ASYMPTOTIC THEORY FOR DENSITY RIDGES

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The large sample theory of estimators for density modes is well understood. In this paper we consider density ridges, which are a higherdimensional extension of modes. Modes correspond to zero-dimensional, local high-density regions in point clouds. Density ridges correspond to *s*dimensional, local high-density regions in point clouds. We establish three main results. First we show that under appropriate regularity conditions, the local variation of the estimated ridge can be approximated by an empirical process. Second, we show that the distribution of the estimated ridge converges to a Gaussian process. Third, we establish that the bootstrap leads to valid confidence sets for density ridges.

1. Introduction. There is a large literature on the problem of estimating the modes of a density. Known results include minimax rates of convergence, limiting distributions and the validity of bootstrap inference [Romano (1988b, 1988a)]. The purpose of the current paper is to establish similar results for the estimation of *ridges*, an extension of modes to higher dimensions.

Intuitively, an *s*-ridge of a density is an *s*-dimensional set of high-density concentration. Modes are just 0-ridges. A density's ridges provide a useful summary of its structure and are features of interest in a variety methods and applications. Figure 1 shows some one-dimensional density ridges. Figure 2 shows two simple datasets and estimates of the ridges.

In this paper, we consider the s = 1 case, and we study the large-sample behavior of the plug-in ridge estimator based on a kernel estimator for the underlying density. Let p be a density, and let \hat{p}_h be a kernel estimator with bandwidth h. The mean $p_h = \mathbb{E}(\hat{p}_h)$ is a smoothed version of the density. We let R = Ridge(p) denote the ridge of a density p, defined formally in Section 2.1. We define $\hat{R}_h \equiv \text{Ridge}(\hat{p}_n)$ as the estimated ridge and $R_h \equiv \text{Ridge}(p_h)$ as the smoothed ridge.

We focus on R_h rather than R for three reasons. First, there is an unavoidable bias in estimating R by \hat{R}_h . This bias originates intrinsically from the ker-

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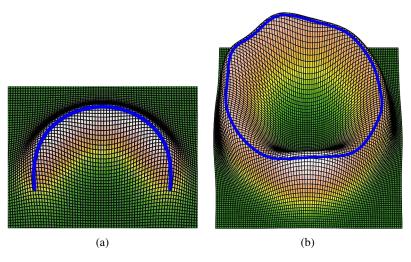


FIG. 1. Examples for the density ridges.

nel density estimator (KDE). In contrast, estimating R_h is unbiased, which allows us to focus on the stochastic variation of \hat{R}_h . Second, as is shown in Genovese et al. (2014), when a topological assumption called tameness is assumed [Cohen-Steiner, Edelsbrunner and Harer (2007), Chazal et al. (2009, 2012)], then R_h and R have the same topology for small h. In addition, for fixed h, the convergence rate for estimating R_h is fast. The third reason is that when the kernel is smooth, R_h is always well defined, while R may be nonsmooth or may not even exist. The main results of the paper focus on characterizing the uncertainty in the ridge estimator. Here is a summary of the main results:

Result 1: Local uncertainty of ridges (Theorem 3). Let $\pi_A(x)$ be the projection of x onto a set A. We define the local uncertainty as the vector $\mathbf{d}(x, \hat{R}_h) = \pi_{\hat{R}_h}(x) - x$ for $x \in R_h$. Note that this vector is unique when \hat{R}_h and R_h are close and \hat{R}_h is sufficiently smooth. We show that the local uncertainty can be approxi-

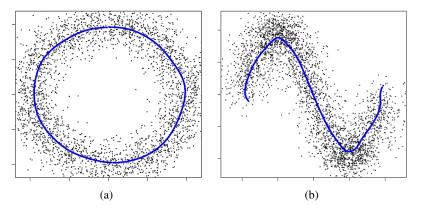


FIG. 2. Examples of estimated ridges (blue curves).

mated by an empirical process \mathbb{G}_n ,

(1)
$$\sup_{x \in R_h} \|\sqrt{nh^{d+2}} \mathbf{d}(x, \widehat{R}_h) - \mathbb{G}_n(f_x)\|_{\infty} = O_P\left(\sqrt{\frac{\log n}{nh^{d+6}}}\right)$$

for some class of functions $y \mapsto f_x(y) \in \mathbb{R}^d$. We use

(2)
$$\rho_n^2(x) = \mathbb{E}(d(x, \widehat{R}_h)^2) = \mathbb{E}(\|\mathbf{d}(x, \widehat{R}_h)\|^2), \quad x \in R_h,$$

to measure the local uncertainty. Note this quantity is essentially a local mean squared error.

Result 2: *Limiting distribution (Theorem* 6). Let \mathbb{B} be a Gaussian process defined on a function space \mathcal{F}_h defined later. If $nh^{d+8}/\log n \to \infty$, then we have the following Berry–Esseen result:

(3)
$$\sup_{t} \left| \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_{h}, R_{h}) \leq t) - \mathbb{P}\left(\sup_{f \in \mathcal{F}_{h}} \left\| \mathbb{B}(f) \right\| \leq t\right) \right|$$
$$= O\left(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}}\right),$$

where Haus(A, B) is the Hausdorff distance between two sets A, B.

Result 3: Bootstrap validity (Theorems 5, 7, 8). Given $h \equiv h_n$ satisfying $nh^{d+8}/\log n \to \infty$, the bootstrap gives valid estimates of uncertainty in three senses. First, the local uncertainty measures $\rho_n^2(x)$ can be estimated by the bootstrap. Second, the distribution of Hausdorff distance Haus(\hat{R}_h, R_h) can be estimated by the bootstrap, in the sense that

$$\sup_{t} \left| \widehat{F}(t) - F(t) \right| = O_P\left(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}}\right),$$

where

$$\widehat{F}(t) = \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_h^*, \widehat{R}_h) \le t | X_1, \dots, X_n),$$

$$F(t) = \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_h, R_h) \le t),$$

where \widehat{R}_n^* is constructed from X_1^*, \ldots, X_n^* drawn i.i.d. from the empirical distribution \mathbb{P}_n . And third, a bootstrap confidence set is consistent, as

(4)
$$\mathbb{P}(R_h \in \widehat{R}_h \oplus \varepsilon_{\alpha}^*) = 1 - \alpha + O\left(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}}\right),$$

where ε_{α}^{*} is an appropriate bootstrap quantile and

$$A \oplus \varepsilon = \left\{ x \in \mathbb{R}^d : d(x, A) \le \varepsilon \right\}$$

denotes the union of ε -balls centered on points in A.

1898

Related work. Much early work on ridge estimation focused on image analysis [Damon (1999), Eberly (1996)]. The concept of ridges in point clouds was introduced by Cheng, Hall and Hartigan (2004), Hall and Peng (2001), Hall, Qian and Titterington (1992), Wegman and Luo (2002). An algorithm for finding density ridges was given by Ozertem and Erdogmus (2011). Recently, Genovese et al. (2014) provided some fundamental results on density ridge estimation, including the convergence rate and some stability properties of plug-in ridge estimators. A similar but distinct concept called *ridgelines* was introduced by Ray and Lindsay (2005) and Li, Ray and Lindsay (2007) for Gaussian mixture models. Metric graph reconstruction [Aanjaneya et al. (2012), Lecci, Rinaldo and Wasserman (2014)], a method based on computational geometry, is another method for modeling ridge structure in a point cloud. This method tends to work best when the data are highly concentrated along filamentary structures and there is little noise. An alternative approach based on minimizing sums of squares subject to a penalty function is proposed by Lu and Slepčev (2013); the statistical properties of this approach are not known. The contour tree [level set tree; Klemelä (2004), Zaliapin and Kovchegov (2012)] is a similar method, but it uses high-density level sets to summarize the distribution rather than ridges.

Ridge estimation is a branch of geometric statistics. Limiting distributions in geometric statistics often involve the Hausdorff distance [Molchanov (2005)]. Examples of using the Hausdorff distance appear in estimating density level sets [Cuevas, González-Manteiga and Rodríguez-Casal (2006), Rinaldo and Wasserman (2010), Tsybakov (1997), Walther (1997)], curves [Cheng et al. (2005), Lee (2000)], filaments [Genovese et al. (2012a, 2014)] and manifolds [Genovese et al. (2012b, 2012c)].

In a recent paper, Qiao and Polonik (2014) give another asymptotic analysis for density ridges (called filaments in that paper). Their approach is quite different; they prove an extreme value distribution as the limiting result for estimating gradient ascent. Also, they focus on the case d = 2.

Outline. We begin with a formal definition of density ridges and ridge estimators in Section 2. Then we define the local uncertainty and confidence sets for the density ridges. Section 3 contains our main results. We first show in Section 3.2 that for each point on the ridge, we can define a d - 1 dimensional subspace normal to the ridge. We show that the local uncertainty can be coupled with an empirical process (Section 3.3). This leads to the Gaussian approximation for the Hausdorff distance (Section 3.4). Finally, we prove the consistency of the bootstrap for constructing the confidence sets (Section 3.5). Some simple simulation results are given in Section 4.

Throughout the paper, we use d for the dimension of ambient space and s for the dimension of ridge. Also, we use \hat{p}_h for the kernel density estimator and p_h for the mean of \hat{p}_h .

2. Background.

2.1. Density ridges. Let X_1, \ldots, X_n be random sample from a distribution P with compact support in \mathbb{R}^d with density p. Let $g(x) = \nabla p(x)$ and H(x) denote the gradient and Hessian, respectively, of p(x). We begin by defining the *ridges* of p, as in Eberly (1996), Genovese et al. (2014), Ozertem and Erdogmus (2011).

While there are many possible definitions of ridges, this definition has many useful properties, including stability to perturbations in the underlying density, estimability at a good rate of convergence and fast reconstruction algorithms, as described in Genovese et al. (2014).

Let $v_1(x), v_2(x), \ldots, v_d(x)$ denote the eigenvectors of the Hessian matrix H(x) corresponding to eigenvalues $\lambda_1(x) \ge \lambda_2(x) \ge \cdots \ge \lambda_d(x)$. Let $V_s(x) = [v_{s+1}(x) \cdots v_d(x)]$, a $d \times (d-s)$ matrix. We define the order-*s projected gradient* $G_s(x)$ by

(5)
$$G_s(x) = V_s(x)V_s(x)^T g(x).$$

The *s*-*ridge* is the collection of points

(6)
$$R \equiv R_s = \{x : G_s(x) = 0, \lambda_{s+1}(x) < 0\}$$

It follows that the 0-ridge, R_0 , is the set of local modes. Under weak conditions, an *s*-ridge is an *s*-dimensional manifold by the implicit function theorem.

From this point forward, we focus on the case s = 1, henceforth writing $G(x) = G_1(x)$ and $V(x) = V_1(x)$. Thus

(7)
$$V(x) = \begin{bmatrix} v_2(x) \cdots v_d(x) \end{bmatrix} \text{ and } G(x) = V(x)V(x)^T g(x).$$

The 1-ridge (or simply ridge) is thus

(8)
$$R \equiv \operatorname{Ridge}(p) = \{x : G(x) = 0, \lambda_2(x) < 0\}.$$

We use "ridge" as an operator that maps a density function to the ridge set. Because the columns of V(x) are orthonormal,

(9)
$$G(x) = 0 \iff V(x)^T g(x) = 0.$$

Intuitively, at points on the ridge, the density curves sharply downward in all but the direction of first eigenvector (corresponding to the eigenvector of the largest eigenvalue) and along the first eigenvector, the density curves more gently. By the implicit function theorem, the ridges are 1-dimensional manifolds if (i.e., a collection of curves)

$$\operatorname{rank}(\nabla(V(x)^T g(x))) = d - 1 \quad \forall x \in R.$$

Claim 4 of Lemma 2 gives a sufficient condition for the ridges to be 1-dimensional manifolds.

