^{1/2} \int_{t=2\alpha}^1 (g(t) - 2g(t-\alpha) + g(t-2\alpha))dtd\alpha}{\int_0^1 g(t)(6t^2 - 6t + 1)dt}$$
  
$$\approx 1.372 \frac{\int_{\alpha=0}^{1/2} \int_{t=2\alpha}^1 (g(t) - 2g(t-\alpha) + g(t-2\alpha))dtd\alpha}{\int_0^1 g(t)(6t^2 - 6t + 1)dt}.$$

When  $g(t) = \rho(t - 1/2)^r$ ,  $r \ge 2$ , r not an odd integer, then

$$\frac{e_S}{e_{LS}} \approx \frac{1.372}{2} \left( 1 + \frac{1}{r+2} \right) \le 0.858.$$

When r = 2, that is, when the least squares test is the ideal test, we see that the relative efficiency is fairly high—over 85%.

While the least squares test always performs better than S under the above assumptions, under some conditions S will perform better than the least squares test. For instance, the convergence of S does not require the existence of moments of  $\epsilon_i$ . Also, for certain functions g, S will be more efficient than the least squares test statistic. In fact, for any positive constant M, we can find a function g so that  $e_{LS} \leq -M$  and  $e_S \geq M$ . (Since we reject the null hypothesis for large values of the test statistics, a positive efficacy indicates a strong tendency to reject the null hypothesis. A negative efficacy indicates that the null hypothesis is not usually rejected.) Let  $\delta$  be a small positive number and, for C > 0, define g with continuous second derivative such that g''(t) = -4C for  $t \in [0, 1/4 - \delta], g''(t) = C$ for  $t \in [1/4 + \delta, 1/2 - \delta], g''(1/2) = 0, g''$  linear on  $[1/4 - \delta, 1/4 + \delta] \cup [1/2 - \delta, 1/2],$ and g''(t) = g''(1 - t) for  $t \in [1/2, 1]$ . To calculate  $e_{LS}$  and  $e_S$  we first rewrite the integral expressions using integration by parts, and then approximate g'' by a step function which equals -4C on  $[0, 1/4] \cup [3/4, 1]$  and equals C on (1/4, 3/4). (The approximation holds for  $\delta$  small.) Thus

$$e_{LS} = \frac{\sqrt{5}}{2\sigma} \int_0^{1/2} [g''(t) + g''(1-t)]t^2(1-t)^2 dt$$
$$\sim \frac{-3\sqrt{5}}{5120\sigma}C$$

and

$$e_{S} = \frac{f_{U}(0)}{12\sigma_{S}^{*}} \int_{0}^{1/2} [g''(t) + g''(1-t)]t^{2}(3-4t)dt$$
$$\sim \frac{f_{U}(0)}{1536\sigma_{S}^{*}}C.$$

Our claim follows by taking C sufficiently large.

#### 5. Simulations

To study the finite sample properties of our asymptotic results and to compare the finite sample characteristics of our test statistics, we carried out simulation studies. Our focus was on testing  $H_0: f''(t) \leq 0$  for all t versus  $H_1: f''(t) > 0$  for some t. In this case, the function  $f^*$  defined prior to Theorem 2.1 is  $f^*(t) \equiv 0$ . This function is "on the boundary" between  $H_0$  and  $H_1$ . Our simulated data followed model (1.2) with the  $\epsilon_i$ 's standard normal random variables. We considered two values of n, n = 50 and n = 100. For each function f considered and for each sample size, we conducted 1000 simulations. In all cases, the statistics  $T_c$  and S were calculated using c = 0. For sample size n = 50, the T statistics were calculated for values of m = 5, 10, and 15. (In the tables, these T statistics are denoted as T(5), T(10) and T(15) respectively.) For sample size n = 100, the Tstatistics were calculated for values of m = 10, 20 and 30. Note that, under  $f^*$ ,  $W_i^{m,2} = I\{\epsilon_i - 2\epsilon_{i-m} + \epsilon_{i-2m} \geq 0\}$ , and thus the null distributions of T and S do not depend on the variance of  $\epsilon_i$ .

Table 1 contains summary information for the T and S statistics under the model (1.2), with  $f(t) \equiv 0$ . The simulated means are given with standard deviations in parentheses. The asymptotic means and accompanying parenthesized standard deviations are those calculated from the results in Theorems 2.1 and 2.2. (The asymptotic means are actually the values of  $E_0(S)$  and  $E_0(T)$ .) The standard errors of T were estimated in the two ways described in Section 3: one using the asymptotic results of Theorem 2.2, and the other via bootstrapping, with 100 bootstrap samples taken in each simulation. The standard errors of Swere calculated only via bootstrapping, again with 100 bootstrap samples taken in each simulation. The averages of the estimates are given, with the standard deviations in parentheses. The simulated means and standard deviations of the test statistics are very close to the true means and asymptotic standard deviations. In addition, the estimated standard errors are extremely accurate. In most cases, the bootstrapped estimate of the standard error is not as accurate as the asymptotic estimate. However, we still recommend the use of the bootstrapped estimate, as it will never yield negative values.

