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On kernel estimation of curves with non-smooth peaks

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Abstract. Nonparametric estimation of the mode of a density function via kernel methods is considered. It is shown that asymptotic normality of the mode estimator can be achieved also if the density has a "kink" at the location at the mode, if there is symmetry up to second order around the kink. Tests for the presence of a smooth or symmetric peak at a preassigned location are also considered.

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1 Introduction and assumptions

An important problem in nonparametric curve estimation consists in estimation of the mode (location of an isolated maximum of the unknown density or regression function). A number of distinguished papers deal with this topic: Parzen (1962), Rüschendorf (1977), Eddy (1980, 1982), Müller (1985, 1989), Romano (1988a,b), Grund and Hall (1995), Ehm (1996) (among many others). In the last few years, an increasing interest in this topic can be observed. Among the most recent evidences of this growing interest are the papers by Mokkadem and Pelletier (2003) as well as Abraham, Biau and Cadre (2003a,b).

The classical procedure is as follows: If $f(x)$ is the unknown curve (x being a real variable, but extensions to the multivariate case are possible) and θ the *mode* of f, i.e.

$$f(\theta) > \sup_{|x-\theta|>\epsilon} f(x) \quad \text{for each } \epsilon > 0, \tag{1}$$

then θ is estimated from the location θ_n of a maximum of a curve estimator $f_n(x)$ for $f(x)$. (Uniqueness of the maximum cannot be expected here, but, in general, this does not affect the validity of asymptotic theory.)

In the present paper, we shall consider f to be a univariate probability density, and we shall estimate it via the Rosenblatt-Parzen kernel estimator

$$f_n(x) = \frac{1}{nh_n} \sum_{i=1}^{n} K(\frac{x - X_i}{h_n}) \tag{2}$$

based on i.i.d. observations X_i having density f, where K is a kernel (i.e. an integrable function satisfying some regularity assumptions to be specified below) and $h_n \to 0$, $h_n > 0$

a bandwidth sequence. We will write but h for h_n in the sequel. Then the mode estimator θ_n is any location fulfilling

$$f_n(\theta_n) = \max_{x \in \mathbb{R}} f(x) \ . \tag{3}$$

In Grund and Hall (1995) and Ziegler (2003) it has been shown that consistency of θ_n can be ensured (under some very mild regularity conditions on kernel and bandwidth), if f is continuous at the point θ only. More specifically, the following holds: If K is a continuous probability density of bounded variation, f is continuous at θ satisfying (1) and h_n fulfills

$$\frac{\log n}{nh} \to 0 \ , \tag{4}$$

then

$$\theta_n \to \theta \quad \text{a.s.} \tag{5}$$

(see Theorem 2.8 in Ziegler, 2002).

In order to determine the speed of convergence, some additional assumptions on the shape of the curve f around θ have to be made (Herrmann and Ziegler, 2003; see also Abraham et al., 2003). In order to achieve asymptotic normality of θ_n (and therefore to be able to construct asymptotic confidence intervals for θ), however, it it is generally believed that rather heavy smoothness conditions are needed (differentiability up to 3rd order at least in a neighborhood of θ, see Romano, 1988a). The main aim of the present paper is to show that this is not the case. The density f may as well exhibit a “kink” at θ, if there is some symmetry around θ and some smoothness in left and right hand neighborhoods. More precisely, the one-sided derivatives have to exist in θ with $f'(\theta - 0) = -f'(\theta + 0)$ and f' has to be quasi-smooth of order $\alpha > 1$ in the sense of Liebscher (1990; we explain below) which, in particular implies the condition $f''(\theta - 0) = f''(\theta + 0)$. Then we can speak of “symmetry of f up to 2nd order around θ”. In the present paper we show that, under appropriate regularity conditions on kernel and bandwidth, an equivalent to the classical asymptotic normality result for θ_n continues to hold in this case.

In section 2 we shall formulate adequate conditions, while section 3 contains the above mentioned asymptotic normality result as well as a sketch of its proof. Finally, in section 4, some tests are suggested for the presence of a smooth or symmetric (up to either 1st or 2nd order) peak at a preassigned location.