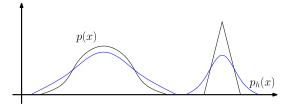


FIG. 3. An example of a density p(x) (black curves) versus the smoothed density $p_h(x)$ (blue curves). Note that even if p(x) is nondifferentiable, its smoothed version is very smooth provided the kernel function is smooth.

2.2. Estimated ridges and smoothed density ridges. Given data X_1, \ldots, X_n drawn i.i.d. from density p, we estimate Ridge(p) by

(10)
$$\widehat{R}_h = \operatorname{Ridge}(\widehat{p}_h).$$

where the kernel density estimator (KDE) \hat{p}_h is defined by

(11)
$$\widehat{p}_h(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{\|x - X_i\|}{h}\right).$$

Here, the kernel K is a smooth, symmetric density function such as a Gaussian and the bandwidth $h \equiv h_n > 0$. Figure 1 shows an example.

Let p_h denote the expected value of the estimated density $p_h(x) = \mathbb{E}(\hat{p}_h(x))$. Thus $p_h = p \star K_h$, where \star denotes convolution. Hence p_h is a smoothed version of p. Figure 3 compares a density p and its smoothed version p_h . We define the *smoothed ridge* set to be the ridge set of p_h :

(12)
$$R_h = \operatorname{Ridge}(p_h) = \{x : V_h(x)^T g_h(x) = 0\},\$$

where $V_h(x) = [v_2(x) \cdots v_d(x)]$, $v_k(x)$ is the eigenvector of Hessian matrix of $p_h(x)$ corresponding to the *k*th eigenvalue and $g_h(x) = \nabla p_h(x)$. Figure 4 compares the smoothed ridge R_h and the original ridge *R*. Our main focus here is on estimating the smoothed ridge R_h .

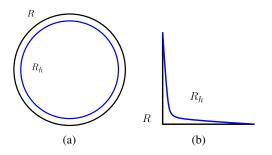


FIG. 4. Examples for ridge R (black) and its smoothed version R_h (blue). Note that in (b), the original ridge is nonsmooth due to the sharp angle, but the smoothed ridge is smooth if the kernel function is smooth enough.

2.3. Distance measures and functional norms. Define the projection from one point x onto a set A by

(13)
$$\pi_A(x) = \underset{y \in A}{\operatorname{argmin}} \|x - y\|.$$

We define the projection vector from *x* onto a set *A* as

(14)
$$\mathbf{d}(x,A) = \pi_A(x) - x.$$

The projection vector may not be unique. A condition related to the uniqueness of the projection is called the *reach* and will be formally introduced in Section 3.1. The projection distance from x onto A is

(15)
$$d(x, A) = \|\mathbf{d}(x, A)\|.$$

The Hausdorff distance between two subsets of \mathbb{R}^d is defined by

(16)
$$\operatorname{Haus}(A, B) = \inf\{\varepsilon > 0 \colon A \subset B \oplus \varepsilon \text{ and } B \subset A \oplus \varepsilon\}$$

where $A \oplus \varepsilon = \bigcup_{x \in A} B(x, \varepsilon)$ and $B(x, \varepsilon) = \{y : ||x - y|| \le \varepsilon\}$. We also define the quasi-Hausdorff distance dist_{Π}(*A*, *B*) as

(17)
$$\operatorname{dist}_{\Pi}(A, B) = \sup_{x \in B} d(x, A),$$

so that

$$(18) B \subseteq A \oplus \mathsf{dist}_{\Pi}(A, B)$$

Note that

(19)
$$\operatorname{Haus}(A, B) = \max\{\operatorname{dist}_{\Pi}(A, B), \operatorname{dist}_{\Pi}(B, A)\}.$$

Now we introduce some norms and semi-norms characterizing the smoothness of the density p. A vector $\alpha = (\alpha_1, \ldots, \alpha_d)$ of nonnegative integers is called a multi-index with $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_d$, and the corresponding derivative operator is

(20)
$$D^{\alpha} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}},$$

where $D^{\alpha} f$ is often written as $f^{(\alpha)}$. For j = 0, ..., 4, define

(21)
$$\|p\|_{\infty}^{(j)} = \max_{\alpha : |\alpha|=j} \sup_{x \in \mathbb{R}^d} |p^{(\alpha)}(x)|.$$

When j = 0, we have the infinity norm of p; for j > 0, these are semi-norms. We also define

(22)
$$\|p\|_{\infty,k}^* = \max_{j=0,\dots,k} \|p\|_{\infty}^{(j)}.$$

It is easy to verify that this is a norm.

1902

Algorithm 1 Local uncertainty estimator

Input: Data $\{X_1, \ldots, X_n\}$. 1. Estimate the ridges from $\{X_1, \ldots, X_n\}$; denote the estimate by \widehat{R}_h . 2. Generate *B* bootstrap samples: $X_1^{*(b)}, \ldots, X_n^{*(b)}$ for $b = 1, \ldots, B$. 3. For each bootstrap sample, estimate the ridges, yielding $\widehat{R}_n^{*(b)}$ for $b = 1, \ldots, B$. 4. For each $x \in \widehat{R}_h$, calculate $\rho_{(b)}^2(x) = d^2(x, \widehat{R}_h^{*(b)}), b = 1, \ldots, B$. 5. Define $\widehat{\rho}_n^2(x) = \text{mean}\{\rho_{(1)}^2(x), \ldots, \rho_{(B)}^2(x)\}$. **Output:** $\widehat{\rho}_n^2(x)$.

2.4. Local uncertainty measures for the density ridges. We define the local uncertainty by

(23)
$$\rho_n^2(x) = \begin{cases} \mathbb{E}(d^2(x, \widehat{R}_h)), & \text{if } x \in R_h, \\ 0, & \text{otherwise.} \end{cases}$$

We estimate the local uncertainty measure by the bootstrap. Let $\mathbb{X}_n = \{X_1, \ldots, X_n\}$ be the given observations. We define \widehat{R}_h^* as the estimated ridge based on the bootstrap [Efron (1979)] sample of \mathbb{X}_n . More precisely, let X_1^*, \ldots, X_n^* be a bootstrap sample from the empirical distribution \mathbb{P}_n . Let $\widehat{p}_h^*(x)$ be the KDE based on the bootstrap sample. The bootstrap ridge is defined as

(24)
$$\widehat{R}_{h}^{*} = \operatorname{Ridge}(\widehat{p}_{h}^{*}(x))$$

We define

(25)
$$\widehat{\rho}_n^2(x) = \begin{cases} \mathbb{E}(d^2(x, \widehat{R}_h^*) | \mathbb{X}_n), & \text{if } x \in \widehat{R}_h, \\ 0, & \text{otherwise,} \end{cases}$$

as the estimated local uncertainty. Algorithm 1 gives a pseudo-code for estimating $\rho_n^2(x)$ by the bootstrap.

2.5. Confidence sets. For making inferences about ridges, we focus on constructing a confidence set for R_h , ignoring the bias Haus (R, R_h) . For suitable h, R_h has essentially the same shape as R and thus serves as a useful target.

We call $\widehat{C}_n \equiv \widehat{C}(X_1, \dots, X_n)$ a valid $(1 - \alpha)$ confidence set if

(26)
$$\liminf_{n \to \infty} \mathbb{P}(R_h \subseteq \widehat{C}_n) \ge 1 - \alpha.$$

Let t_{α} be the value such that

$$\mathbb{P}(R_h \subseteq \widehat{R}_h \oplus t_\alpha) \ge 1 - \alpha.$$

Thus $t_{\alpha} = F^{-1}(1 - \alpha)$ where

(27)
$$F(t) = \mathbb{P}(\operatorname{dist}_{\Pi}(\widehat{R}_h, R_h) \le t).$$

Algorithm 2 Confidence sets

Input: Data $\{X_1, \ldots, X_n\}$, significance level α . 1. Estimate the ridge from $\{X_1, \ldots, X_n\}$; denote this by \widehat{R}_h . 2. Generates bootstrap samples $\{X_1^{*(b)}, \ldots, X_n^{*(b)}\}$ for $b = 1, \ldots, B$. 3. For each bootstrap sample, estimate the ridge, call this $\widehat{R}_h^{*(b)}$. 4. For $i = 1, \ldots, B$, calculate $t_i = \{\text{dist}_{\Pi}(\widehat{R}_i^*, \widehat{R}_h)\}$. 5. Let \widehat{t}_{α} be the α -upper quantile of t_1, \ldots, t_B . **Output:** $\widehat{R}_h \oplus \widehat{t}_{\alpha}$.

Although t_{α} is unknown, we can estimate it by the bootstrap. We define $\hat{t}_{\alpha} = \hat{F}^{-1}(1-\alpha)$ where

(28)
$$\widehat{F}(t) = \mathbb{P}\left(\operatorname{dist}_{\Pi}\left(\widehat{R}_{h}^{*}, \widehat{R}_{h}\right) \le t | \mathbb{X}_{n}\right)$$

and where \widehat{R}_{h}^{*} is constructed from an i.i.d. sample $X_{1}^{*}, \ldots, X_{n}^{*}$ from the empirical distribution $\widehat{\mathbb{P}}_{n}$. Algorithm 2 provides a pseudo-code for constructing the confidence sets and Theorem 8 shows its consistency.

3. Main results. For a vector $v \in \mathbb{R}^d$, ||v|| is the usual \mathcal{L}^2 norm for the vector, and $||v||_{\infty}$ is the supremum norm for v; that is,

$$||v||_{\infty} = \max\{||v_1||, \dots, ||v_d||\}.$$

For a matrix M, let $||M||_{max} = \max_{i,j} ||M_{ij}||$. When M is symmetric, we define $||M||_2 = \max_v \frac{||Mv||}{||v||}$.

We define \mathbb{C}^{r} to be the collection of *r*-times continuously differentiable functions. For a vector value function $f = (f_1, \ldots, f_k) : \mathbb{R}^d \mapsto \mathbb{R}^k$, we define the gradient $\nabla f(x)$ as a $d \times k$ matrix given by

(29)
$$\nabla f(x) = (\nabla f_1(x), \dots, \nabla f_k(x)).$$

3.1. Assumptions. We begin by defining the tangent vector e(x) to R_h at each $x \in R_h$. Let

(30)
$$M(x) = \nabla (V_h(x)^T g_h(x)),$$

which is a $d \times (d-1)$ matrix. We define e(x) to be the eigenvector corresponding to the largest eigenvalue of $\mathbf{I}_d - M(x)(M(x)^T M(x))^{-1}M(x)^T$. As long as M(x) has rank d-1, e(x) is unique.

LEMMA 1. Assume the matrix M(x) has rank d-1. Then e(x), the first eigenvector of

$$\mathbf{I}_d - M(x) (M(x)^T M(x))^{-1} M(x)^T,$$

is tangent to R_h at $x \in R_h$. The column space of M(x) is normal to R_h at each $x \in R_h$.

The proof can be found in the supplementary material [Chen, Genovese and Wasserman (2015)]. By Lemma 1, the vector e(x) defined as above is always tangent to R_h whenever $x \in R_h$. Later we will see in claim 4 of Lemma 2, condition (P1) with smoothness on p_h [guaranteed by conditions (K1)–(K2)] implies Lemma 1.

With the above notation, we now formally describe our assumptions.