Table 2 contains simulation results for a 0.05 level test of  $H_0$ . We considered the model (1.2) for the functions  $f(t) = -t^2$ , 0,  $t^2$ , and  $t^3$ . Using the statistic S, we reject  $H_0$  at this level if  $S \ge E_0(S) + 1.645\hat{\sigma}_S$ , where  $\hat{\sigma}_S$  is our bootstrapped estimate of the standard error of S. We considered two tests based on T(m): one test rejects  $H_0$  if  $T(m) \ge n/2 - m + 1.645\hat{\sigma}_T$ , where  $\hat{\sigma}_T$  is the asymptotics-based estimate of the standard error of T(m). The other test rejects  $H_0$  if  $T(m) \ge n/2 - m + 1.645\hat{\sigma}_{TB}$ , where  $\hat{\sigma}_{TB}$  is the bootstrapped estimate. These two tests are denoted T(m) and TB(m), respectively. The least-squares regression based test, denoted LS, rejects  $H_0$  if  $\hat{\beta}_2 \ge t_{0.05}\hat{\sigma}_{\beta_2}$ , where  $t_{0.05}$  is the upper 5th percentile of a t distribution with degrees of freedom n-3, and  $\hat{\sigma}_{\beta_2}$  is the usual estimate of the standard error of  $\hat{\beta}_2$ . As expected, we see that the least squares test is the best, but that the test using S is comparable. The tests based on T do not perform very well.

In each of the studies of T(5) with a sample size of n = 50, the estimate of

n = 50	T(5)	$\overline{T(10)}$	T(15)	S
Simulated mean	20.00 (1.91)	14.97 (1.90)	10.03 (1.93)	299.84 (20.25)
Asymptotic mean	20.00(1.86)	15.00(1.84)	10.00(1.94)	300.00(18.77)
SE estimate/asymptotic	1.82(0.31)	1.83(0.13)	1.94~(0.06)	
SE estimate/bootstrap	1.85~(0.14)	1.83 (0.12)	1.95~(0.13)	19.58(1.46)
n = 100	T(10)	T(20)	T(30)	S
n = 100 Simulated mean	$\frac{T(10)}{40.22 \ (2.76)}$	$\frac{T(20)}{30.07 \ (2.62)}$	T(30) 19.97 (2.74)	<i>S</i> 1223.6 (52.5)
n = 100 Simulated mean Asymptotic mean	T(10) 40.22 (2.76) 40.00 (2.63)	$T(20) \\ 30.07 (2.62) \\ 30.00 (2.60)$	$T(30) \\19.97 (2.74) \\20.00 (2.76)$	<i>S</i> 1223.6 (52.5) 1225.0 (53.1)
n = 100 Simulated mean Asymptotic mean SE estimate/asymptotic	$\begin{array}{c} T(10) \\ \hline 40.22 \ (2.76) \\ 40.00 \ (2.63) \\ 2.60 \ (0.29) \end{array}$	$\begin{array}{c} T(20)\\ \hline 30.07 \ (2.62)\\ 30.00 \ (2.60)\\ \hline 2.60 \ (0.12) \end{array}$	$\begin{array}{c} T(30) \\ 19.97 \ (2.74) \\ 20.00 \ (2.76) \\ 2.76 \ (0.05) \end{array}$	<i>S</i> 1223.6 (52.5) 1225.0 (53.1) —
n = 100 Simulated mean Asymptotic mean SE estimate/asymptotic SE estimate/bootstrap	$\begin{array}{c} T(10) \\ \hline 40.22 \ (2.76) \\ 40.00 \ (2.63) \\ 2.60 \ (0.29) \\ 2.62 \ (0.19) \end{array}$	T(20) = 10000000000000000000000000000000000	$\begin{array}{c} T(30) \\ 19.97 \ (2.74) \\ 20.00 \ (2.76) \\ 2.76 \ (0.05) \\ 2.75 \ (0.19) \end{array}$	$\begin{array}{c} S \\ \hline 1223.6 (52.5) \\ 1225.0 (53.1) \\ - \\ 54.27 (3.99) \end{array}$

Table 1. Distribution of the test statistics with  $f(t) \equiv 0$ .

Simulation results are based on 1000 simulation runs, with observations  $X_i = \epsilon_i$ ,  $\epsilon_i$  standard normal.

Table 2.	Percent of ti	mes $H_0$ is	s rejected i	n a level	0.05 test.

Sample size	Statistic	$f(t) = -t^2$	f(t) = 0	$f(t) = t^2$	$f(t) = t^3$
n = 50	S	2.4(0.5)	5.1 (0.7)	11.4 (1.0)	14.2 (1.1)
	T(5)	7.2(0.8)	6.0(0.8)	6.4(0.8)	6.8(0.8)
	TB(5)	6.2(0.8)	4.7(0.7)	5.2(0.7)	4.8(0.7)
	T(10)	5.8(0.7)	6.1(0.8)	5.7(0.7)	6.0(0.8)
	TB(10)	5.3(0.7)	4.8(0.7)	5.4(0.7)	5.9(0.7)
	T(15)	4.2(0.6)	3.8(0.6)	4.4(0.6)	4.4(0.6)
	TB(15)	5.4(0.7)	4.5(0.7)	4.8(0.7)	5.0(0.7)
	LS	1.8(0.4)	5.5(0.7)	13.5(1.1)	17.9(1.2)
n = 100	$\overline{S}$	0.6(0.2)	4.5 (0.7)	14.0 (1.1)	22.0 (1.3)
	T(10)	5.3 (0.7)	7.4(0.8)	7.1(0.8)	7.5(0.8)
	TB(10)	5.1 (0.7)	6.4(0.8)	6.5(0.8)	6.8(0.8)
	T(20)	4.6(0.7)	5.2(0.7)	5.4(0.7)	6.0(0.8)
	TB(20)	4.8(0.7)	5.9(0.7)	5.8(0.7)	5.8(0.7)
	T(30)	5.1  (0.7)	4.7(0.7)	4.8(0.7)	4.1(0.6)
	TB(30)	5.1  (0.7)	4.7(0.7)	4.8(0.7)	4.0(0.6)
	LS	0.9(0.3)	5.2(0.7)	17.7(1.2)	28.3(1.4)

