Multivariate goodness-of-fit on flat and curved spaces via nearest neighbor distances

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Abstract

We present a unified approach to goodness-of-fit testing in \mathbb{R}^d and on lowerdimensional manifolds embedded in \mathbb{R}^d based on sums of powers of weighted volumes of k-th nearest neighbor spheres. We prove asymptotic normality of a class of test statistics under the null hypothesis and under fixed alternatives. Under such alternatives, scaled versions of the test statistics converge to the α -entropy between probability distributions. A simulation study shows that the procedures are serious competitors to established goodness-of-fit tests.

1 Introduction and summary

Nearest neighbor methods have been successfully applied in a variety of fields, such as classification (see [10]), density and regression function estimation (see [5], [8]), and multivariate two-sample testing (see, e.g., [12], [21], and [26]). Moreover, nearest neighbor

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methods have also been employed in the context of testing the goodness-of-fit of given data with a distributional model (see [6], [11] and [15]).

This paper is devoted to a class of universally consistent goodness-of-fit tests based on nearest neighbors. These tests can be applied not only to test for uniformity on a compact domain in \mathbb{R}^d , but also to test for a specified density on a *m*-dimensional manifold embedded in \mathbb{R}^d , where $m \leq d$. Here, prominent special cases involve testing for uniformity on a circle or on a sphere.

To be specific, let \mathcal{M} denote a C^1 *m*-dimensional manifold embedded in \mathbb{R}^d , where $m \leq d$. \mathcal{M} is endowed with the subset topology and is a closed subset of \mathbb{R}^d . Let dx be the Riemannian volume element on \mathcal{M} . A probability density function on \mathcal{M} is a measurable non-negative real-valued function f on \mathcal{M} satisfying $\int_{\mathcal{M}} f(x) dx = 1$. The support $\mathcal{K}(f)$ of f is the smallest closed set $K \subset \mathcal{M}$ such that $\int_K f(x) dx = 1$.

Let $\mathcal{P}(\mathcal{M})$ denote the class of bounded probability density functions f on \mathcal{M} , and write $\mathcal{P}_b(\mathcal{M}) \subset \mathcal{P}(\mathcal{M})$ for the subset of probability density functions f such that $\mathcal{K}(f)$ is compact and either (i) $\mathcal{K}(f)$ has no boundary or (ii) $\mathcal{K}(f)$ is a C^1 submanifold-withboundary of \mathcal{M} ; we refer to Section 2 of [23] for details. Notice that $\mathcal{K}(f)$ could be an *m*-sphere (or any ellipsoid) embedded in \mathbb{R}^d . Let $\mathcal{P}_c(\mathcal{M})$ denote those probability density functions $f \in \mathcal{P}_b(\mathcal{M})$ which are bounded away from zero on their support.

In what follows we let X_i , $i \ge 1$, be independent and identically distributed (i.i.d.) random variables with density f, defined on a common probability space $(\Omega, \mathcal{A}, \mathbb{P})$, and we put $\mathcal{X}_n := \{X_1, ..., X_n\}$.

Given a locally finite subset \mathcal{X} of \mathcal{M} and $x \in \mathcal{X}$, we write $x^{(k)}$ for the kth nearest neighbor (with respect to the Euclidean norm $|\cdot|$) of x among $\mathcal{X} \setminus \{x\}$. Let $v_m := \pi^{m/2}/\Gamma(m/2+1)$ be the volume of the unit m-sphere.