- (K1) The kernel K is in \mathbb{C}^4 and $||K||_{\infty}^* < \infty$.
- (K2) Let

$$\mathcal{K}_r = \left\{ y \mapsto K^{(\alpha)} \left(\frac{x - y}{h} \right) : x \in \mathbb{R}^d, \, |\alpha| = r \right\},\$$

where $K^{(\alpha)}$ is defined in (20), and let $\mathcal{K}_l^* = \bigcup_{r=0}^l \mathcal{K}_r$. We assume that \mathcal{K}_4^* is a VC-type class; that is, there exist constants A, v and a constant envelope b_0 such that

(31)
$$\sup_{Q} N(\mathcal{K}_{4}^{*}, \mathcal{L}^{2}(Q), b_{0}\varepsilon) \leq \left(\frac{A}{\varepsilon}\right)^{\nu},$$

where $N(T, d_T, \varepsilon)$ is the ε -covering number for an semi-metric set T with metric d_T , and $\mathcal{L}^2(Q)$ is the L_2 norm with respect to the probability measure Q.

(P1) There exist constants β_0 , β_1 , β_2 , $\delta_0 > 0$ such that

(32)
$$\lambda_{2}(x) \leq -\beta_{1},$$
$$\lambda_{1}(x) \geq \beta_{0} - \beta_{1},$$
$$\|g_{h}(x)\| \max_{|\alpha|=3} |p_{h}^{(\alpha)}(x)| \leq \beta_{0}(\beta_{1} - \beta_{2}),$$

for all $x \in R_h \oplus \delta_0$. We call δ_0 the *gap*. Note that $V_h(x)$ defined in equation (12). (P2) For each $x \in R_h$, $|e(x)^T g_h(x)|^2 \ge \frac{\lambda_1(x)}{\lambda_1(x) - \lambda_2(x)}$ where e(x) is the direction of R_h at point $x \in R_h$ defined in Lemma 1. of R_h at point $x \in R_h$ defined in Lemma 1.

(P3) Conditions (P1), (P2) hold for all small *h*.

Now we discuss the conditions. (K1) is needed since the definition of density ridge requires twice differentiability. We need additional smoothness for making sure the estimated ridges are smooth. (K2) regularizes the complexity of kernel functions and its partial derivatives. This is to ensure the fourth derivatives of the KDE will converge; we need the fourth derivative since the reach of R_h depends on the fourth derivative of \hat{p}_h by claim 7 in Lemma 2. Note that similar conditions to (K2) appear in Einmahl and Mason (2000, 2005), Giné and Guillou (2002). The Gaussian kernel satisfies this condition.

(P1) is the eigen condition which also appears in Genovese et al. (2014). This implies that the projected gradient near the ridge is smooth. This leads to a welldefined local normal coordinate along ridges; see Lemma 2. We require a slightly stronger condition (existence of β_2) than Genovese et al. (2014).

We use (P2) to make sure the density ridge is also a generalized local mode in the normal space; see Lemma 9. Note that whenever $\lambda_1(x) < 0$ for some $x \in R_h$, x must be a local mode in the normal space of R_h at x since all eigenvalues are negative. (P3) is required if we allow $h \rightarrow 0$; otherwise we do not need to assume it. Note that if we say a density p satisfies (P1) or (P2), we mean that the condition holds for p_h .

Finally, we consider the following assumption that will not be assumed in our main result but is useful and frequently assumed in working lemmas.

(A1) The density $p \in \mathbb{C}^4$ and has uniformly bounded derivatives to the fourth order.

This condition will not be assumed in our main results since conditions (K1)–(K2) imply (A1) for p_h .

3.2. The normal space for density ridges. In this section, we show that under suitable conditions, for each point x on the density ridge we can construct a matrix N(x) whose columns span the normal space of the density ridge at x.

Let *L* be a $d \times q$ matrix with orthonormal columns. For such an *L*, we define the subspace derivative by $\nabla_L = L^T \nabla$, which in turn gives the subspace gradient

$$g(x; L) = \nabla_L p(x)$$

and the subspace Hessian

$$H(x; L) = \nabla_L \nabla_L p(x).$$

Thus g(x; L) and H(x; L) are the gradient and Hessian generated by the partial derivatives along columns of L; this is the partial derivative in the subspace spanned by columns of L. If L is a unit vector, then ∇_L is the *directional derivative* along L.

Now we construct a local normal coordinate for the ridge. Note in this subsection, all notation with subscript q (e.g., g_q , H_q , V_q) denote the quantities defined for the smooth density q. For any smooth density q, let $g_q(x)$, $H_q(x)$ denote the gradient and Hessian of q. For simplicity, we denote the eigenvectors and eigenvalues of $H_q(x)$ using the same notation as before. Let $v_1(x), \ldots, v_d(x)$ be the eigenvectors of $H_q(x)$ corresponding to eigenvalues $\lambda_1(x) \ge \cdots \ge \lambda_d(x)$. As before, the ridge set $R_q = \text{Ridge}(q)$ is defined as the collection of x such that $V_q(x)^T g_q(x) = 0$ with $\lambda_2(x) < 0$. By Lemma 1, the gradient of $V_q(x)^T g_q(x)$ forms a matrix whose columns space spans the normal space to R_q at each $x \in R_q$.

Define $M_q(x) = \nabla(V_q(x)^T g_q(x)) = [m_2(x) \cdots m_d(x)]$ which is a $d \times (d-1)$ matrix. Eberly (1996) (page 65) shows that

(33)
$$m_k(x) = \left(\lambda_k(x)\mathbf{I}_d + \frac{v_1(x)^T g_q(x)}{\lambda_k(x) - \lambda_1(x)} \nabla_{v_1(x)} H_q(x)\right) v_k(x),$$

where \mathbf{I}_d is the $d \times d$ identity matrix. The columns of $M_q(x)$ span the normal space to R_q at x. However, the columns of $M_q(x)$ are not orthonormal. Thus we perform an orthonormalization to $M_q(x)$ to construct $N_q(x)$ by the following steps: We have that $M_q(x) = \nabla V_q(x)^T g_q(x)$. There exists a lower triangular matrix $L_q(x)$ such that

$$L_q(x)L_q(x)^T = M_q(x)^T M_q(x).$$

We then define

(34)
$$N_q(x) = M_q(x) [L_q(x)^T]^{-1}.$$

Note that $M_q(x)$ might not be unique since the eigenvalues of $H_q(x)$ can have multiplicities. When $H_q(x)$ has multiplicities, any choice of linearly independent eigenvectors for $H_q(x)$ will work in the above construction. As will be shown later, what we need is the smoothness of $N_q(x)N_q(x)^T$ or $M_q(x)M_q(x)^T$, which is unaffected by multiplicities.

The *reach* [Federer (1959)] for a set A, denoted by reach(A), is the largest real number r such that each $x \in \{y : d(y, A) \le r\}$ has a unique projection onto A. The reach measures the smoothness of a set.

LEMMA 2 (Properties of the normal space). Let q be a density that satisfies (A1) and (P1), and denote $R_q = \text{Ridge}(q)$. Let $R_q^{\delta} = R_q \oplus \delta_0$ where δ_0 is the gap defined in (P1). Let $M_q(x)$, $N_q(x)$ be constructed from (34). Then:

(1) N_q and M_q have the same column space. Also,

(35)
$$N_q(x)N_q(x)^T = M_q(x)[M_q(x)^T M_q(x)]^{-1}M_q(x)^T.$$

That is, $N_q(x)N_q(x)^T$ is the projection matrix onto columns of $M_q(x)$.

(2) The columns of $N_q(x)$ are orthonormal to each other.

(3) For $x \in R_q$, the column space of $N_q(x)$ is normal to the direction of R_q at x.

(4) For all $x \in R_q$, rank $(N_q(x)) = \operatorname{rank}(M_q(x)) = d - 1$. Moreover, R_q is a 1-dimensional manifold that contains no intersection and no endpoints. Namely, R_q is a finite union of connected, closed curves.

(5) When ||x - y|| is sufficiently small and $x, y \in R_a^{\delta}$,

$$\|N_q(x)N_q(x)^T - N_q(y)N_q(y)^T\|_{\max} \le A_0(\|q^{(3)}\|_{\infty} + \|q^{(4)}\|_{\infty})^2\|x - y\|,$$

for some constant A_0 .

(6) Assume q' also satisfies (A1) and (P1) and $||q - q'||_{\infty,3}^*$ is sufficiently small. Then

$$||N_q(x)N_q(x)^T - N_{q'}(x)N_{q'}(x)^T||_{\max} \le A_1(||q - q'||_{\infty,3}^*)$$

for some constant A_1 .

(7) The reach of R_q satisfies

$$\operatorname{reach}(R_q) \ge \min\left\{\frac{\delta_0}{2}, \frac{\beta_2^2}{A_2(\|q^{(3)}\|_{\infty} + \|q^{(4)}\|_{\infty})}\right\}$$

for some constant A_2 .

The proof can be found the supplementary material [Chen, Genovese and Wasserman (2015)]. We call $N_q(x)$ the *normal matrix* since by claims 2 and 3 of the lemma, the columns of $N_q(x)$ span the normal space to Ridge(q) at x. By claim 4, the ridge is a 1-dimensional manifold and by claim 1–3 and Lemma 1, at each $x \in R_h$, the column space of $N_q(x)$, $M_q(x)$ spans the normal space to R_h at x.

Claim 4 avoids cases in density ridges that are not well defined: endpoints and intersections. The eigenvectors near endpoints or intersections will be ill-defined. Claim 5 proves that the projection matrix, $N_q(x)N_q(x)^T$, changes smoothly near R_q . Claim 6 shows that when two density functions are sufficiently close, the column space of $N_q(x)$ will also be close. Claim 7 gives the smoothness of R_q in terms of the reach.

In the following sections, we work primarily on the ridge generated from p_h and \hat{p}_h , so for simplicity we define

(36)
$$N(x) = N_{p_h}(x), \qquad \widehat{N}_n(x) = N_{\widehat{p}_h}(x).$$

3.3. Local uncertainty for ridges. Let

$$H_N(x) = H(x; N(x)), \qquad x \in R_h,$$

which is the subspace Hessian matrix in the normal space along R_h at x. Recall that N(x) is not uniquely defined (due to possible multiplicities of eigenvalues), but any choice of N(x) constructed from (34) can be used in the definition of H_N . Lemma 4 guarantees this invariance.

Let \mathcal{F} be the class of vector valued functions defined by

(37)
$$\mathcal{F} = \left\{ f_x(\cdot) = \frac{1}{\sqrt{h^{d+2}}} N(x) H_N^{-1}(x) N(x)^T (\nabla K) \left(\frac{x-\cdot}{h}\right), x \in R_h \right\}.$$

Define the empirical process $(\mathbb{G}_n(f) : f \in \mathcal{F})$ where

(38)
$$\mathbb{G}_n(f) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left(f(X_i) - \mathbb{E}(f(X_i)) \right).$$

THEOREM 3 (Local uncertainty theorem). Assume (K1)–(K2), (P1)–(P2). Suppose that $\frac{hh^{d+8}}{\log n} \to \infty$. If $h \to 0$, then we further assume (P3). Then for all $x \in R_h$, when $\|\hat{p}_h - p_h\|_{\infty,4}^*$ is sufficiently small,

$$\sup_{x\in R_h} \left\|\sqrt{nh^{d+2}}\mathbf{d}(x,\,\widehat{R}_h) - \mathbb{G}_n(f_x)\right\|_{\infty} = O\left(\|\widehat{p}_h - p_h\|_{\infty,3}^*\right) = O_P\left(\sqrt{\frac{\log n}{nh^{d+6}}}\right)$$

1908

and $nh^{d+2}\rho_n^2(x) = \text{Trace}(\Sigma(x)) + o(1)$, where

$$\Sigma(x) = \operatorname{Cov}(N(x)H_N^{-1}(x)N(x)^T \nabla K(x-X_i)).$$

We used Theorem 10 to convert the rate $O(\|\hat{p}_h - p_h\|_{\infty,3}^*)$ into $O_P(\sqrt{\frac{\log n}{nh^{d+6}}})$ in the first equality. An intuitive explanation for the approximation error rate $\|\hat{p}_h - p_h\|_{\infty,3}^*$ comes from difference in normal matrices $N(x)N(x)^T$ and $\hat{N}_n(x)\hat{N}_n(x)$ by claim 6 in Lemma 2.