Results are based on 1000 simulation runs, with observations  $X_i = f(t_i) + \epsilon_i$ , where  $t_i = i/(n+1)$  and  $\epsilon_i$  is standard normal. The entries in the table are  $\pi =$  percent of times  $H_0$  is rejected and, in parenthesis, the standard error  $\sqrt{\pi(1-\pi)/1000} \times 100$ .

the variance of T(5) based on the asymptotics was negative in one of the thousand simulation runs. The figures given in Tables 1 and 2 for T(5) are based on the 999 simulations that resulted in positive estimates of the variance.

Table 3 contains simulation results for comparing the least squares procedure with the test based on S in the presence of outliers. The sample size was n =50. The simulations were identical to those presented in Table 2, except for the distribution of the  $\epsilon_i$ 's. Here, we generated fifty standard normal random variables, then chose N of these at random, replacing them with normal random variables with mean zero and standard deviation ten. We considered N = 10 and N = 20. As one would expect, the statistic S is much less influenced by outliers than the least squares procedure. For sample size 100 (not presented here), the differences between the two procedures were less striking.

Under all simulation configurations, the distributions of the test statistics were very close to normal.

Number of outliers	Statistic	$f(t) = -t^2$	f(t) = 0	$f(t) = t^2$	$f(t) = t^3$
10	S	2.5  (0.5)	4.7(0.7)	8.9(0.9)	10.5(1.0)
	LS	4.0(0.6)	4.9(0.7)	6.6(0.8)	7.4(0.8)
20	S	4.8(0.7)	5.9(0.7)	8.0(0.9)	9.6(0.9)
	LS	3.8  (0.6)	4.4(0.6)	5.2(0.7)	5.6(0.7)

Table 3. Percent of times  $H_0$  is rejected in a level 0.05 test.

Results are based on 1000 simulation runs, with observations  $X_i = f(t_i) + \epsilon_i$ , where  $t_i = i/(n+1)$  and  $\epsilon_i$  is standard normal, except that outliers are normal with mean 0 and standard deviation 10. The entries in the table are  $\pi$  = percent of times  $H_0$  is rejected and, in parenthesis, the standard error  $\sqrt{\pi(1-\pi)/1000} \times 100$ .

# Appendix

## Proofs of Theorems

We first prove that  $f^*$  is the "worst case" function in  $\mathcal{F}$ , that is that

$$\sup_{f \in \mathcal{F}} P_f\{S_c^n \ge s\} = P_{f^*}\{S_c^n \ge s\}$$

and

$$\sup_{f \in \mathcal{F}} P_f\{T_c^n \ge s\} = P_{f^*}\{T_c^n \ge s\}.$$

This is an immediate consequence of the following lemma.

LEMMA A.1. Let  $f \in \mathcal{F}$ , and  $X_i$  as in (1.2) with  $t_i = i/(n+1)$ . Define  $X_i^* = f^*(t_i) + \epsilon_i$ . Then  $I\{(\Delta^{m,k} \boldsymbol{X})_i \ge c\} \le I\{(\Delta^{m,k} \boldsymbol{X}^*)_i \ge c\}$ .

PROOF. Let  $\boldsymbol{f} = (f(t_1), \dots, f(t_n))^t$ , and  $\boldsymbol{f}^*$  defined similarly. Since  $(\Delta^{m,k}\boldsymbol{f})_i = f^{(k)}(\xi)$  for some  $\xi \in [t_{i-km}, t_i], (\Delta^{m,k}\boldsymbol{f})_i \leq \gamma \equiv (\Delta^{m,k}\boldsymbol{f}^*)_i$ . Therefore

$$I\{(\Delta^{m,k}\boldsymbol{X})_i \ge c\}$$
  
=  $I\{(\Delta^{m,k}\boldsymbol{f})_i + (\Delta^{m,k}\boldsymbol{\epsilon})_i \ge c\} \le I\{(\Delta^{m,k}\boldsymbol{f}^*)_i + (\Delta^{m,k}\boldsymbol{\epsilon})_i \ge c\}$   
=  $I\{(\Delta^{m,k}\boldsymbol{X}^*)_i \ge c\}.$ 

We now study the distribution of  $S_c^n$  under the model

$$X_i^n = f_n\left(\frac{i}{n+1}\right) + \epsilon_i$$

where the  $\epsilon_i$ 's are independent and identically distributed and  $\{f_n\}$  is any sequence of functions in  $\mathcal{F}$  (see Theorem A.1). In Theorem A.2, we study the distribution for a fixed function f, calculating the asymptotic mean and variance. Theorem A.3 states the efficacy of  $S_c^n$ . The analogous results for the distribution of  $T_c^n$  are in Theorems A.4–A.6.