Given a fixed $\alpha \in (0, \infty)$ and a fixed positive integer J, consider the volume score function induced by the J nearest neighbor distances:

$$\xi_J^{(\alpha)}(x,\mathcal{X}) := \sum_{k=1}^J (v_m | x - x^{(k)} |^m)^{\alpha}, \qquad (1.1)$$

i.e., sums of volumes (to power α) of the k nearest neighbor balls around $x, k \in \{1, ..., J\}$. When \mathcal{X} consists of $\Theta(n)$ elements in a compact subset of \mathcal{M} , where $an \leq \Theta(n) \leq bn$, $n \ge 1$, for some $0 < a < b < \infty$, we study the re-scaled volume scores

$$\xi_{n,J}^{(\alpha)}(x,\mathcal{X}) := \sum_{k=1}^{J} (v_m | n^{1/m} (x - x^{(k)}) |^m)^{\alpha}.$$

Recalling that $\mathcal{X}_n := \{X_1, ..., X_n\}$, we consider the random measure

$$\mu_{n,J}^{(\alpha)} := \sum_{X_i \in \mathcal{X}_n} \xi_{n,J}^{(\alpha)}(X_i, \mathcal{X}_n) \delta_{X_i}, \qquad (1.2)$$

with δ_x denoting the Dirac point mass at x. If h is an arbitrary measurable bounded function on \mathcal{M} , we write $\langle \mu_{n,J}^{(\alpha)}, h \rangle$ for $\int_{\mathcal{M}} h(x) \, \mathrm{d} \mu_{n,J}^{(\alpha)}(x)$.

Given a fixed $f_0 \in \mathcal{P}(\mathcal{M})$, this paper considers testing goodness-of-fit of the hypothesis

 H_0 : the unknown density of X_i is f_0 , (1.3)

against general alternatives, based on the statistic

$$T_{n,J}^{(\alpha)} := \langle \mu_{n,J}^{(\alpha)}, f_0^{\alpha} \rangle := \sum_{X_i \in \mathcal{X}_n} \xi_{n,J}^{(\alpha)}(X_i, \mathcal{X}_n) (f_0(X_i))^{\alpha}.$$
(1.4)

Notice that for the special case m = d and J = 1, this type of statistic has been studied in [6] and [15], but without allowing for lower-dimensional manifolds, and without considering fixed alternatives to H_0 .

In Section 2, we prove the asymptotic normality of $T_{n,J}^{(\alpha)}$ as n tends to infinity both under H_0 and under fixed alternatives to H_0 , and we show that $T_{n,J}^{(\alpha)}/n$ has an almost sure limit under a fixed alternative to H_0 . In the case $0 < \alpha < 1$, this limit is, apart from a multiplicative constant, the α -entropy between f and f_0 . As a consequence, the statistic $T_{n,J}^{(\alpha)}$ yields a universally goodness-of-fit test of H_0 for each $\alpha \in (0, \infty), \alpha \neq 1$, and each J. The versatility of this class of tests is demonstrated in Section 3, which presents the results of a simulation study comparing our tests with several well-known competitors. The paper concludes with some remarks and open problems.

2 Main results

The limit theory for the statistic (1.4) may be deduced from general theorems established in [23] and goes as follows. **Theorem 2.1** If $f \in \mathcal{P}_c(\mathcal{M})$, $\alpha \in (0, \infty)$, then as $n \to \infty$ we have

$$\frac{T_{n,J}^{(\alpha)}}{n} \to \sum_{k=1}^{J} \frac{\Gamma(\alpha+k)}{\Gamma(k)} \int_{\mathcal{M}} f_0(x)^{\alpha} f(x)^{1-\alpha} \,\mathrm{d}x$$
(2.1)

in L^2 and also \mathbb{P} -a.s.

Remarks. (i) Notice that the right-hand side of (2.1) is distribution-free if $\alpha = 1$. Thus, in view of the testing problem (1.3), it is indispensable to have $\alpha \neq 1$.

(ii) If dim $\mathcal{M} = d$, if the support $\mathcal{K}(f)$ of f is a convex polyhedron, and if f_0 is the uniform density over \mathcal{M} , then the asserted L^2 convergence in (2.1) is given by Theorem 2 of [29]. That paper, which is based on [22], shows that

$$\mathbb{E}\,\xi_{n,J}^{(\alpha)}(X_1,\mathcal{X}_n) \to \int_{\mathcal{K}(f)} \mathbb{E}\,\xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_{f(x)})\,f(x)\,\mathrm{d}x\tag{2.2}$$