REMARK 1. For a fixed x, $\mathbb{G}_n(f_x)$ is a vector and converges to a mean 0 multivariate-normal distribution with covariance matrix $\Sigma(x)$ having rank d - 1. This theorem also shows the asymptotic result for the local uncertainty measure $\rho_n^2(x)$. The matrix $\Sigma(x)$ determines the behavior of $\rho_n^2(x)$ and depends on three quantities: the normal matrix N(x), the inverse of subspace Hessian $H_N^{-1}(x)$ and the kernel function $\nabla K(x - X_i)$. The normal matrix comes from the fact that $\mathbf{d}(x, \hat{R}_h)$ is asymptotically in the normal space of R_h at x. The inverse of subspace Hessian to a local mode. We will discuss its properties later. The last term comes from the kernel density estimator that depends on the kernel function we use.

Theorem 3 shows that the uncertainty measure has a limiting distribution that is similar to KDE for estimating the gradient. The difference is the matrix $N(x)H_N^{-1}(x)N(x)^T$ whose properties are given in the following lemma.

LEMMA 4. Assume (P1)-(P2). Let

$$W(x) = N(x)^{T} H_{N}^{-1}(x) N(x)^{T} = N(x)^{T} (N(x)^{T} H(x) N(x))^{-1} N(x)^{T}$$

Then:

(1) For any other $d \times (d-1)$ matrix N'(x) such that $N'(x)^T N'(x) = \mathbf{I}_{d-1}$ and $N'(x)N'(x)^T = N(x)N(x)^T$,

$$N(x)^{T} (N(x)^{T} H(x) N(x))^{-1} N(x)^{T} = N'(x)^{T} (N'(x)^{T} H(x) N'(x))^{-1} N'(x)^{T}$$

when $x \in R_h \oplus \delta_0$.

(2) When ||x - y|| is sufficiently small,

$$||W(x) - W(y)||_{\max} \le A_3 (||q^{(3)}||_{\infty} + ||q^{(4)}||_{\infty})^2 ||x - y||$$

for some constant A_3 .

(3) Assume another density q satisfies (A1) and (P1), and let $W_q(x)$ be the counterpart of W(x) for density q. When $||p_h - q||_{\infty,3}^*$ is sufficiently small,

$$\|W(x) - W_q(x)\|_{\max} \le A_4 \|p_h - q\|_{\infty,3}^*$$

for some constant A_4 .

The proof can be found the supplementary material [Chen, Genovese and Wasserman (2015)]. The first result shows that the matrix $N(x)^T H_N^{-1}(x)N(x)^T$ is the same for any orthonormal matrix N'(x) whose column space spans the same space. This shows that W(x) is unaffected if multiplicity of eigenvalues occur. The second result gives the smoothness for $N(x)^T H_N^{-1}(x)N(x)^T$, and the third result shows stability under small perturbation on the density.

Now we show that the uncertainty measure $\rho_n^2(x)$ can be estimated by the bootstrap. Given the observed data $\mathbb{X}_n = \{X_1, \dots, X_n\}$, we generate the bootstrap sample $\mathbb{X}_n^* = \{X_1^*, \dots, X_n^*\}$. We use the bootstrap sample to construct the bootstrap KDE

(39)
$$\widehat{p}_h^*(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{x - X_i^*}{h}\right)$$

The bootstrap ridge is

(40)
$$\widehat{R}_h^* = \operatorname{Ridge}(\widehat{p}_h^*).$$

Let

(41)
$$\widehat{\rho}_n^2(x) = \begin{cases} \mathbb{E}(d(x, \widehat{R}_h^*)^2 | X_1, \dots, X_n), & \text{for } x \in \widehat{R}_h, \\ 0, & \text{otherwise,} \end{cases}$$

be the bootstrap estimate to the local uncertainty measure.

THEOREM 5 (Bootstrap consistency). Assume (K1)–(K2), (P1)–(P2). For all large *n* the following is true. There exists an event \mathcal{X}_n such that $\mathbb{P}(\mathcal{X}_n) \ge 1 - 5e^{-nh^{d+8}D_1}$ for some constant D_1 , and for $\mathbb{X}_n \in \mathcal{X}_n$, when $\|\widehat{p}_h - p_h\|_{\infty,4}^*$ is sufficiently small, for all $x \in R_h$:

- (1) The set $\widehat{R}_h \cap B(x, \operatorname{Haus}(\widehat{R}_h, R_h)) \neq \phi$.
- (2) The estimated ridge satisfies: $\widehat{R}_h = \bigcup_{x \in R_h} (\widehat{R}_h \cap B(x, \text{Haus}(\widehat{R}_h, R_h))).$

(3) Suppose that $\frac{nh^{d+8}}{\log n} \to \infty$. The estimated local uncertainty measure is consistent in the sense that for any $y \in \widehat{R}_h \cap B(x, \text{Haus}(\widehat{R}_h, R_h))$,

$$nh^{d+2}|\hat{\rho}_n^2(y) - \rho_n^2(x)| = O(\|\hat{p}_h - p_h\|_{\infty,3}^*) = O_P(\sqrt{\frac{\log n}{nh^{d+6}}}).$$

[If we allow $h \rightarrow 0$, we need to assume (P3).]

Note that we need the above set-based argument because $\rho_n(x)$ and $\hat{\rho}_n(x)$ are defined on different supports: $\rho_n(x)$ is defined on R_h while $\hat{\rho}_n(x)$ is defined on \hat{R}_h . This theorem shows that as \hat{R}_h is approaching R_h , the estimated local uncertainty on \hat{R}_h will converge to the local uncertainty defined on R_h .

1910

3.4. *Gaussian approximation*. In this section, we derive the limiting distribution of the Hausdorff distance. Let \mathbb{B} be a centered, tight Gaussian process defined on \mathcal{F} with covariance function

(42)
$$\operatorname{Cov}(\mathbb{B}(f_1), \mathbb{B}(f_2)) = \mathbb{E}[f_1(X_i), f_2(X_i)] - \mathbb{E}[f_1(X_i)]\mathbb{E}[f_2(X_i)].$$

Such Gaussian processes exists if \mathcal{F} is pre-Gaussian. The kernel functions and its derivatives of order less than four are pre-Gaussian by assumption (K2).

THEOREM 6 (Gaussian approximation). Assume conditions (K1)–(K2), (P1)–(P2) and that $\frac{nh^{d+8}}{\log n} \to \infty$. Then there exists a Gaussian process \mathbb{B} defined on a function space \mathcal{F}_h [see equation (69)] such that, when n is sufficiently large,

$$\sup_{t} \left| \mathbb{P}\left(\sqrt{nh^{d+2}}\mathsf{Haus}(\widehat{R}_{h}, R_{h}) < t\right) - \mathbb{P}\left(\sup_{f \in \mathcal{F}_{h}} \left|\mathbb{B}(f)\right| < t\right) \right| = O\left(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}}\right)$$

We can replace Haus(\widehat{R}_h, R_h) with dist $_{\Pi}(\widehat{R}_h, R_h)$ in the above. If we allow $h \to 0$, we need to assume (P3).

Here we provide an intuitive explanation. From Theorem 3, the local uncertainty vector $\mathbf{d}(x, \hat{R}_h)$ can be approximated by an empirical process. Recall from equations (14), (15), (17), we have

(43)
$$\operatorname{dist}_{\Pi}(\widehat{R}_h, R_h) = \sup_{x \in R_h} \left\| \mathbf{d}(x, \widehat{R}_h) \right\|$$

The Hausdorff distance and the quasi-Hausdorff distance will be the same when the two ridges are close enough; see Lemma 14. The above argument shows the connection between Hausdorff distance and the empirical process. The rest of the proof of Theorem 6 establishes the approximation of the empirical process by the Gaussian process and applies an anti-concentration argument due to Chernozhukov, Chetverikov and Kato (2014a) to construct the Berry–Esseen type bound.

REMARK 2. As a referee points out, the Hausdorff distance is usually unstable. Here we obtain a nice concentration because of assumption (P1)–(P2) along with the fact that p_h has fourth derivatives. These conditions ensure the density near ridges is well behaved.

3.5. Asymptotic validity of the confidence set. To show our confidence set is consistent, we need to show that

$$\widehat{F}(t) = \mathbb{P}\big(\sqrt{nh^{d+2}}\mathsf{dist}_{\Pi}\big(\widehat{R}_h^*, \widehat{R}_h\big) < t \,|\,\mathbb{X}_n\big)$$

has the same limit as

$$F(t) = \mathbb{P}(\sqrt{nh^{d+2}} \mathsf{dist}_{\Pi}(\widehat{R}_h, R_h) < t).$$

THEOREM 7 (Gaussian approximation for bootstrapping). Assume conditions (K1)–(K2) and (P1)–(P2) and that $\frac{nh^{d+8}}{\log n} \to \infty$. For all large *n* the following is true. There exists an event \mathcal{X}_n such that $\mathbb{P}(\mathcal{X}_n) \ge 1 - 5e^{-nh^{d+8}D_1}$ for some constant D_1 , and for $\mathbb{X}_n \in \mathcal{X}_n$, there exists a Gaussian process \mathbb{B} defined on a space \mathcal{F}_h [see equation (69)] such that

$$\sup_{t} \left| \mathbb{P}\left(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_{h}^{*}, \widehat{R}_{h}) < t | \mathbb{X}_{n}\right) - \mathbb{P}\left(\sup_{f \in \mathcal{F}_{h}} \left|\mathbb{B}(f)\right| < t\right) \right|$$
$$= O\left(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}}\right) + O\left(\left(\frac{\log n}{nh^{d+6}}\right)^{1/6}\right).$$

A similar result also holds when replacing $\operatorname{Haus}(\widehat{R}_h^*, \widehat{R}_h)$ by $\operatorname{dist}_{\Pi}(\widehat{R}_h^*, \widehat{R}_h)$. Note that if we allow $h \to 0$, we need to assume (P3).

The above result, together with Theorem 6, establishes a Berry–Esseen result for the bootstrap estimate for the distribution of $\text{Haus}(\widehat{R}_h, R_h)$. Theorem 7 gives the rate for the bootstrap case.

REMARK 3. One might expect the rate to be $O_P(\frac{\sqrt{\log n}}{(nh^{d+2})^{1/8}})$ in light of Theorem 6. The second term $O_P((\frac{\log n}{nh^{d+6}})^{1/6})$ comes from the difference in support of the two ridges R_h , \hat{R}_h . The rate is related to the rate estimating the third derivative of a density, which contributes to the difference in normal spaces between points of R_h and \hat{R}_h .

We now have the following result on the coverage of the confidence set.

THEOREM 8. Assume (K1)–(K2), (P1)–(P2) and that $\frac{nh^{d+8}}{\log n} \to \infty$. Let $\hat{t}_{\alpha} = \widehat{F}^{-1}(1-\alpha)$. Then

$$\mathbb{P}(R_h \subset \widehat{R}_h \oplus \widehat{t}_{\alpha}/\sqrt{nh^{d+2}}) \ge 1 - \alpha + O\left(\frac{\log n}{(nh^{d+2})^{1/8}}\right) + O\left(\left(\frac{\log n}{nh^{d+6}}\right)^{1/6}\right).$$

If we allow $h \rightarrow 0$, we need to assume (P3).