THEOREM A.1. Let  $\hat{S}_c^n$  be the Hájek projection of  $S_c^n$  (Hájek (1968)):

$$\hat{S}_c^n = \sum_{j=1}^n \mathcal{E}(S_c^n \mid \epsilon_j) \equiv \sum_{j=1}^n \eta_j$$

Suppose that there exists a sequence  $\rho_n \to 0$  such that

$$\liminf_{n \to \infty} \rho_n n^{-2} \operatorname{var}(\hat{S}_c^n) > 0.$$

Then

$$\frac{\operatorname{var}(S_c^n)}{\operatorname{var}(\hat{S}_c^n)} \to 1$$

and

$$\frac{S_c^n - \mathcal{E}(S_c^n)}{\operatorname{var}^{1/2}(S_c^n)} \Longrightarrow N(0, 1).$$

PROOF. For convenience, the superscripts and subscripts n and c will be omitted.

To prove the first statement, we show that

(A.1) 
$$\rho n^{-2} (\operatorname{var}(S) - \operatorname{var}(\hat{S})) \to 0.$$

Write

$$\operatorname{var}(S) = \sum_{m,m'=1}^{[(n-1)/k]} \sum_{i=km+1}^{n} \sum_{i'=km'+1}^{n} \operatorname{cov}(W_i^m, W_{i'}^{m'})$$

and

$$\operatorname{var}(\hat{S}) = \sum_{j=1}^{n} \operatorname{var}(\eta_j)$$
  
= 
$$\sum_{m,m'=1}^{[(n-1)/k]} \sum_{i=km+1}^{n} \sum_{i'=km'+1}^{n} \sum_{j=1}^{n} \operatorname{cov}(\operatorname{E}(W_i^m \mid \epsilon_j), \operatorname{E}(W_{i'}^{m'} \mid \epsilon_j)).$$

Since  $W_i^m = I\{(\Delta^{m,k} \mathbf{X})_i \ge c\}$  involves  $X_{i-km}, \ldots, X_i$ , the calculation of the individual terms in the variances of S and  $\hat{S}$  will depend upon

$$A(m, i, m', i') = \{i - km, \dots, i - m, i\} \cap \{i' - km', \dots, i' - m', i'\}$$

for  $1 \le m, m' \le [(n-1)/k], km+1 \le i \le n$ , and  $km'+1 \le i' \le n$ . We partition the indices (m, i, m', i') as follows.

$$egin{aligned} &A_0 = \{(m,i,m',i'):A(m,i,m',i') = \emptyset\}, \ &A_1 = \{(m,i,m',i'): ext{ the cardinality of } A(m,i,m',i') = 1\}, \ &A_2 = \{(m,i,m',i'): ext{ the cardinality of } A(m,i,m',i') \geq 2\}. \end{aligned}$$

We first study the variance of S. If  $(m, i, m', i') \in A_0$ , then  $W_i^m$  and  $W_{i'}^{m'}$  are independent and so  $\operatorname{cov}(W_i^m, W_{i'}^{m'}) = 0$ . One easily shows that the cardinality of  $A_2$  is  $O(n^2)$ . Therefore

$$\operatorname{var}(S) = \sum_{(m,i,m',i') \in A_1} \operatorname{cov}(W_i^m, W_{i'}^{m'}) + O(n^2).$$

To study the variance of  $\hat{S}$ , first note that if  $j \notin A(m, i, m', i')$ , then either  $\epsilon_j$ and  $W_i^m$  are independent, or  $\epsilon_j$  and  $W_{i'}^{m'}$  are independent, or both. Thus, either  $E(W_i^m | \epsilon_j) = E(W_i^m)$  or  $E(W_{i'}^{m'} | \epsilon_j) = E(W_{i'}^{m'})$  or both, and so  $cov(E(W_i^m | \epsilon_j), E(W_{i'}^{m'} | \epsilon_j)) = 0$ .

Therefore

$$\begin{aligned} \operatorname{var}(\hat{S}) &= \left[ \sum_{(m,i,m',i')\in A_1} \sum_{j\in A(m,i,m',i')} + \sum_{(m,i,m',i')\in A_2} \sum_{j\in A(m,i,m',i')} \right] \operatorname{cov}(\operatorname{E}(W_i^m \mid \epsilon_j), \operatorname{E}(W_{i'}^{m'} \mid \epsilon_j)). \end{aligned}$$

If  $(m, i, m', i') \in A_1$ , then there exists exactly one j in A(m, i, m', i'). For this value of  $j, W_i^m$  and  $W_{i'}^{m'}$  are conditionally independent given  $\epsilon_j$ . Therefore  $\operatorname{cov}(\operatorname{E}(W_i^m | \epsilon_j), \operatorname{E}(W_{i'}^{m'} | \epsilon_j)) = \operatorname{cov}(W_i^m, W_{i'}^{m'})$ . Since the cardinality of  $A_2$  is  $O(n^2)$  and the cardinality of A(m, i, m', i') is at most k + 1,

$$\operatorname{var}(\hat{S}) = \sum_{(m,i,m',i') \in A_1} \operatorname{cov}(W_i^m, W_{i'}^{m'}) + O(n^2) = \operatorname{var}(S) + O(n^2).$$

This completes the proof of (A.1).