holds in L^2 as $n \to \infty$. Here, **0** denotes a point at the origin of \mathbb{R}^m , and $\mathcal{H}_{\tau}, \tau \in (0, \infty)$, stands for a homogeneous Poisson process of intensity τ in \mathbb{R}^m , with \mathbb{R}^m embedded in \mathbb{R}^d so that the random variable $\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{\tau})$ is well-defined. As will be shown in the upcoming proof, the paper [23] upgrades (2.2) to give convergence of the measures at (1.2), it provides L^2 and a.s. convergence, and also allows $\mathcal{K}(f)$ to be replaced by a C^1 *m*-dimensional submanifold of \mathbb{R}^d .

(iii) The statistic $T_{n,J}^{(\alpha)}$ may be considered a multivariate analogue of the statistic $\sum_{i=1}^{n+1} U_i^{\alpha}$ introduced in [18] for testing the hypothesis of a uniform distribution in the unit interval [0, 1]. Here, $U_i = F(X_{(i)}) - F(X_{(i-1)})$, where $0 := X_{(0)} \leq X_{(1)} \leq \ldots \leq X_{(n)} \leq X_{(n+1)} := 1$ are the order statistics of i.i.d. random variables X_1, \ldots, X_n with common density function f. From the asymptotic distribution of $\sum_{i=1}^{n+1} U_i^{\alpha}$ (see, e.g., [31]), it follows that

$$\frac{1}{n}\sum_{i=1}^{n+1}(nU_i)^{\alpha} \to \Gamma(\alpha+1)\int_0^1 f(x)^{1-\alpha} \,\mathrm{d}x$$

in probability as $n \to \infty$. This result obviously corresponds to (2.1) for J = 1 and f_0 being the uniform density over \mathcal{M} , where m = d and \mathcal{M} has Lebesgue measure one.

(iv) If $\alpha \in (0, 1)$, the integral

$$r_{\alpha}(f_0, f) := \int_{\mathcal{M}} f_0(x)^{\alpha} f(x)^{1-\alpha} \, \mathrm{d}x$$

figuring on the right-hand side of (2.1) is known as the α -entropy between (the distributions associated with) f_0 and f, see [28]. Notice that $1 - r_{1/2}(f_0, f) = H^2(f_0, f)$, where $H(f_0, f)$ is the Hellinger distance of f_0 and f. By Hölder's inequality, $r_{\alpha}(f_0, f) \leq 1$, with equality if and only if the distributions pertaining to f_0 and f coincide. If $\alpha \in (1, \infty)$, put $W := f_0(X_1)/f(X_1)$, and recall that X_1 has density f. Then

$$r_{\alpha}(f_0, f) = \mathbb{E}\left[W^{\alpha}\right],$$

and, by Jensen's inequality, $r_{\alpha}(f_0, f) \geq (\mathbb{E}W)^{\alpha} = 1$. As above, equality holds if the distributions associated with f_0 and f are the same.

(v) It follows from (iii) and Theorem 2.1 that, for fixed $\alpha \in (0, 1)$, a test of fit that rejects the hypothesis H_0 figuring in (1.3) for *small* values of $T_{n,J}^{(\alpha)}$ is consistent against each fixed alternative density f. If $\alpha \in (1, \infty)$, rejection of H_0 is for *large* values of $T_{n,J}^{(\alpha)}$, and the resulting test is universally consistent.

Before stating variance asymptotics and a central limit theorem we introduce more notation from [23], especially (3.8) and (3.9) of that paper. Given $u \in \mathbb{R}^m$, abbreviate $H_{\tau} \cup \{u\}$ by H_{τ}^u . We consider an integrated 'covariance' of scores

$$V(\tau) := V^{\xi_J^{(\alpha)}}(\tau) := \mathbb{E} \,\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{\tau})^2 + \tau \int_{\mathbb{R}^m} \left\{ \mathbb{E} \,\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{\tau}^u) \xi_J^{(\alpha)}(u, \mathcal{H}_{\tau}^\mathbf{0}) - (\mathbb{E} \,\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{\tau}))^2 \right\} \,\mathrm{d}u$$

and an integrated 'add-one cost'

$$\delta(\tau) := \delta^{\xi_J^{(\alpha)}}(\tau) := \mathbb{E}\,\xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_\tau) + \tau \int_{\mathbb{R}^m} \mathbb{E}\left[\xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_\tau^u) - \xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_\tau)\right] \mathrm{d}u.$$

As shown in Theorem 3.2 of [23], these integrals are finite. Let $N(0, \sigma^2)$ denote a mean zero normal random variable with variance σ^2 .