This theorem is a direct result of Theorems 6 and 7, so we omit the proof. Note that here \hat{t}_{α} differs to the one defined in Algorithm 2 (and Section 2.5) by a factor $\sqrt{nh^{d+2}}$. This is because we rescale dist $_{\Pi}(\hat{R}_{h}^{*}, \hat{R}_{h})$ when defining $\hat{F}(t)$.

REMARK 4. As a referee points out, one can use

$$\psi_h = \max_{x \in R_h} \frac{d(x, R_h)}{p_h(x)}$$

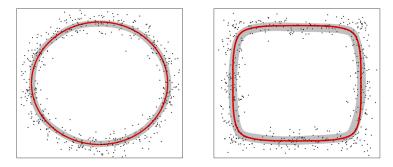


FIG. 5. 90% confidence sets for the circle data (left) and box data (right). The red curve is the smoothed ridge R_h , and the gray regions are confidence sets.

as a replacement for dist_{Π}(\hat{R}_h , R_h) and use the bootstrap to construct a confidence set. This is a variance-stabilizing version for the original confidence set. This confidence set is also valid by a simple modification of Theorems 6–8.

4. Examples. We consider two simulation settings: the circle data and the smoothed box data. For all simulations, we use a sample size of 500. We choose the bandwidth h using Silverman's rule [Silverman (1986)].

The first dataset is the circle data. See Figure 5. We show the true smoothed ridge (red) and the estimated ridge (blue) along with the 90% confidence sets (gray regions).

The second dataset is the box data; see Figure 5. Notice that the original box data has corners that violate condition (P1), but the ridge of the smoothed density p_h obeys (P1). We show the 90% confidence sets. The box data has a large angle near its corner, but our confidence set still has good behavior over these regions.

5. Proofs. We prove the main theorems in this section. The proofs for the lemmas (including those used for proving the main theorems) are given in the supplementary material; see Supplementary proofs and Chen, Genovese and Wasserman (2015). Before we prove Theorem 3, we state three useful lemmas.

LEMMA 9. Let *R* be the ridge of a density *p*. For $x \in R$, let the Hessian at *x* be H(x) with eigenvectors $[v_1, \ldots, v_d]$ and eigenvalues $0 > \lambda_2 \ge \cdots \ge \lambda_d$. Consider any subspace \mathbb{L} spanned by a basis $[e_2, \ldots, e_d]$ with e_1 in the normal direction of that subspace. Then a sufficient condition for *x* being a local mode of *p* constrained to \mathbb{L} is

(44)
$$(v_1^T e_1)^2 > \frac{\lambda_1}{\lambda_1 - \lambda_2}.$$

The proof can be found in the supplementary material [Chen, Genovese and Wasserman (2015)].

The following lemma is a uniform bound for the KDE.

LEMMA 10 [Giné and Guillou (2002); version of Genovese et al. (2014)]. Assume (K1)–(K2) and that $\log n/n \le h^d \le b$ for some 0 < b < 1. Then we have

(45)
$$\|\widehat{p}_n - p\|_{\infty,k} = O(h^2) + O_P\left(\sqrt{\frac{\log n}{nh^{d+2k}}}\right)$$

for k = 0, ..., 4. In particular, if we consider the smoothed version of density, p_h , for the same kernel function, then we have

$$\|\widehat{p}_n - p_h\|_{\infty,k} = O_P\left(\sqrt{\frac{\log n}{nh^{d+2k}}}\right)$$

for k = 0, ..., 4.

LEMMA 11. Assume (K1)–(K2). Then we have

(46)
$$\mathbb{E}\left(\left(\|\widehat{p}_n - p_h\|_{\infty,k}^*\right)^2\right) = O\left(\frac{\log n}{nh^{d+2k}}\right)$$

for k = 0, ..., 4.

This lemma follows directly from Talagrand's inequality [Talagrand (1996)], which proves an exponential concentration inequality for random variable $\|\hat{p}_n - p_h\|_{\infty,k}^*$. Thus the second moment is bounded at the specified rate.

In the next proof, we will frequently use the following theorem that links the uniform derivative difference to the Hausdorff distance.

THEOREM 12 [Theorem 6 in Genovese et al. (2014)]. Assume condition (A1), (P1) for two densities p_1, p_2 . When $||p_1 - p_2||_{\infty,3}^*$ is sufficiently small, we have Haus $(R_1, R_2) = O(||p_1 - p_2||_{\infty,2}^*)$.

PROOF OF THEOREM 3. Theorem 3 makes two claims: the first claim is an empirical approximation

$$\sup_{x\in R_h} \|\sqrt{nh^{d+2}}\mathbf{d}(x,\widehat{R}_h) - \mathbb{G}_n(f_x)\|_{\infty} = O(\|\widehat{p}_h - p_h\|_{\infty,3}^*),$$

and the second claim is the limiting behavior for the uncertainty measure $\rho_n^2(x)$. We prove the empirical approximation first and then use it to show the asymptotic theory for the uncertainty measure.

Proof for the empirical approximation. Let $g_h(x) = \nabla p_h(x)$ and $\widehat{g}_n(x) = \nabla \widehat{p}_h(x)$, and define N(x), $\widehat{N}_n(x)$ to be the normal space at $x \in R_h$ and $x \in \widehat{R}_h$, respectively. Note that when $\|\widehat{p}_h - p_h\|_{\infty,2}^*$ is sufficiently small, we have (P1) for \widehat{p}_h . This implies that N(x), $\widehat{N}_n(x)$ can be defined (but they are not necessarily unique) for points near R_h , \widehat{R}_h by claim 3 of Lemma 2. Condition (P3) ensures that the constants in (P1) and the reach of p_h have positive lower bound as $h \to 0$ for p_h .

By (P2) and Lemma 9, the ridges are the local modes in the subspace N(x). Note that despite the fact that N(x) may not be unique, the column space of N(x) is unique by claim 5 in Lemma 2. Hence we have

(47)
$$N(x)^T g_h(x) = 0, \qquad \widehat{N}_n(z)\widehat{g}_n(z) = 0$$

for all $x \in R_h$ and $z \in \widehat{R}_h$. This shows that ridges are generalized local modes with respect to their local normal coordinate.

Let $\tilde{x} = \pi_{\hat{R}_h}(x) \in \hat{R}_h$. When $\|\tilde{x} - x\|$ is smaller than the reach of \hat{R}_h , the projection \tilde{x} is unique. By claim 7 in Lemma 2 and the fact that $\text{Haus}(\hat{R}_h, R_h) = O(\|\hat{p}_h - p_h\|_{\infty,2}^*)$ from Theorem 12, the reach of \hat{R}_h and the reach of R_h will be close once $\|\hat{p}_h - p_h\|_{\infty,4}^*$ is sufficiently small. Accordingly, $\mathbf{d}(x, \hat{R}_h) = x - \tilde{x}$ is unique once $\|x - \tilde{x}\| \leq \text{Haus}(\hat{R}_h, R_h) = O(\|\hat{p}_h - p_h\|_{\infty,2}^*)$ is sufficiently small. This leads to

(48)

$$\widehat{g}_{n}(\widetilde{x}) - g_{h}(x) = \widehat{g}_{n}(\widetilde{x}) - g_{h}(\widetilde{x}) + g_{h}(\widetilde{x}) - g_{h}(x)$$

$$\leq O(\|\widehat{p}_{h} - p_{h}\|_{\infty,1}^{*} + \operatorname{Haus}(\widehat{R}_{h}, R_{h}))$$

$$\leq O(\|\widehat{p}_{h} - p_{h}\|_{\infty,2}^{*}) \quad \text{by Theorem 12.}$$

We use the fact that $g_h(x)$ has bounded derivatives from (K1). Accordingly, $\widehat{g}_n(\widetilde{x})$ converges to $g_h(x)$. Hence, when $\|\widehat{p}_h - p_h\|_{\infty,2}^*$ is sufficiently small, $N(x)^T \widehat{g}_n(\widetilde{x}) = 0$ by Lemma 9. Since $N(x)^T \widehat{g}_n(\widetilde{x}) = 0$,

(49)
$$N(x)^T \widehat{g}_n(\widetilde{x}) = 0 = N(x)^T [\widehat{g}_n(\widetilde{x}) - \widehat{g}_n(x) + \widehat{g}_n(x) - g_h(x)],$$

which leads to

(50)
$$N(x)^{T} [\widehat{g}_{n}(\widetilde{x}) - \widehat{g}_{n}(x)] = -N(x)^{T} [\widehat{g}_{n}(x) - g_{h}(x)]$$
$$= -N(x)^{T} [\widehat{g}_{n}(x) - \mathbb{E}(\widehat{g}_{n}(x))].$$

We used $g_h(x) = \mathbb{E}(\widehat{g}_n(x))$ in the last equality. Since $\|\widetilde{x} - x\|$ is small due to Theorem 12, and $\|\widehat{p}_h - p\|_{\infty}^*$ is small, we use Taylor's theorem for the first term which yields

(51)

$$N(x)^{T} [\widehat{g}_{n}(\widetilde{x}) - \widehat{g}_{n}(x)] = N(x)^{T} \int_{0}^{1} \widehat{H}_{n} (x + (\widetilde{x} - x)t) dt (\widetilde{x} - x)$$

$$= N(x)^{T} H(x) (1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty, 2}^{*}) + O(\|\widetilde{x} - x\|)) (\widetilde{x} - x)$$

$$= N(x)^{T} H(x) (\widetilde{x} - x) (1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty, 2}^{*})).$$

We use the fact that

$$\int_0^1 \widehat{H}_n(x + (\widetilde{x} - x)t) dt = H(x) (1 + O(\|\widehat{p}_h - p_h\|_{\infty,2}^*) + O(\|\widetilde{x} - x\|))$$

in the second equality and apply Theorem 12 to absorb $O(\|\tilde{x} - x\|)$ into the other term. By claims 5, 6 in Lemma 2 and the fact that the line segment joining \tilde{x} and x is contained in $R_h \oplus \delta_0$ by (P1), we have

(52)
$$\left\|\widehat{N}_{n}(\widetilde{x})\widehat{N}_{n}(\widetilde{x})^{T}-N(x)N(x)^{T}\right\|_{\max}=O\left(\left\|\widehat{p}_{h}-p_{h}\right\|_{\infty,3}^{*}\right).$$

Now $\tilde{x} - x = \hat{N}_n(\tilde{x})\hat{N}_n(\tilde{x})^T(\tilde{x} - x)$. Combining this with equations (50), (51) and (52) we obtain

(53)

$$-N(x)^{T} [\widehat{g}_{n}(x) - \mathbb{E}(\widehat{g}_{n}(x))] = N(x)^{T} [\widehat{g}_{n}(\widehat{x}) - \widehat{g}_{n}(x)] = N(x)^{T} H(x)(\widehat{x} - x)(1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty,2}^{*})) = N(x)^{T} H(x)\widehat{N}_{n}(\widehat{x})\widehat{N}_{n}(\widehat{x})^{T}(\widehat{x} - x)(1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty,2}^{*})) = N(x)^{T} H(x)N(x)N(x)^{T}(\widehat{x} - x)(1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty,3}^{*})) = H_{N}(x)N(x)^{T}(\widehat{x} - x)(1 + O(\|\widehat{p}_{h} - p_{h}\|_{\infty,3}^{*})),$$

where

(54)
$$H_N(x) = N(x)^T H(x)N(x).$$

In the fourth equality, we used (52). Multiplying the matrix $H_N(x)$ to the left of both sides and moving $O(\|\hat{p}_h - p_h\|_{\infty,3}^*)$ to the other side,