Since

$$\frac{\mathrm{E}(S-\hat{S})^2}{\mathrm{var}(S)} = \frac{\mathrm{var}(S) - \mathrm{var}(\hat{S})}{\mathrm{var}(S)} \to 0$$

the asymptotic normality of S will follow once we show that

$$\frac{\hat{S} - \mathcal{E}(\hat{S})}{\operatorname{var}^{1/2}(\hat{S})} \Longrightarrow N(0, 1).$$

By the Lindeberg-Feller Theorem (see e.g. Serfling (1980)), it suffices to show that

$$\lim_{n} \operatorname{var}^{-1}(\hat{S}) \sum_{j=1}^{n} \operatorname{E}((\eta_{j} - \operatorname{E}\eta_{j})^{2} I\{|\eta_{j} - \operatorname{E}\eta_{j}| \ge \phi \operatorname{var}^{1/2}(\hat{S})\}) = 0$$

for all  $\phi > 0$ . We show that  $I\{|\eta_j - E\eta_j| \ge \phi \operatorname{var}^{1/2}(\hat{S})\} = 0$  for all j, for n sufficiently large. Now

$$\eta_j - \mathrm{E}(\eta_j) = \sum_{m=1}^{[(n-1)/k]} \sum_{i=km+1}^n [\mathrm{E}(W_i^m \mid \epsilon_j) - \mathrm{E}(W_i^m)].$$

Since, for fixed j,  $E(W_i^m | \epsilon_j) = E(W_i^m)$  unless j = i - lm for some l = 0, ..., k, the inner summation over i in the above contains at most k + 1 terms. Thus  $\eta_j - E\eta_j$  is a sum of O(n) bounded random variables. But the variance of  $\hat{S}$  grows quickly: by assumption, there exists C such that  $n^{-2} \operatorname{var}(\hat{S}) \ge C/\rho \to \infty$ .  $\Box$ 

We now consider the asymptotic distribution of  $S_c^n$  for a fixed function f. Recall the definitions of  $\Delta_f^{\alpha,k}$ , U,  $U_1(l,l')$ , and  $U_2(l,l')$  in Section 2. Let

$$\begin{split} \mu_S &= \mu_S(f) = \int_{\alpha=0}^{1/k} \int_{t=k\alpha}^1 P\{U \ge \alpha^k (c - \Delta_f^{\alpha,k}(t))\} dt d\alpha, \\ \sigma_f^2(l,l',\alpha,\alpha',t) &= \operatorname{cov}(I\{U_1(l,l') \ge \alpha^k (c - \Delta_f^{\alpha,k}(t+l\alpha))\}, \\ I\{U_2(l,l') \ge \alpha'^k (c - \Delta_f^{\alpha',k}(t+l'\alpha'))\}), \\ \beta(l,l',\alpha,\alpha',t) &= I\{\max\{(k-l)\alpha, (k-l')\alpha'\} < t < 1 - \max\{l\alpha, l'\alpha'\}\}, \end{split}$$

and

$$\sigma_S^2 = \sigma_S^2(f) = \sum_{l,l'=0}^k \int_{\alpha,\alpha'=0}^{1/k} \int_{t=0}^1 \beta(l,l',\alpha,\alpha',t) \sigma_f^2(l,l',\alpha,\alpha',t) dt d\alpha d\alpha'.$$

In Theorems A.2 and A.3, we require that the integrands of  $\mu_S(f)$  and  $\sigma_S^2(f)$  be Riemann integrable. It suffices that f has k continuous derivatives and the distributions of U and  $(U_1(l, l'), U_2(l, l'))$  be continuous. One easily shows that the distributions of U and  $(U_1(l, l'), U_2(l, l'))$  are continuous if the distribution of  $\epsilon_1$  is continuous.

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THEOREM A.2. Suppose that  $f_n \equiv f$ ,  $\sigma_S^2(f) > 0$ , and that the integrands in  $\sigma_S^2(f)$  and  $\mu_S(f)$  are Riemann integrable. Then, under f,

$$\begin{split} & \frac{S_c^n - \mathbf{E}(S_c^n)}{\operatorname{var}^{1/2}(S_c^n)} \Longrightarrow N(0, 1), \\ & n^{-3} \operatorname{var}(\hat{S}_c^n) \sim n^{-3} \operatorname{var}(S_c^n) \to \sigma_S^2, \end{split}$$

and

$$\mathcal{E}(S_c^n) = n^2 \mu_S + o(n^2)$$

where  $\hat{S}_c^n$  is the projection of  $S_c^n$ , as defined in Theorem A.1. If  $f = f^*$ , as defined in Theorem 2.1, and if U has a continuous density, then

$$\mathcal{E}(S_c^n) = n^2 \mu_S + O(n).$$

PROOF. Write

$$W_i^m = I\left\{\left(\frac{m}{n+1}\right)^k (\Delta^{m,k}\boldsymbol{\epsilon})_i \ge \left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k}\left(\frac{i}{n+1}\right)\right)\right\}.$$