Theorem 2.2 If $f \in \mathcal{P}_c(\mathcal{M})$ is a.e. continuous and $\alpha \in (0, \infty)$, then

$$\lim_{n \to \infty} n^{-1} \operatorname{Var}(T_{n,J}^{(\alpha)}) = \sigma^2(f_0, f)$$

$$:= \int_{\mathcal{M}} f_0(x)^{2\alpha} V(f(x)) f(x) \, \mathrm{d}x - \left(\int_{\mathcal{M}} \delta(f(x)) f_0(x)^{\alpha} f(x) \, \mathrm{d}x\right)^2 \in (0, \infty).$$

Moreover, as $n \to \infty$,

$$\frac{T_{n,J}^{(\alpha)} - \mathbb{E} T_{n,J}^{(\alpha)}}{\sqrt{n}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2(f_0, f)).$$

Remark. Theorem 2.1 of [1] provides variance asymptotics and a central limit theorem for sums of functions of kth nearest neighbor distances in the special case m = d.

Proof of Theorem 2.1. We deduce this from Theorem 3.1 of [23] with $\rho = \infty$, especially display (3.16) of [23], with the f in (3.16) of [23] set to f_0^{α} and with the κ in (3.16) of [23] set to f. Observe that $\xi_J^{(\alpha)}$ belongs to the class $\Sigma(k, r)$ of that paper, and notice that

$$\sup_{n} \mathbb{E} \left(\xi_{n,J}^{(\alpha)}(X_1, \mathcal{X}_n) \right)^p < \infty$$

holds for all $p \in [1, \infty)$, i.e., the moment condition (3.4) of [23] holds for all p.

The limit (3.16) of [23] tells us that as $n \to \infty$ we have convergence in L^2

$$\frac{T_{n,J}^{(\alpha)}}{n} \to \int_{\mathcal{M}} f_0(x)^{\alpha} \mathbb{E} \,\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{f(x)}) f(x) \,\mathrm{d}x,\tag{2.3}$$

where $\xi_J^{(\alpha)}(\mathbf{0}, \mathcal{H}_{f(x)})$ is defined at (1.1). The last assertion in Theorem 3.1 of [23] also gives a.s. convergence in (2.3).

Given $\tau \in (0, \infty)$ and \mathcal{H}_{τ} , we let $X_{\tau}^{(k)} \in \mathcal{H}_{\tau}$ be the *k*th nearest neighbor to the origin. We compute

$$\mathbb{E}\,\xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_{\tau}) = \sum_{k=1}^J \mathbb{E}\,(v_m | X_{\tau}^{(k)} |^m)^{\alpha}$$
$$= \sum_{k=1}^J v_m^{\alpha} (\tau^{-1/m})^{\alpha m} \mathbb{E}\,(|X_1^{(k)}|)^{\alpha m}$$
$$= \left(\frac{v_m}{\tau}\right)^{\alpha} \sum_{k=1}^J v_m^{-(\alpha m)/m} \frac{\Gamma(k+\alpha)}{\Gamma(k)}$$
$$= \tau^{-\alpha} \sum_{k=1}^J \frac{\Gamma(k+\alpha)}{\Gamma(k)},$$

where the penultimate equality follows by display (15) of [29] (with α replaced by αm , d replaced by m). We have thus shown

$$\mathbb{E}\,\xi_J^{(\alpha)}(\mathbf{0},\mathcal{H}_\tau) = \tau^{-\alpha} \sum_{k=1}^J \frac{\Gamma(k+\alpha)}{\Gamma(k)}.$$
(2.4)

Letting τ equal f(x) in (2.3) and applying (2.4) gives the claimed limit (2.1).