(55)
$$N(x)^{T}(\tilde{x}-x) = -H_{N}(x)^{-1}N(x)^{T}[\hat{g}_{n}(x) - \mathbb{E}(\hat{g}_{n}(x))](1 + O(\|\hat{p}_{h} - p_{h}\|_{\infty,3}^{*})).$$

We multiply by N(x) and use (52) again to obtain

(56)
$$N(x)N(x)^{T}(\tilde{x}-x) = \widehat{N}_{n}(\tilde{x})\widehat{N}_{n}(\tilde{x})^{T}(\tilde{x}-x)(1+O(\|\widehat{p}_{h}-p_{h}\|_{\infty,2}^{*})) = (\tilde{x}-x)(1+O(\|\widehat{p}_{h}-p_{h}\|_{\infty,3}^{*})).$$

Let $W_2(x) = N(x)H_N(x)^{-1}N(x)^T$, and define $\mathbf{d}(x, \widehat{R}_h) = \widetilde{x} - x$. Combining (55) and (56),

(57)
$$\mathbf{d}(x, \widehat{R}_h) = W_2(x) \big[\widehat{g}_n(x) - \mathbb{E} \big(\widehat{g}_n(x) \big) \big] \big(1 + O \big(\| \widehat{p}_h - p_h \|_{\infty, 3}^* \big) \big).$$

Notice that the KDE can be expressed in terms of the empirical process via

(58)
$$\widehat{g}_{n}(x) - \mathbb{E}(\widehat{g}_{n}(x))\left(\frac{x-X_{i}}{h}\right) - \mathbb{E}\left(\frac{1}{h^{d+2}}(\nabla K)\left(\frac{x-X_{i}}{h}\right)\right)$$
$$= \frac{1}{\sqrt{n}}\mathbb{G}_{n}(\tau_{x}),$$

where $y \mapsto \tau_x(y) = \frac{1}{h^{d+1}} (\nabla K)(\frac{x-y}{h})$. From equation (37),

(59)
$$f_x(y) = \sqrt{h^{d+2}} W_2(x) \tau_x(y)$$

for all $x \in R_h$. Hence, multiplying (57) by $\sqrt{nh^{d+2}}$ and using (58) and (59),

(60)
$$\sqrt{nh^{d+2}}\mathbf{d}(x,\widehat{R}_h) - \mathbb{G}_n(f_x) = O\big(\|\widehat{p}_h - p_h\|_{\infty,3}^*\big),$$

for each $x \in R_h$. Note that the bound $O(\|\hat{p}_h - p_h\|_{\infty,3}^*)$ is independent of x and the above construction is valid for all $x \in R_h$. Hence

$$\sup_{x\in R_h} \|\sqrt{nh^{d+2}}\mathbf{d}(x,\widehat{R}_h) - \mathbb{G}_n(f_x)\|_{\infty} = O\big(\|\widehat{p}_h - p_h\|_{\infty,3}^*\big).$$

This proves the approximation for $\mathbf{d}(x, \hat{R}_h)$.

Proof for the uncertainty measures. We first prove that the local uncertainty measure $nh^{d+2}\rho_n(x)$ converges to $\mathbb{E}(\|\mathbb{G}_n(f_x)\|^2)$. Then we show the limiting behavior for $\|\mathbb{G}_n(f_x)\|$. We have

(61)

$$|nh^{d+2}\rho_n(x) - \mathbb{E}(||\mathbb{G}_n(f_x)||^2)|$$

$$= |\mathbb{E}(nh^{d+2}d^2(x,\widehat{R}_h) - ||\mathbb{G}_n(f_x)||^2)|$$

$$(\text{Jensen's}) \leq \mathbb{E}|nh^{d+2}d^2(x,\widehat{R}_h) - ||\mathbb{G}_n(f_x)||^2|$$

$$= \mathbb{E}|nh^{d+2}||\mathbf{d}(x,\widehat{R}_h)||^2 - ||\mathbb{G}_n(f_x)||^2|$$

$$= \mathbb{E}|(D_n - G_n)^T(D_n + G_n)|$$

$$(\text{Cauchy-Schwarz}) \leq \sqrt{\mathbb{E}(||D_n - G_n||^2)\mathbb{E}(||D_n + G_n||^2)},$$

where $D_n = \sqrt{nh^{d+2}} \mathbf{d}(x, \widehat{R}_h) \in \mathbb{R}^d$ and $G_n = \mathbb{G}_n(f_x) \in \mathbb{R}^d$. Now by (60) and Lemma 11,

(62)
$$\mathbb{E}(\|D_n - G_n\|^2) = O\left(\frac{1}{nh^{d+6}}\right).$$

Note $D_n + G_n \le 2G_n + (D_n - G_n)$, which implies $||D_n + G_n||^2 \le (||2G_n|| + ||D_n - G_n||)^2$. Taking expectation on both sides and using the fact that $\sqrt{\mathbb{E}(A^2)}$ is \mathcal{L}^2 norm for the random variable A,

(63)
$$\mathbb{E}(\|D_n + G_n\|^2) \le \mathbb{E}((\|2G_n\| + \|D_n - G_n\|)^2) \le (\sqrt{\mathbb{E}(\|2G_n\|^2)} + \sqrt{\mathbb{E}(\|D_n - G_n\|^2)})^2.$$

Again by (60) and Lemma 11,

(64)
$$\mathbb{E}(\|D_n + G_n\|^2) = 2\mathbb{E}(\|G_n\|^2) + O\left(\sqrt{\frac{1}{nh^{d+6}}}\right).$$

Here we derive $\mathbb{E}(||G_n||^2)$. Recall that $G_n = \mathbb{G}_n(f_x)$, where

$$f_x(\cdot) = \frac{1}{\sqrt{h^{d+2}}} N(x) H_N^{-1}(x) N(x)^T (\nabla K) \left(\frac{x-\cdot}{h}\right)$$

for each $x \in R_h$ by (37). Note that $||G_n||^2 = G_n^T G_n$ and $\mathbb{E}(G_n) = 0$. Hence

(65)

$$\mathbb{E}(\|G_n\|^2) = \mathbb{E}(G_n^T G_n)$$

$$= \mathbb{E}((G_n - \mathbb{E}(G_n))^T (G_n - \mathbb{E}(G_n)))$$

$$= \operatorname{Trace}(\operatorname{Cov}(G_n))$$

$$= \operatorname{Trace}(\Sigma(x)),$$

where

$$\Sigma(x) = \operatorname{Cov}(G_n) = \operatorname{Cov}\left(N(x)H_N^{-1}(x)N(x)^T(\nabla K)\left(\frac{x-X_i}{h}\right)\right)$$

is bounded. Thus by (61)–(65) we conclude that

$$|nh^{d+2}\rho_n(x) - \mathbb{E}(\|\mathbb{G}_n(f_x)\|^2)|$$

$$\leq \sqrt{\mathbb{E}(\|D_n - G_n\|^2)\mathbb{E}(\|D_n + G_n\|^2)}$$

$$= O\left(\sqrt{\frac{1}{nh^{d+6}}}\right).$$

Thus the uncertainty measure $\rho_n(x)$ can be approximated by $\mathbb{E}(\|\mathbb{G}_n(f_x)\|^2) = \mathbb{E}(\|G_n\|^2)$. Now by (65), the result follows. \Box

Before we prove the bootstrap result, we need the following lemma.

LEMMA 13. Let p_h be the smoothed density and R_h be the associated ridges. Let \hat{p}_h be the KDE based on the observed data $\mathbb{X}_n = \{X_1, \ldots, X_n\}$ and \hat{R}_h be the estimated ridge. Consider these two conditions:

- (T1) (P1)–(P2) holds for \hat{p}_h .
- (T2) $\|\hat{p}_h p_h\|_{\infty,4}^* < s_0$ for a small constant s_0 .

Let $\mathcal{X}_n = \{\mathbb{X}_n : (T1), (T2) \text{ holds}\}$. Then, when n is sufficiently large,

$$\mathbb{P}(\mathcal{X}_n) \ge 1 - 5e^{-nh^{d+8}D_1},$$

for some constant D_1 .

The proof can be found in the supplementary material [Chen, Genovese and Wasserman (2015)].

1918

PROOF OF THEOREM 5. To prove the bootstrap result, we use a technique of Romano (1988a) by first considering a sequence of nonrandom distributions $\{Q_m : m = 1, ...\}$. In the last step, we replace Q_m by the empirical distribution \mathbb{P}_n . Let q_m be the density of the smoothed distribution $Q_m \star K_h$ where $K_h(x) = \frac{1}{h^d} K(\frac{x}{h})$ is the kernel function used in the KDE and \star is the convolution operator. If we replace Q_m with the sample distribution \mathbb{P} , the smoothed distribution has density p_h . If we replace Q_m with the empirical distribution $\widehat{\mathbb{P}}_n$, we obtain the KDE \widehat{p}_h .

We assume that each smoothed density q_m satisfies conditions (P1)–(P2) and $||q_m - p_h||_{\infty,4}^* \to 0$, and $||q_m - p_h||_{\infty,4}^*$ is sufficiently small for all m. Let $R(q_m) = \text{Ridge}(q_n)$. Let $\mathbb{Y}_{m,n} = \{Y_{m,1}, \ldots, Y_{m,n}\}$ where $Y_{m,1}, \ldots, Y_{m,n} \sim Q_m$. Let $\hat{q}_{m,n}$ be the KDE based on $\mathbb{Y}_{m,n}$, and let $\hat{R}_h(q_m) = \text{Ridge}(\hat{q}_{m,n})$.

Let $\rho_{m,n}^2(x)$ for $x \in R(q_m)$ be the local uncertainty measure. When $||q_m - p_h||_{\infty,3}^*$ is sufficiently small, we can apply Theorem 3 to $R(q_m)$ so that

$$\rho_{m,n}^2(x) = \frac{1}{nh^{d+2}} \operatorname{Trace} \Sigma(x; q_m) + o\left(\frac{1}{nh^{d+2}}\right),$$

where

$$\Sigma(x; q_m) = \operatorname{Cov} \left[N_{q_m}(x) H_N(x; q_m)^{-1} N_{q_m}(x)^T \nabla K(x - Y_{m,i}) \right]$$

for $x \in R(q_m)$. Note that although we do not assume (P3) for q_m , Theorem 3 is still valid once the gap constants in (P1) have positive lower bound. In this case, because $\|\hat{p}_h - p_h\|_{\infty,3}^*$ is sufficiently small and we assume (P3) for p_h , the gap constants have a lower bound for q_m as q_m approaching p_h .

Now we proceed with the proof. Claims 1 and 2 are trivially true by the definition of Hausdorff distance. Now we prove claim 3. When $||q_m - p_h||_{\infty,3}^*$ is sufficiently small,

Haus
$$(R(q_m), R_h) = O(||q_m - p_h||_{\infty,2}^*).$$

For any point $x \in R_h$, and any $y \in R_h \cap B(x, \text{Haus}(R(q_m), R_h))$,

$$\|y-x\| \leq \operatorname{Haus}(R(q_m), R_h).$$

Since y is on $R(q_m)$, the local uncertainty $\rho_{m,n}^2(y)$ is well defined. Then

$$\|\rho_{m,n}^{2}(y) - \rho_{n}^{2}(x)\| = \frac{1}{nh^{d+2}} \operatorname{Trace}(\Sigma(y; q_{m}) - \Sigma(x)) + o\left(\frac{1}{nh^{d+2}}\right)$$
$$\leq \frac{d}{nh^{d+2}} \|\Sigma(y; q_{m}) - \Sigma(x)\|_{\max} + o\left(\frac{1}{nh^{d+2}}\right).$$

Since the terms in $\Sigma(x)$ involve only the derivatives of the smoothed density up to the third order and since $||y - x|| \le \text{Haus}(R(q_m), R_h)$, we conclude that

$$\begin{split} \|\Sigma(y;q_m) - \Sigma(x)\|_{\max} &= O(\mathsf{Haus}(R(q_m),R_h) + \|q_m - p_h\|_{\infty,3}^*) \\ &= O(\|q_m - p_h\|_{\infty,3}^*). \end{split}$$

The $O(||q_m - p_h||_{\infty,3}^*)$ term does not depend on x so that this can be taken uniformly for all $x \in R_h$. This proves claim 3.