By Theorem A.1, the asymptotic normality of S and the asymptotic variance expression will follow if we show that  $\operatorname{var}(\hat{S}) \sim n^3 \sigma_S^2$ . Since  $\operatorname{E}(W_i^m \mid \epsilon_j) = \operatorname{E}(W_i^m)$  if  $j \neq i - lm, l = 0, \ldots, k$ ,

$$\eta_j - \mathcal{E}(\eta_j) = \sum_{l=0}^k \sum_{m=1}^{[(n-1)/k]} (\mathcal{E}(W_{j+lm}^m \mid \epsilon_j) - \mathcal{E}(W_{j+lm}^m)) I\{km+1 \le j+lm \le n\}$$

and so

$$\begin{aligned} \text{(A.2)} \quad & \text{var}(\hat{S}) = \sum_{j=1}^{n} \sum_{l,l'=0}^{k} \sum_{m,m'=1}^{[(n-1)/k]} [I\{\max\{(k-l)m,(k-l')m'\} \\ & < j < n+1 - \max\{lm,l'm'\}\} \\ & \text{cov}(\text{E}(W_{j+lm}^{m} \mid \epsilon_{j}),\text{E}(W_{j+l'm'}^{m'} \mid \epsilon_{j}))] \\ & = \sum_{l,l'=0}^{k} \sum_{j=1}^{n} \sum_{m,m'=1}^{[(n-1)/k]} \beta\left(l,l',\frac{m}{n+1},\frac{m'}{n+1},\frac{j}{n+1}\right) \\ & \quad \cdot \sigma_{f}^{2}\left(l,l',\frac{m}{n+1},\frac{m'}{n+1},\frac{j}{n+1}\right) \\ & \sim n^{3}\sigma_{S}^{2}. \end{aligned}$$

To study the asymptotic expected value of S, write

$$\mathbf{E}(S) = \sum_{m=1}^{[(n-1)/k]} \sum_{i=mk+1}^{n} P\left\{ U \ge \left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k}\left(\frac{i}{n+1}\right)\right) \right\}$$
  
~  $n^2 \mu_S.$ 

The stronger statement concerning E(S) is easily shown.  $\Box$ 

THEOREM A.3. Let  $f_n(x) = f(x) + \delta_n n^{-1/2} g(x)$ , where f and g have k continuous derivatives,  $\sigma_S^2(f) > 0$ , and  $\delta_n \to \delta < \infty$ . Assume that  $(U_1(l, l'), U_2(l, l'))$  have continuous joint densities and that U has a continuous density,  $f_U$ . Then

$$n^{-3/2}(\mathcal{E}_{f_n}(S_c^n) - \mathcal{E}_f(S_c^n)) \to \delta \int_{\alpha=0}^{1/k} \int_{t=k\alpha}^1 \alpha^k \Delta_g^{\alpha,k}(t) f_U(\alpha^k(c - \Delta_f^{\alpha,k}(t))) dt d\alpha$$

and under  $f_n$ 

$$\frac{S_c^n - \mathcal{E}_{f_n}(S_c^n)}{n^{3/2} \sigma_S(f)} \Longrightarrow N(0, 1)$$

**PROOF.** To prove the statement concerning the means of  $S_c^n$ , write

$$\begin{split} \mathbf{E}_{f_n}(W_i^m) - \mathbf{E}_f(W_i^m) &= \mathbf{E}(W_i^m) - \mathbf{E}(W_i^{*m}) \\ &= P\{(\Delta^{m,k}\boldsymbol{\epsilon})_i \geq c - (\Delta^{m,k}\boldsymbol{f})_i - \frac{\delta}{\sqrt{n}}(\Delta^{m,k}\boldsymbol{g})_i\} \\ &- P\{(\Delta^{m,k}\boldsymbol{\epsilon})_i \geq c - (\Delta^{m,k}\boldsymbol{f})_i\} \\ &= P\left\{U \geq \left(\frac{m}{n+1}\right)^k \left(c - (\Delta^{m,k}\boldsymbol{f})_i - \frac{\delta}{\sqrt{n}}(\Delta^{m,k}\boldsymbol{g})_i\right)\right\} \\ &- P\left\{U \geq \left(\frac{m}{n+1}\right)^k (c - (\Delta^{m,k}\boldsymbol{f})_i)\right\} \\ &= \frac{\delta}{\sqrt{n}} \left(\frac{m}{n+1}\right)^k \Delta_g^{m/(n+1),k} \left(\frac{i}{n+1}\right) \\ &\cdot f_U\left[\left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k} \left(\frac{i}{n+1}\right)\right)\right] \\ &+ o(n^{-1/2}) \end{split}$$

uniformly in *i* and *m*. Thus the statement concerning  $E_{f_n}(S_c^n) - E_f(S_c^n)$  holds. Similarly

$$\sigma_{f_n}^2\left(l,l',\frac{m}{n+1},\frac{m'}{n+1},\frac{j}{n+1}\right) - \sigma_f^2\left(l,l',\frac{m}{n+1},\frac{m'}{n+1},\frac{j}{n+1}\right) = O(n^{-1/2})$$

and so, using A.2,

$$n^{-3}(\operatorname{var}(\hat{S}_c^n) - \operatorname{var}(\hat{S}_c^{*n})) \to 0$$

where  $\hat{S}_c^n$  and  $\hat{S}_c^{*n}$  are the projections of  $S_c^n$  and  $S_c^{*n}$  respectively. By Theorem A.2,  $n^{-3} \operatorname{var}(\hat{S}_c^n) \to \sigma_S^2(f)$ , and so  $n^{-3} \operatorname{var}(\hat{S}_c^n) \to \sigma_S^2(f)$ . The theorem follows from Theorem A.1.  $\Box$ 

We now study  $T_c^n$ . Assume that  $m = m_n$  as in (2.2).