2 Assumptions

First we recall the definition of quasi-smoothness of a function g (we write here g rather than f, since our g will be f' later) which has apparently been introduced by Liebscher (1990) in generalization of a concept due to Woodroofe (1970). g is called quasi-smooth of order $\alpha > 0$ at a point θ, if the following conditions are fulfilled:

- Let m be the greatest integer being smaller than α. Then there exists a neighborhood U of θ such that $g^{(m)}$ exists and is continuous on $U \setminus \{\theta\}$. Furthermore, $g^{(m)}(\theta - 0)$ and $g^{(m)}(\theta + 0)$ exist.
- $g^{(i)}(\theta - 0) = g^{(i)}(\theta + 0)$ for $i = 1, \dots, m$ (this condition is empty if $\alpha \le 1$).
- The limits

$$\lim_{z \to 0+0} |z|^{-\alpha} \left(g(\theta + z) - \sum_{i=0}^{m} g^{(i)}(\theta + 0) \frac{z^i}{i!} \right) =: g_\alpha^+(\theta)$$

$$\lim_{z \to 0-0} |z|^{-\alpha} \left(g(\theta + z) - \sum_{i=0}^{m} g^{(i)}(\theta - 0) \frac{z^i}{i!} \right) =: g_\alpha^-(\theta)$$

  exist and are finite.

  We put

$$g_\alpha(\theta) := g_\alpha^+(\theta + 0) + g_\alpha^-(\theta - 0) \ .$$

Note that g itself may be discontinuous at θ. Note further the following: If g'' exists on $U \setminus \{\theta\}$ and is continuous with existing limits $g''(\theta - 0)$ and $g''(\theta - 0)$, and if additionally $g'(\theta - 0) = g'(\theta - 0)$, then g is quasi-smooth of order $\alpha = 2$ with $g_2^+(\theta) = \frac{1}{2} g''(\theta + 0)$ and $g_2^-(\theta) = \frac{1}{2} g''(\theta - 0)$, so that in this case

$$g_2(\theta) = \frac{1}{2}(g''(\theta - 0) + g''(\theta + 0)) \ .$$

In the sequel, this will form an important special case.

Now we are in the position to state our conditions on the unknown density f. Additionally to (1), we assume the following:

Assumption $\mathcal{F}$

$$f \text{ is continuous at } \theta \tag{6}$$

$$f \text{ is twice continuously differentiable in } U \setminus \{\theta\}, \tag{7}$$

where U is an appropriate neighborhood of θ

$$f'(\theta - 0), f'(\theta - 0) \text{ exist with } f'(\theta - 0) = -f'(\theta - 0) \tag{8}$$

$$f''(\theta - 0), f''(\theta - 0) \text{ exist with } f''(\theta - 0) = f''(\theta - 0) \neq 0 \tag{9}$$

$$f' \text{ is quasi-smooth at } \theta \text{ of order } 1 < \alpha \le 2 \tag{10}$$

Remarks (a) (10) implies part of (9).
(b) (9) together with (7), in turn, implies that f'' may be considered as a continuous function on the whole of U (by setting $f''(\theta) := f''(\theta - 0)$).
(c) In the present case, in strict contrast to the smooth one, it is possible that $f''(\theta) > 0$ in spite of the fact that θ is a maximum.
(d) In case of existence and continuity of f''' on $U \setminus \{\theta\}$ with existing limits $f'''(\theta - 0)$ and $f'''(\theta + 0)$, it holds that $\alpha = 2$ and $(f')_2(\theta) = \frac{1}{2}(f'''(\theta - 0) + f'''(\theta + 0))$.

Now we turn to the kernel:

Assumption $\mathcal{K}$

$$K \text{ is twice continuously differentiable with } K'' \text{ being of bounded variation} \tag{11}$$

$$\operatorname{supp} \mathrm{K} \subset [-1, 1] \tag{12}$$

$$K(-u) = K(u) \text{ for all } u \tag{13}$$

$$K(0) = 0 \tag{14}$$

$$K \geq 0 \tag{15}$$

$$\int_{-1}^{1} K(u)du = 1 \tag{16}$$

Remarks (a) (11) is needed since a consistent estimate of $f''(\theta)$ is required for our procedure. So the curve estimator f_n will not exhibit a kink at θ.
(b) (12) is not needed and can, as so often, be replaced with appropriate tail conditions, rendering the proofs more technical (see Romano, 1988, Ziegler, 2002, for different types of such conditions and the corresponding techniques of proof).
(c) (14) is not standard, but needed here in order to be able to estimate f'' consistently uniformly in a neighborhood of θ. The kink at θ would disturb this procedure if (14) is not imposed.
(d) (15) is needed only to ensure consistency of θ_n under the condition that f is continuous only at the point θ. As indicated in Ziegler (2002), (15) can be dispensed with if global continuity of f is assumed.