For the bootstrap case, we replace Q_m by $\widehat{\mathbb{P}}_n$. Thus q_m is replaced by \widehat{p}_h so that we obtain the result. Notice that we require that \hat{p}_h satisfies (P1)–(P2) and that $\|\widehat{p}_h - p_h\|_{\infty,4}^*$ be sufficient small. Recall that \mathcal{X}_n is the collection of \mathbb{X}_n such that \hat{p}_h satisfies conditions (P1)–(P2) and $\|\hat{p}_h - p_h\|_{\infty,4}^*$ is sufficiently small. Applying Lemma 13 we conclude that

$$\mathbb{P}(\mathcal{X}_n) \ge 1 - 5e^{-nh^{d+8}D}$$

for some constant D_1 . \Box

Before we prove the Gaussian approximation, we need the following lemma that links the quasi-Hausdorff distance to the Hausdorff distance.

LEMMA 14. Let R_1 , R_2 be two closed, nonself-intersecting curves with positive reach. If

Haus
$$(R_1, R_2) < (2 - \sqrt{2}) \min\{ \operatorname{reach}(R_1), \operatorname{reach}(R_2) \},\$$

then

(66)
$$\operatorname{dist}_{\Pi}(R_2, R_1) = \operatorname{dist}_{\Pi}(R_1, R_2) = \operatorname{Haus}(R_1, R_2).$$

The proof can be found in the supplementary material [Chen, Genovese and Wasserman (2015)].

PROOF OF THEOREM 6. Our proof consists of three steps. The first step establishes a coupling between the Hausdorff distance $Haus(\widehat{R}_h, R_h)$ and the supremum of an empirical process. The second step shows that the distribution of the maxima of the empirical process can be approximated by the maxima of a Gaussian process. The last step uses anti-concentration to bound the distributions between Haus(\widehat{R}_h, R_h) and the maxima of a Gaussian process.

Step 1—Empirical process approximation.

Recall that \mathbb{G}_n is the empirical process defined by

(67)
$$\mathbb{G}_n(f_k) = \frac{1}{\sqrt{n}} \Big(f_k(X_i) - \mathbb{E} \big(f_k(X_i) \big) \Big),$$
$$\mathbb{E} \Big(f_k(X_i) - \mathbb{E} \big(f_k(X_i) \big) \Big) = \mathbb{E} \Big(f_k(X_i) f_k(X_i) \Big)$$

$$\operatorname{Cov}(\mathbb{G}_n(f_1),\mathbb{G}_n(f_2)) = \mathbb{E}(f_1(X_1)f_2(X_1))$$

for any two functions f_1 , f_2 . We also recall the function $f_x(y)$ in (37),

(68)
$$y \mapsto f_x(y) = \frac{1}{\sqrt{h^{d+2}}} N(x) H_N^{-1}(x) N(x)^T (\nabla K) \left(\frac{x-y}{h}\right), \qquad x \in R_h.$$

Note that $f_x(y) \in \mathbb{R}^d$ is a vector. Let

(69)
$$\mathcal{F}_h = \{ \mathbf{w}^T f_x(y) : \mathbf{w} \in \mathbb{R}^d, \|\mathbf{w}\| = 1, f_x(y) \text{ defined in (68)}, x \in R_h \}.$$

1920

By Theorem 3,

$$\sup_{x\in R_h} \left\|\sqrt{nh^{d+2}}\mathbf{d}(x,\widehat{R}_h) - \mathbb{G}_n(f_x)\right\|_{\infty} = O\left(\|\widehat{p}_h - p_h\|_{\infty,3}^*\right).$$

Since the \mathcal{L}^2 norm is bounded by *d* times the infinity norm for a vector,

$$\sup_{x \in R_h} |\sqrt{nh^{d+2}} d(x, \widehat{R}_h) - \|\mathbb{G}_n(f_x)\|| = \sup_{x \in R_h} |\sqrt{nh^{d+2}} \|\mathbf{d}(x, \widehat{R}_h)\| - \|\mathbb{G}_n(f_x)\||$$
$$= O(\|\widehat{p}_h - p_h\|_{\infty,3}^*).$$

For any vector $v \in \mathbb{R}^d$, $||v|| = \sup_{||\mathbf{w}||=1} \mathbf{w}^T v$ where $\mathbf{w} \in \mathbb{R}^d$. Hence

$$\left|\sup_{x\in R_h}\sqrt{nh^{d+2}}d(x,\widehat{R}_h)-\sup_{x\in R_h,\|\mathbf{w}\|=1}\mathbf{w}^T\mathbb{G}_n(f_x)\right|=O(\|\widehat{p}_h-p_h\|_{\infty,3}^*).$$

Define $\|\mathbb{G}_n\|_{\mathcal{F}} = \sup_{f \in \mathcal{F}} \|\mathbb{G}_n(f)\|$. Recall that the asymptotic Hausdorff distance is dist $_{\Pi}(A, B) = \sup_{x \in B} d(x, A)$. Then

(70)
$$\left|\sqrt{nh^{d+2}}\operatorname{dist}_{\Pi}(\widehat{R}_{h},R_{h})-\|\mathbb{G}_{n}\|_{\mathcal{F}_{h}}\right|=O(\|\widehat{p}_{h}-p_{h}\|_{\infty,3}^{*}).$$

This shows that the quasi-Hausdorff distance can be approximated by the supremum of an empirical process over the functional space \mathcal{F}_h .

When $\|\widehat{p}_h - p_h\|_{\infty,4}^*$ is sufficiently small, the reach of \widehat{R}_h is close to the reach of R_h by claim 7 of Lemma 2, and the Hausdorff distance is much smaller than the reach. By Lemma 14, the quasi-Hausdorff distance is the same as the Hausdorff distance so that

(71)
$$\left|\sqrt{nh^{d+2}}\operatorname{Haus}(\widehat{R}_h, R_h) - \|\mathbb{G}_n\|_{\mathcal{F}_h}\right| = O\left(\|\widehat{p}_h - p_h\|_{\infty,3}^*\right).$$

Equation (71) is the coupling between Hausdorff distance and the supremum of an empirical process and is the main result for step 1. Note that a sufficient condition for $\|\hat{p}_h - p_h\|_{\infty,4}^*$ being small is that $\frac{nh^{d+8}}{\log n} \to \infty$. This is the bandwidth condition we require.

Step 2—Gaussian approximation.

In this step, we use a theorem of Chernozhukov, Chetverikov and Kato (2014a) to show that the supremum of the empirical process can be approximated by the supremum of a centered, tight Gaussian process \mathbb{B} defined on \mathcal{F}_h with covariance function

(72)
$$\operatorname{Cov}(\mathbb{B}(f_1), \mathbb{B}(f_2)) = \mathbb{E}[f_1(X_i)f_2(X_i)] - \mathbb{E}[f_1(X_i)]\mathbb{E}[f_2(X_i)]$$

for $f_1, f_2 \in \mathcal{F}_h$. We first recall the theorem of Chernozhukov, Chetverikov and Kato (2014a).

THEOREM 15 [Theorem 3.1 in Chernozhukov, Chetverikov and Kato (2014a)]. Let G be a collection of functions that is a VC-type class [see condition (K2)] with a constant envelope function b. Let σ^2 be a constant such that $\sup_{g \in \mathcal{G}} \mathbb{E}[g(X_i)^2] \le \sigma^2 \le b^2$. Let \mathbb{B} be a centered, tight Gaussian process defined on \mathcal{G} with covariance function

(73)
$$\operatorname{Cov}(\mathbb{B}(g_1), \mathbb{B}(g_2)) = \mathbb{E}[g_1(X_i)g_2(X_i)] - \mathbb{E}[g_1(X_i)]\mathbb{E}[g_2(X_i)],$$

where $g_1, g_2 \in \mathcal{G}$. Then for any $\gamma \in (0, 1)$ as *n* is sufficiently large, there exists a random variable $\mathbf{B} \stackrel{d}{=} \|\mathbb{B}\|_{\mathcal{G}}$ such that

(74)
$$\mathbb{P}\left(\left|\|\mathbb{G}_{n}\|_{\mathcal{G}}-\mathbf{B}\right|>A_{1}\frac{b^{1/3}\sigma^{2/3}\log^{2/3}n}{\gamma^{1/3}n^{1/6}}\right)\leq A_{2}\gamma,$$

where A_1 , A_2 are two universal constants.

Now we show that \mathcal{G} in Theorem 15 can be linked to \mathcal{F}_h with a proper scaling. From condition (K2), the collection

$$\left\{t \to \left(\frac{\partial}{\partial x_i} K\right) \left(\frac{x-t}{h}\right) : x \in \mathbb{R}^d, i = 1, \dots, d\right\}$$

is a VC-type pre-Gaussian class with a constant envelope b_0 . Recall equation (68):

$$f_x(y) = \frac{1}{\sqrt{h^{d+2}}} N(x) H_N^{-1}(x) N(x)^T (\nabla K) \left(\frac{x-y}{h}\right), \qquad x \in R_h.$$

This function will not be uniformly bounded as $h \rightarrow 0$, so we consider

(75)
$$g_x(y) = \sqrt{h^{d+2}} f_x(y)$$
$$= N(x) H_N^{-1}(x) N(x)^T (\nabla K) \left(\frac{x-y}{h}\right), \qquad x \in R_h$$

Note that each element of the vector $g_x(y)$ is uniformly bounded. This is because $N(x)H_N^{-1}(x)N(x)^T \le c_1 < \infty$ for some universal constant since N(x) is generated by the derivatives of p_h with order less than four and by (K1) is uniformly bounded.

Now we define

(76)
$$\mathcal{G}_{h} = \{ \mathbf{w}^{T} g_{x}(y) : \mathbf{w} \in \mathbb{R}^{d}, \|\mathbf{w}\| = 1, x \in R_{h} \}$$
$$= \{ \sqrt{h^{d+2}} f : f \in \mathcal{F}_{h} \}.$$

Since $\|\mathbf{w}\| = 1$ and $N(x)H_N^{-1}(x)N(x)^T \le c_1$ and b_0 is a constant envelope for the partial derivatives of kernel functions, $b_1 = c_1b_0$ is a constant envelope for \mathcal{G}_h and \mathcal{G}_h is a VC-type class. In addition,

(77)
$$\sup_{g \in \mathcal{G}_h} \mathbb{E}[g^2(X_i)] \le h^{d+2} b_1^2 \le b_1^2$$

as h < 1. So we can choose $\sigma^2 = h^{d+2}b_1^2$ in Theorem 15. Applying Theorem 15 and (76), there exist random variables

(78)
$$\mathbf{B}_{1} \stackrel{d}{=} \|\mathbb{B}\|_{\mathcal{G}_{h}},$$
$$\mathbf{B}_{2} \stackrel{d}{=} \|\mathbb{B}\|_{\mathcal{F}_{h}}$$

such that

(79)

$$\mathbb{P}\left(\left|\|\mathbb{G}_{n}\|_{\mathcal{G}_{h}}-\mathbf{B}_{1}\right| > A_{1}\frac{b_{1}h^{(d+2)/3}\log^{2/3}n}{\gamma^{1/3}n^{1/6}}\right) \le A_{2}\gamma,$$

$$\mathbb{P}\left(\left|\|\mathbb{G}_{n}\|_{\mathcal{F}_{h}}-\mathbf{B}_{2}\right| > A_{1}\frac{b_{1}\log^{2/3}n}{\gamma^{1/3}(nh^{d+2})^{1/6}}\right) \le A_{2}\gamma$$

for two universal constants, when *n* is sufficiently large and $\gamma \in (0, 1)$. The second result comes from the one-to-one correspondence between \mathcal{G}_h and \mathcal{F}_h with a constant scaling.