THEOREM A.4. Suppose that

$$\liminf_{n \to \infty} \operatorname{var}(T_c^n) = \infty.$$

Then

$$\frac{T_c^n - \mathcal{E}(T_c^n)}{\operatorname{var}^{1/2}(T_c^n)} \Longrightarrow N(0, 1)$$

PROOF.  $T_c^n$  can be rewritten

$$T_c^n = \sum_{i=1}^m Z_i$$

where

$$Z_{i} = Z_{i}(n, c, m, k) = W_{i+km}^{m} + W_{i+(k+1)m}^{m} + \dots + W_{i+(k+l(i))m}^{m}$$

and l(i) = l(i, n, m, k) is as large as possible, that is  $i + (k + l(i))m \leq n < i + (k + l(i) + 1)m$ .  $Z_1, Z_2, \ldots, Z_m$  are independent.

By the Lindeberg-Feller Theorem it suffices to show that, for all  $\phi > 0$ ,

$$\operatorname{var}^{-1}(T) \sum_{i=1}^{m} \operatorname{E}((Z_i - \operatorname{E}(Z_i))^2 I\{|Z_i - \operatorname{E}(Z_i)| \ge \phi \operatorname{var}^{1/2}(T)\}) \to 0$$

This follows immediately, since  $Z_i$  is a sum of at most  $n/m = O(1/\alpha_0) = O(1)$ bounded terms and  $\operatorname{var}(T) \to \infty$  by assumption. Thus, for *n* sufficiently large,  $I\{|Z_i - E(Z_i)| \ge \phi \operatorname{var}^{1/2}(T)\} = 0$  for all  $i = 1, \ldots, m$ .  $\Box$ 

As in the study of  $S_c^n$ , the study of the asymptotic mean and variance of  $T_c^n$  requires the partitioning of index sets via A(m, i, m', i'). However, here the "overlapping" sets are much simpler since, for each n, m is fixed. Thus we need only consider A(m, i, m, i'):

$$A(m,i,m,i')=\{i,i-m,\ldots,i-km\}\cap\{i',i'-m,\ldots,i'-km\}$$

for  $km + 1 \le i, i' \le n$ . If  $A(m, i, m, i') = \emptyset$  then  $W_i^m$  and  $W_{i'}^m$  are independent, so we can neglect these terms when studying the variance of  $T_c^n$ . We partition  $\{(i, i') : A(m, i, m, i') \ne \emptyset\}$ :

$$\{(i,i'): A(m,i,m,i') \neq \emptyset\} = \left[\bigcup_{l=0}^{k-1} (B_1(l) \cup B_2(l))\right] \cup \left[\bigcup_{i=km+1}^n \{(i,i)\}\right]$$

where

$$B_1(l) = \{(i,i') : A(m,i,m,i') = \{i',i'-m,\ldots,i'-lm\} \\ = \{i-(k-l)m,\ldots,i-km\}\}$$

and

$$egin{aligned} B_2(l) &= \{(i,i'): A(m,i,m,i') = \{i,i-m,\ldots,i-lm\} \ &= \{i'-(k-l)m,\ldots,i'-km\} \}. \end{aligned}$$

The dependence of  $B_1(l)$  and  $B_2(l)$  upon n, k, and m is suppressed. Note that  $(i, i') \in B_1(l)$  if and only if  $W_i^m$  and  $W_{i'}^m$  involve the l + 1 common observations:  $X_{i'} = X_{i-(k-l)m}, \ldots, X_{i'-lm} = X_{i-km}$ .

Recall the definition of  $(V_1(l), V_2(l))$  in Section 2. We thus have

$$(V_1(l), V_2(l)) \sim \left(\frac{m}{n+1}\right)^k ((\Delta^{m,k} \boldsymbol{\epsilon})_i, (\Delta^{m,k} \boldsymbol{\epsilon})_{i'}), \quad (i,i') \in B_1(l),$$

and

$$(V_2(l), V_1(l)) \sim \left(\frac{m}{n+1}\right)^k ((\Delta^{m,k} \boldsymbol{\epsilon})_i, (\Delta^{m,k} \boldsymbol{\epsilon})_{i'}), \quad (i,i') \in B_2(l).$$

Let

$$\mu_T = \mu_T(f, \alpha) = \int_{t=k\alpha}^1 P\{U \ge \alpha^k (c - \Delta_f^{\alpha, k}(t))\} dt$$

and

$$\sigma_f^2(k,\alpha,t) = \operatorname{var}(I\{U \ge \alpha^k(c - \Delta_f^{\alpha,k}(t))\}).$$