Finally, we state the conditions on the bandwidth:

Assumption $\mathcal{H}$

$$h \to 0 \tag{17}$$

$$\frac{nh^5}{\log n} \to \infty \tag{18}$$

$$nh^{3+2\alpha} \to c^2 \geq 0 \tag{19}$$

where α stems from (10).

Remarks (a) (18) is stronger than (4) and needed for consistent estimation of f'' (uniformly in a neighborhood of θ.
(b) Even with $c = 0$, (18) and (19) can be fulfilled simultaneously since $\alpha > 1$.

3 Toward an asymptotic normality result

Recall the definitions (2) and (3). Then, since $f_n'(\theta_n) = 0$, we obtain by the mean value theorem the classical representation

$$\theta_n - \theta = -\frac{f_n'(\theta)}{f_n''(\theta^*)} \tag{20}$$

with some θ^* between θ_n and θ. As usual, asymptotic normality is then gained by proving consistency of $f_n''(\theta^*)$ and asymptotic normality of $f_n'(\theta)$. Now it is well known (and a simple consequence of Ljapunov's CLT together with Parzen's lemma) that

$$\frac{f_n'(\theta) - \mathbb{E}f_n'(\theta)}{\sqrt{Var(f_n'(\theta))}} \xrightarrow{\mathcal{L}} N(0,1) \ ,$$

where only continuity of f at θ, some properties of K (contained in $\mathcal{K}$) and $nh \to \infty$ is needed (see Parzen, 1962). Since, again by Parzen's lemma

$$nh^3 Var(f_n'(\theta)) \to f(\theta) \int_{\mathbb{R}} (K'(z))^2 dz \ ,$$

we have

$$\sqrt{nh^3}(f_n'(\theta) - \mathbb{E}f_n'(\theta)) \xrightarrow{\mathcal{L}} N(0, f(\theta) \int_{\mathbb{R}} (K'(z))^2 dz) \ . \tag{21}$$

The following proposition is crucial in order to derive asymptotic normality from (20) and (21). In the proof, we shall, in essence, only give the steps that are different from the smooth case:

Proposition Under $\mathcal{F}$, $\mathcal{K}$ and $\mathcal{H}$ it holds that

$$\mathbb{E}f_n'(\theta) = h^\alpha (f')_\alpha(\theta) \int_0^1 z^\alpha K(z)dz + o(h^\alpha) \tag{22}$$

and that

$$\sup_{x\in V} |f_n''(x) - f''(x)| \to 0 \quad \text{f.s.} \; , \tag{23}$$

where V is an appropriate neighborhood of θ.

Sketch of proof As to (22), we first observe that in

$$\mathbb{E}f_n'(\theta) = \frac{1}{h^2}\int_{-\infty}^{\theta} K'(\frac{\theta-u}{h})f(u)du + \frac{1}{h^2}\int_{\theta}^{\infty} K'(\frac{\theta-u}{h})f(u)du$$

the domains of integration are in fact subsets of U if h is small enough since we have (12). Hence, by (7) and (8) we can regard f as continuously differentiable on the respective region of integration, and we can perform integration by parts to obtain

$$\begin{aligned}\mathbb{E}f_n'(\theta) \;&=\; \Big[-\frac{1}{h}K(\frac{\theta-u}{h})f(u)du\Big]_{-\infty}^{\theta} + \frac{1}{h}\int_{-\infty}^{\theta} K(\frac{\theta-u}{h})f'(u)du \\ &+\; \Big[-\frac{1}{h}K(\frac{\theta-u}{h})f(u)du\Big]_{\theta}^{\infty} + \frac{1}{h}\int_{\theta}^{\infty} K(\frac{\theta-u}{h})f'(u)du \; ,\end{aligned}$$

which by (6) equals

$$\frac{1}{h}\int_{-\infty}^{\theta} K(\frac{\theta-u}{h})f'(u)du + \frac{1}{h}\int_{\theta}^{\infty} K(\frac{\theta-u}{h})f'(u)du \; .$$