Now recall (71) from the end of step 1:

$$\left|\sqrt{nh^{d+2}}\operatorname{Haus}(\widehat{R}_h,R_h)-\|\mathbb{G}_n\|_{\mathcal{F}_h}\right| \leq O\big(\|\widehat{p}_h-p_h\|_{\infty,3}^*\big),$$

which implies that there exists a constant $C_0 > 0$ such that for any $a_0 > 0$,

(80)

$$\mathbb{P}(|\sqrt{nh^{d+2}}\operatorname{Haus}(\widehat{R}_h, R_h) - ||\mathbb{G}_n||_{\mathcal{F}_h}| > a_0)$$

$$\leq \mathbb{P}(||\widehat{p}_h - p_h||_{\infty,3}^* > C_0 \cdot a_0)$$

$$\leq 4e^{-nh^{d+6}C_1a_0}$$

for some constant C_1 as *n* is sufficiently large. Note that we apply Talagrand's inequality (see Lemma 13) in the last inequality.

Choose $a_0 = \frac{1}{\sqrt{nh^{d+6}}}$ in (80), combine it with (79) and use the fact that $\frac{1}{\sqrt{nh^{d+6}}}$ converges much faster than $\frac{1}{(nh^{d+2})^{1/6}}$, to conclude that

(81)
$$\mathbb{P}\left(\left|\sqrt{nh^{d+2}}\mathsf{Haus}(\widehat{R}_h, R_h) - \mathbf{B}_2\right| > A_3 \frac{\log^{2/3} n}{\gamma^{1/3} (nh^{d+2})^{1/6}}\right) \le A_4 \gamma$$

for some constants A_2 , A_4 . We can replace A_1 by A_3 and A_2 by A_4 to absorb the extra small terms from (80) and the envelope b_1 .

Step 3—Anti-concentration bound.

To convert the above result into a Berry–Esseen type bound, we use the anticoncentration inequality in (Corollary 2.1) in Chernozhukov, Chetverikov and Kato (2014a); a similar result appears in Chernozhukov, Chetverikov and Kato (2013, 2014b). Here we use a modification of the anti-concentration inequality. LEMMA 16 [Modification of Corollary 2.1 in Chernozhukov, Chetverikov and Kato (2014a)]. Let X_t be a Gaussian process with index $t \in T$, and with semimetric d_T such that $\mathbb{E}(X_t) = 0$, $\mathbb{E}(X_t^2) = 1$ for all $t \in T$. Assume that $\sup_{t \in T} X_t < \infty$ a.s. and there exists a random variable Y such that $\mathbb{P}(|Y - \sup_{t \in T} |X_t|| > \eta) < \delta(\eta)$. If $A(|X|) = \mathbb{E}(\sup_{t \in T} |X_t|) < \infty$, then

$$\sup_{t} \left| \mathbb{P}(Y < t) - \mathbb{P}\left(\sup_{t \in T} |X_t| < t \right) \right| \le A_5(\eta + \delta(\eta)) A(|X|)$$

for some constant A₅.

This lemma is a direct application of Corollary 2.1 of Chernozhukov, Chetverikov and Kato (2014a), so we omit the proof. We apply Lemma 16 to equation (81) which yields

(82)
$$\sup_{t} \left| \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(R_{h}, \widehat{R}_{h}) < t) - \mathbb{P}(\|\mathbb{B}\|_{\mathcal{F}_{h}} < t) \right| = A_{6} \left(A_{3} \frac{\log^{2/3} n}{\gamma^{1/3} (nh^{d+2})^{1/6}} + A_{4} \gamma \right),$$

where $A_6 = A_5 \times A(\|\mathbb{B}\|_{\mathcal{F}_h}) < \infty$ is a constant. We use the fact that \mathbf{B}_2 and $\|\mathbb{B}\|_{\mathcal{F}_h}$ have the same distribution. Choosing $\gamma = O((\frac{\log^4 n}{nh^{d+2}})^{1/8})$ completes the proof.

For the case of dist_{Π}(\hat{R}_h , R_h), the result follows by using (70) rather than (71) in the empirical approximation. \Box

PROOF OF THEOREM 7. The proof for the bootstrap result is very similar to the previous theorem. The major difference is that the estimated ridges and the smoothed ridges have different supports. This makes the functional spaces different. Our strategy for proving this theorem has three steps. First, we show that the Hausdorff distance Haus (\hat{R}_h^*, \hat{R}_h) conditioned on the observed data can be approximated by an empirical process. This is the same as step 1 in proof of Theorem 6. Second, we apply the result of Theorem 6 to bound the difference between the distributions of Haus (\hat{R}_h^*, \hat{R}_h) and a Gaussian process defined on the \hat{R}_h . This uses the second and the third steps of the previous proof. The last step shows that the Gaussian process defined on \hat{R}_h is asymptotically the same as being defined on R_h . Let $X_n \in X_n$, and recall that by Lemma 13, $\mathbb{P}(X_n) > 1 - 5e^{-nh^{d+8}D_1}$.

Step 1—Empirical approximation.

Let $\mathbb{X}_n = \{X_1, \dots, X_n\}$ be the observed data. Let $\mathbb{G}_n^*(\mathbb{X}_n) = \sqrt{n}(\mathbb{P}_n^* - \mathbb{P}_n)$. Let \hat{p}_h^* be the bootstrap KDE (KDE based on the bootstrap sample).

In the following, we assume that $X_n \in \mathcal{X}_n$ and treat X_n as fixed. Hence, \hat{p}_h and \hat{R}_h are fixed. In this case, Theorem 3 can be applied to the local uncertainty vector, that is,

(83)
$$\|\mathbf{d}(x,\widehat{R}_h^*) - \mathbb{G}_n^*(\mathbb{X}_n)(\widehat{f}_{n,x})\| = \|\widehat{p}_h^* - \widehat{p}_h\|_{\infty,3}^*, \qquad x \in \widehat{R}_h,$$

where

(84)
$$y \mapsto \widehat{f}_{n,x}(y) = \frac{1}{\sqrt{h^{d+2}}} \widehat{N}_n(x) \widehat{H}_{N,n}(x)^{-1} \widehat{N}_n(x)^T (\nabla K) \left(\frac{x-y}{h}\right) \in \mathbb{R}^d.$$

Note that $\widehat{N}_n(x)$ is the matrix with column space equal to the normal space of \widehat{R}_h at x, and $\widehat{H}_{N,n}(x)$ is the corresponding subspace Hessian matrix of the space spanned by columns of $\widehat{N}_n(x)$. Define

(85)
$$\widehat{\mathcal{F}}_{h}(\mathbb{X}_{n}) = \{ \mathbf{w}^{T} \, \widehat{f}_{n,x} : \mathbf{w} \in \mathbb{R}^{d}, \, \|\mathbf{w}\| = 1, \, x \in \widehat{R}_{h} \}$$

Then by the same argument as in the paragraph before the proof of Theorem 6, we have a similar result to (71),

(86)
$$|\operatorname{Haus}(\widehat{R}_h^*, \widehat{R}_h) - ||\mathbb{G}_n^*(\mathbb{X}_n)||_{\widehat{\mathcal{F}}_h(\mathbb{X}_n)}| = O(||\widehat{p}_h^* - \widehat{p}_h||_{\infty,3}^*).$$

Step 2—*Gaussian approximation.*

We use the same proof as in Theorem 6. We apply Theorem 6 to conclude that

(87)
$$\sup_{t} \left| \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_{h}^{*}, \widehat{R}_{h}) < t | \mathbb{X}_{n}) - \mathbb{P}(\|\mathbb{B}\|_{\widehat{\mathcal{F}}_{h}(\mathbb{X}_{n})} < t | \mathbb{X}_{n}) \right|$$
$$= O\left(\left(\frac{\log^{4} n}{nh^{d+2}}\right)^{1/8}\right).$$

Step 3—Support approximation.

In the previous step, the approximating distribution is a Gaussian process over the function space $\widehat{\mathcal{F}}_h(\mathbb{X}_n)$, which is not the same as \mathcal{F}_h . Now we apply Lemma 17 and the fact that $\|\widehat{p}_h - p\|_{\infty,2}^*/h = O(\|\widehat{p}_h - p\|_{\infty,3}^*)$ to get

(88)
$$\sup_{t} |\mathbb{P}(||\mathbb{B}||_{\widehat{\mathcal{F}}_{h}(\mathbb{X}_{n})} < t|\mathbb{X}_{n}) - \mathbb{P}(||\mathbb{B}||_{\mathcal{F}_{h}} < t)| = O((||\widehat{p}_{h} - p||_{\infty,3}^{*})^{1/3}).$$

Combining (87), (88) and the fact that $\|\widehat{p}_h - p\|_{\infty,3}^* = O(\frac{\log n}{nh^{d+6}})$, we conclude

$$\sup_{t} \left| \mathbb{P}(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_{h}^{*}, \widehat{R}_{h}) < t | \mathbb{X}_{n}) - \mathbb{P}(\|\mathbb{B}\|_{\mathcal{F}_{h}} < t) \right|$$
$$= O\left(\frac{\log n}{(nh^{d+2})^{1/8}}\right) + O\left(\left(\frac{\log n}{nh^{d+6}}\right)^{1/6}\right).$$

Consider two densities p_1 , p_2 satisfying conditions (A1), (P1)–(P2). Let R_1 , R_2 be the density ridges for p_1 , p_2 , respectively. We assume conditions (K1)–(K2). Define

(89)
$$\mathcal{F}_k = \{ \mathbf{w}^T f_{x,k} : \mathbf{w} \in \mathbb{R}^d, \|\mathbf{w}\| = 1, x \in R_k \}, \qquad k = 1, 2,$$

where

(90)
$$f_{x,k} = \frac{1}{\sqrt{h^{d+2}}} N_k(x) H_{N,k}(x)^{-1} N_k(x)^T (\nabla K) \left(\frac{x-y}{h}\right) \in \mathbb{R}^d.$$

Note that we have two indices x, \mathbf{w} for each element in \mathcal{F}_1 and \mathcal{F}_2 . The first index x is the *location*, and the second index \mathbf{w} is the *direction*. $N_k(x)$ is the normal matrix (as $x \in R_k$, its column space is the normal space) defined by Lemma 2 at x, and $H_{N,k}(x)$ is the subspace Hessian in the columns space of $N_k(x)$.

LEMMA 17 (Gaussian comparison on two ridges). When $||p_1 - p_2||_{\infty,3}^*$ is sufficiently small, we have

$$\sup_{t} \left| \mathbb{P}(\|\mathbb{B}\|_{\mathcal{F}_{1}} < t) - \mathbb{P}(\|\mathbb{B}\|_{\mathcal{F}_{2}} < t) \right| = O((\|p_{1} - p_{2}\|_{\infty,3}^{*} + \operatorname{Haus}(R_{1}, R_{2})/h)^{1/3}).$$

The proof can be found in the supplementary material [Chen, Genovese and Wasserman (2015)].

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SUPPLEMENTARY MATERIAL

Supplementary proofs: Asymptotic theory for density ridges (DOI: 10. 1214/15-AOS1329SUPP; .pdf). The supplementary material contains proofs of Lemmas 1, 2, 4, 9, 13, 14, 17.

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