For l = 0, k - 1, let

$$\sigma_f^2(l,\alpha,t) = \operatorname{cov}(I\{V_1(l) \ge \alpha^k(c - \Delta_f^{\alpha,k}(t))\},$$
$$I\{V_2(l) \ge \alpha^k(c - \Delta_f^{\alpha,k}(t - (k - l)\alpha))\})$$

and

$$b(l, \alpha, t) = I\{(2k - l)\alpha < t < 1\}.$$

Let

$$\sigma_T^2 = \sigma_T^2(f,\alpha) = 2\sum_{l=0}^{k-1} \int_{t=k\alpha}^1 \sigma_f^2(l,\alpha,t)b(l,\alpha,t)dt + \int_{t=k\alpha}^1 \sigma_f^2(k,\alpha,t)dt.$$

For the remainder of the section, assume that  $\sigma_T^2(f, \alpha_0)$  is positive, and that there exists a neighborhood of  $\alpha_0$  such that  $\sigma_f^2(l, \alpha, t)$ ,  $l = 0, \ldots, k$ , and  $P\{U \ge \alpha^k(c - \Delta_f^{\alpha,k}(t))\}$  are continuous in  $(\alpha, t)$  for all t and all  $\alpha$  in that neighborhood. For instance, it suffices to assume that f has k continuous derivatives and that the distributions of  $(V_1(l), V_2(l))$  and U are continuous. This will be true if the distribution of  $\epsilon_1$  is continuous.

THEOREM A.5. Suppose that  $f_n = f$  is fixed. Then

$$\begin{split} & \frac{T_c^n - \mathrm{E}(T_c^n)}{\mathrm{var}^{1/2}(T_c^n)} \Longrightarrow N(0,1), \\ & n^{-1} \operatorname{var}(T_c^n) \to \sigma_T^2(f,\alpha_0), \end{split}$$

and

$$\mathcal{E}(T_c^n) = n\mu_T(f,\alpha_0) + o(n).$$

If  $f = f^*$  and U has a continuous density then

$$\mathbf{E}(T_c^n) = n\mu_T(f, \alpha_0) + O(1).$$

PROOF. We first prove the second statement.

$$\operatorname{var}(T_{c}^{n}) = \sum_{i,i'=km+1}^{n} \operatorname{cov}(W_{i}^{m}, W_{i'}^{m}) = \sum_{(i,i'):A(m,i,m,i')\neq\emptyset} \operatorname{cov}(W_{i}^{m}, W_{i'}^{m})$$
$$= \sum_{l=0}^{k-1} \sum_{(i,i')\in B_{1}(l)\cup B_{2}(l)} \operatorname{cov}(W_{i}^{m}, W_{i'}^{m}) + \sum_{i=km+1}^{n} \operatorname{var}(W_{i}^{m}).$$

For l = 0, ..., k - 1,

$$\begin{split} \sum_{(i,i')\in B_1(l)} \operatorname{cov}(W_i^m, W_{i'}^m) \\ &= \sum_{(i,i')\in B_2(l)} \operatorname{cov}(W_i^m, W_{i'}^m) \\ &= \sum_i \operatorname{cov}\left(I\left\{V_1(l) \ge \left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k}\left(\frac{i}{n+1}\right)\right)\right\}, \\ &\quad I\left\{V_2(l) \ge \left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k}\left(\frac{i - (k-l)m}{n+1}\right)\right)\right\}\right) \\ &= \sum_i \sigma_f^2\left(l, \frac{m}{n+1}, \frac{i}{n+1}\right) \end{split}$$

where the summation is over all i with  $km + 1 \le i$ ,  $i - (k - l)m \le n$ , that is with  $(2k - l)m < i \le n$ , or equivalently, over all i with b(l, m/(n + 1), i/(n + 1)) = 1. Also,

$$\operatorname{var}(W^m_i) = \sigma_f^2\left(k, rac{m}{n+1}, rac{i}{n+1}
ight).$$

The second statement of the theorem follows immediately, by calculating Riemann integrals.

The asymptotic normality of T follows from Theorem A.4.

The third statement, concerning the expected value of T, follows from

$$\mathbf{E}(T_c^n) = \sum_{i=mk+1}^n P\left\{ U \ge \left(\frac{m}{n+1}\right)^k \left(c - \Delta_f^{m/(n+1),k}\left(\frac{i}{n+1}\right)\right) \right\} \sim n\mu_T.$$

The fourth statement follows easily.  $\Box$ 

THEOREM A.6. Let  $f_n(x) = f(x) + \delta_n n^{-1/2} g(x)$ , where f and g have k continuous derivatives. Suppose that U has a continuous density  $f_U$  and that  $\delta_n \to \delta < \infty$ . Then

$$\frac{T_c^n - \mathcal{E}_{f_n}(T_c^n)}{n^{1/2} \sigma_T(f, \alpha_0)} \Longrightarrow N(0, 1)$$

and

$$n^{-1/2}(\mathcal{E}_{f_n}(T_c^n) - \mathcal{E}_f(T_c^n)) \to \delta\alpha_0^k \int_{t=\alpha_0 k}^1 \Delta_g^{\alpha_0,k}(t) f_U(\alpha_0^k(c - \Delta_f^{\alpha_0,k}(t))) dt.$$

The proof is similar to that of Theorem A.3 and is omitted.

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