If we assign an arbitrary value to $f'(\theta)$, we can write the latter quantity as

$$\frac{1}{h}\int_{-\infty}^{\infty} K(\frac{\theta-u}{h})f'(u)du = \int_{-1}^{1} K(u)f'(\theta-zh)dz \; ,$$

where we have performed a change of variable (recall again (12)). Now, since f' is quasi-smooth of order α at θ, an obvious modification of Lemma 2 in Liebscher (1990) implies that

$$\mathbb{E}f_n'(\theta) = \frac{1}{2}(f'(\theta-0)+f'(\theta+0)) + h^\alpha (f')_\alpha(\theta)\int_0^1 z^\alpha K(z)dz + o(h^\alpha) \; .$$

By (8), (22) follows.

Since the mere application of Liebscher's lemma does not give much insight in where (9) comes in, we sketch a direct proof here in the special case mentioned above where f''' is thrice continuously differentiable on $V \setminus \{\theta\}$ and $f'''(\theta-0)$ and $f'''(\theta+0)$ exist. A Taylor expansion of $f'(\theta - zh)$ on the left hand side of θ gives (for $h > 0$ small enough), by (13) and (16) and Lebesgue's theorem

$$\begin{aligned}\int_0^1 K(u)f'(\theta - zh)dz &= \frac{1}{2}f'(\theta - 0) + hf''(\theta - 0)\int_0^1 zK(z)dz \\ &+ \frac{1}{2}h^2 f'''(\theta - 0)\int_0^1 z^2K(z)dz + o(h^2)\ .\end{aligned}$$

An analogous expansion for $\int_{-1}^0 K(u)f'(\theta - zh)dz$ (obtained by a Taylor expansion on the right hand side of θ), together with $\int_{-1}^0 zK(z)dz = -\int_0^1 zK(z)dz$ and $\int_{-1}^0 z^2K(z)dz = \int_0^1 z^2K(z)dz$ finally leads to

$$\begin{aligned}\mathbb{E}f_n'(\theta) &= \frac{1}{2}(f'(\theta - 0) + f'(\theta + 0)) + h(f''(\theta - 0) - f''(\theta + 0))\int_0^1 zK(z)dz \\ &+ \frac{1}{2}h^2(f'''(\theta - 0) + f'''(\theta + 0))\int_0^1 z^2K(z)dz + o(h^2)\ ,\end{aligned}$$

whence from (8) and (9) the assertion (22) follows in the special case considered.

As to (23), we first note that under (11) and (18) we have

$$\sup_{x\in\mathbb{R}} |f_n''(x) - \mathbb{E}f_n''(x)| \to 0 \quad \text{a.s.}$$

(see, e.g. Theorem 1.1. in Ziegler, 2002; recall that f is bounded). Hence, we have only to show that

$$\sup_{x\in V} |\mathbb{E}f_n''(x) - f''(x)| \to 0\ .$$

Since f is not twice continuously differentiable on a neighborhood of θ (f' is discontinuous at θ), we cannot resort to known results here. But now consider $\mathbb{E}f_n''(x) = \frac{1}{h^3}\int_{-\infty}^{\infty} K'(\frac{x-u}{h})f(u)du$. If $x \neq \theta$, then f is twice continuously differentiable in a neighborhood of x. With h being small enough, integration extends in fact only over this neighborhood and a double integration by parts yields

$$\mathbb{E}f_n''(x) = \frac{1}{h}\int_{-\infty}^{\infty} K(\frac{x-u}{h})f''(u)du\ . \tag{24}$$

For $x = \theta$, we split the integral $\int_{-\infty}^{\infty} K'(\frac{x-u}{h})f(u)du$ into the two regions $]-\infty, \theta[$ and $]\theta, \infty[$, as above. A first integration by parts leads, by (6), to

$$\frac{1}{h^2}\int_{-\infty}^{\theta} K'(\frac{\theta - u}{h})f'(u)du + \frac{1}{h^2}\int_{\theta}^{\infty} K'(\frac{\theta - u}{h})f'(u)du\ ,$$

while a further integration by parts shows the latter quantity to be equal to

$$\begin{aligned}\mathbb{E}f_n''(\theta) &= \left[-\frac{1}{h}K(\frac{\theta - u}{h})f'(u)du\right]_{-\infty}^{\theta} + \frac{1}{h}\int_{-\infty}^{\theta} K(\frac{\theta - u}{h})f''(u)du \\ &+ \left[-\frac{1}{h}K(\frac{\theta - u}{h})f'(u)du\right]_{\theta}^{\infty} + \frac{1}{h}\int_{\theta}^{\infty} K(\frac{\theta - u}{h})f''(u)du\ .\end{aligned}$$

Now, due to the discontinuity of f' at θ, we need (14) to make the undesirable terms vanish, and hence to prove $\mathbb{E}f_n'(\theta) = \int_{-\infty}^{\infty} K(\frac{\theta-u}{h})f''(u)du$, so that (24) holds for each $x \in U$.

From (24), in turn, we see, by standard arguments, that $\mathbb{E}f_n''(x) \to f''(x)$ holds uniformly on each interval where f'' is uniformly continuous. Now, by (7) and (9) this is the case on $V \subset U$ if we choose V to be a compact neighborhood of θ. (23) is proven. $\square$

Since, under $(\mathcal{F})$, $(\mathcal{K})$ and $(\mathcal{H})$, we have in particular (5), this implies together with (24) and the fact that f'' is continuous at θ that $f_n''(\theta^*) \to f''(\theta^*)$ a.s. From this, (20), (21) and (22) we obtain immediately:

Theorem Under $(\mathcal{F})$, $(\mathcal{K})$ and $(\mathcal{H})$, we have

$$\sqrt{nh^3}(\theta_n - \theta) \xrightarrow{\mathcal{L}} N(\mu, \sigma^2)$$

with

$$\begin{aligned} \mu &= -c(f')_\alpha(\theta) \int_0^1 z^\alpha K(z)dz \\ \sigma^2 &= \frac{f(\theta)}{f''(\theta)^2} \int_{-1}^1 (K'(z))^2 dz \ . \end{aligned}$$

Remarks (a) The proof of the proposition shows that $\mathbb{E}f_n'(\theta)$ explodes if either (8) or (9) is violated. Hence, the assumption of f being locally symmetric up to 2nd order around θ is also necessary for asymptotic normality of θ_n. In the case of non-symmetric kinks, a different estimator will have to be considered correcting the non-symmetry.

(b) The theorem shows that in our case of a symmetric kink, a confidence interval for θ can be constructed in quite the same manner as in the smooth case, since $f_n(\theta_n)$ and $f_n''(\theta_n)$ are consistent estimators for $f(\theta)$ and $f''(\theta)$, respectively. (Namely, f_n is also uniformly consistent for f locally in a neighborhood of θ, with the same reasoning as exposed above for f_n'' and f'').

(c) With appropriate modifications of the proofs, our result takes over to regression analysis.

(d) In practice, h will be chosen such that $c = 0$ in order to get a confidence interval being symmetric around θ. Otherwise, one would also have to estimate the bias which would require estimation of $(f')_\alpha(\theta)$. The estimation of this quantity, however, seems to be quite a challenge. Even in the case $\alpha = 2$, where $(f')_\alpha(\theta) = \frac{1}{2}(f'''(\theta-0) + f'''(\theta+0))$, there is a major difficulty: At a known point x, the one-sided derivatives $f'''(x-0)$, $f'''(x+0)$ can be estimated by pilot kernel estimators $f_{n,-}'''(x)$, $f_{n,+}'''(x)$ employing one-sided kernels (having support only on $[-1, 0]$ and $[0, 1]$, respectively, see Müller, 1992). However, we cannot estimate $f'''(\theta - 0)$ consistently by the plug-in estimator $f_{n,-}'''(\theta_n)$ since, of course, $f'''(x-0)$ is not continuous at θ, but only left-continuous and there is not necessarily $\theta_n < \theta$.

(e) The question of bandwidth choice must also remain unanswered here. An optimal choice in the sense of minimizing the MSE of the asymptotic distribution would lead to a rate of $n^{-1/(3+2\alpha)}$, but the constant would contain $(f')_\alpha(\theta)$, so that, in order to render this choice feasible, we would again arrive at the problem of estimating this quantity consistently.

(f) For computational reasons, Abraham et al. (2003a,b) consider a different mode estimator which maximizes f_n only over the finite data set $X_1, \ldots, X_n$. They show an asymptotic equivalence result of their estimator to the classical one, so that, in the smooth case, the asymptotic normality of their estimator follows. Since their proof relies heavily on the usual smoothness and regularity conditions (including f to be twice continuously differentiable with a negative definite Hessian; they consider the multivariate case), we do not know if their result would continue to hold in the situation of the present paper.

(g) Concerning asymptotic normality of $f_n(\theta_n)$, it is known that there are even problems in the smooth case. Under the usual regularity conditions, only a degenerate asymptotic normal law of $\sqrt{nh^3}(f_n(\theta_n) - f(\theta))$ can be obtained (Ziegler, 2003, Theorem 3.10). Higher order kernels are required if one wants to have a non-degenerate asymptotic normality result for $\sqrt{nh}(f_n(\theta_n) - f(\theta))$ (Ziegler, 2003, Theorem 4.1). However, none of these results seems to take over to the non-smooth case since the continuity of f' at θ has been crucial in the proofs.

4 Testing for the presence of a smooth or symmetric peak

Consider now the situation that we want to know if there is a nice symmetric (or even smooth) local peak at a given location θ. Using the methods described above, we can easily construct a test for the null hypothesis that f is either smooth with $f'(\theta)$ or symmetric up to 1st or 2nd order, respectively around θ. (This test will not be able to separate smoothness from certain symmetry.) First we observe that $Var f_n'(\theta) \to 0$ if $nh^3 \to \infty$ and hence, under some mild conditions on K and f (not including (8) and (9)) we have

$$f_n'(\theta) \to \frac{1}{2}(f'(\theta - 0) + f'(\theta + 0)) \quad \text{in probability .}$$

If f has a smooth or 1st order symmetric peak at θ, this limit equals zero, and, vice versa, we should expect to be $|f_n'(\theta)|$ "too large" if there is too much lack of symmetry. Under appropriate conditions we have (see the proof of the first part of the proposition)

$$\sqrt{nh^3}\mathbb{E}f_n'(\theta) \sim \sqrt{nh^3}\frac{1}{2}(f'(\theta - 0) + f'(\theta + 0)) + \sqrt{nh^5}\int_0^1 zK(z)dz(f''(\theta - 0) - f''(\theta + 0)) \;, \tag{25}$$

which, under $nh^5 \not\to 0$, is asymptotically zero if and only if the null hypothesis

$$H_0 : \; f'(\theta - 0) = -f'(\theta + 0) \text{ and } f''(\theta - 0) = f''(\theta + 0)$$

(i.e. local symmetry up to 2nd order around θ) is fulfilled. Under H_0 then we can easily conclude from (21) that

$$\frac{\sqrt{nh^3} f_n'(\theta)}{\sqrt{f_n(\theta)\int (K')^2}} \to N(0,1) \tag{26}$$

in distribution, so that an asymptotic level-γ test is given by

$$\text{Reject } H_0, \text{ iff } |f_n'(\theta)| > c_{n,\gamma}$$

with

$$c_{n,\gamma} := u_{1-\gamma/2}\sqrt{\frac{f_n(\theta)\int (K')^2}{nh^3}}$$

where u_β denotes the β-quantile of the standard normal distribution.

The test has a very wide alternative; perhaps it is more natural testing only for 1st order symmetry, i.e. to set up the null hypothesis

$$H_0' : \ f'(\theta - 0) = -f'(\theta + 0) \ .$$

If we take h smaller, i.e. $nh^5 \to 0$, the 2nd order term in (25) vanishes, and (26) holds still under H_0', so that the above test is in this case a level-γ test for H_0'.

For the validity of (26) under H_0', it is only needed that

$$\sqrt{nh^3}\mathbb{E} f_n'(\theta) \sim \sqrt{nh^3}\frac{1}{2}(f'(\theta - 0) + f'(\theta + 0))$$

which continues to hold if f' is only quasi-smooth of order $\alpha > 0$ and if $nh^{3+2\alpha} \to 0$. So the test for H_0' will work under those circumstances, too.

If we know about smoothness of the curve in advance, the test becomes a test for the presence of a local peak at θ.

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