Proof of Theorem 2.2. This is an immediate consequence of Theorem 3.2 of [23] as well as remark (iv) on p. 2174 of [23]. In that remark we may set the function f there to f_0^{α} , we set $\rho = \infty$, and we put $\mu_{n,k,\rho}^{\xi}$ equal to $\mu_{n,J}^{(\alpha)}$. Keeping ρ set to infinity, it is a straightforward matter to show that $\mu_{n,J}^{(\alpha)}$ satisfies the moment conditions (3.5) and (3.6) of [23]. Since $\mu_{n,J}^{(\alpha)}$ satisfies all the conditions of remark (iv) on p. 2174 of [23], Theorem 2.2 follows as desired.

3 Simulations

By means of a simulation study, this section compares the finite-sample power performance of the test based on $T_{n,J}^{(\alpha)}$ with that of several competitors. All simulations are performed using the statistical computing environment R, see [25]. We consider testing for uniformity on the unit square $[0, 1]^2$, on the unit circle $S^1 = \{x \in \mathbb{R}^2 : |x| = 1\}$, and on the unit sphere $S^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$. Since, strictly speaking, there is not only one new test, but a whole family of tests that depend on the choice of the power α and the number J of neighbors taken into account, the impact on finite-sample power of α and J will be of particular interest. In each scenario, we consider the sample sizes n = 50, n = 100 and n = 200, and the nominal level of significance is set to 0.05. Throughout, critical values for $T_{n,J}^{(\alpha)}$ under H_0 (see Tables 7 – 9) have been simulated with 100 000 replications, and each entry in a table referring to the power of the test is based on 10 000 replications.

3.1 Unit square $[0,1]^2$

For testing the hypothesis H_0 that the distribution of X_1 is uniform over the unit square $[0, 1]^2$, we considered the following competitors to the new test statistic.

(i) The Distance to Boundary Test DB (see [2]), which is based on the distance of X_1, \ldots, X_n to the boundary ∂W of $W := [0, 1]^2$. Writing $D_B(y, \partial W) := \min\{|x - y| : x \in \partial W\}$ for the distance of $y \in W$ to ∂W and $R := \max\{D_B(x, \partial W) : x \in W\}$ for the largest of such distances (which equals 0.5 in our case), the test statistic computes the values

$$Y_j := \frac{D_B(X_j, \partial W)}{R}, \quad j = 1, \dots, n$$

Under H_0 the random variables Y_1, \ldots, Y_n have a Beta(1, 2)-distribution. The test employs the Kolmogorov-Smirnov type statistic

$$DB_n = \sqrt{n} \sup_{y \in [0,1]} |G_n(y) - G_0(y)|$$

Here, G_n is the empirical distribution function of Y_1, \ldots, Y_n , and G_0 is the distribution function of the Beta(1, 2)-distribution. Rejection of H_0 is for large values of DB_n , and critical values can be taken from the Kolmogorov distribution. Note that this test is not consistent against some easily computable alternatives, e.g., the uniform distribution on the subset $[0.5, 1]^2$ of W.

(ii) The Maximal Spacing Test MS, see [3]. Writing B(x, r) for an open circle centered at x with radius r, this test considers the maximum radius

$$\Delta_n := \sup\{r > 0: \text{ there is some } x \text{ with } B(x, r) \subset [0, 1]^2 \setminus \mathcal{X}_n\}$$

of a circle that does not contain any of X_1, \ldots, X_n as an inner point. Rejection of H_0 is for large values of the test statistic $V_n := \pi \Delta_n^2$. The limit distribution of V_n under H_0 follows from (2.5) of [13], which states that

$$nV_n - \log n - \log \log n \xrightarrow{\mathcal{D}} G, \quad n \to \infty,$$

where the random variable G follows a Gumbel distribution with distribution function $\exp(-\exp(-x))$, $x \in \mathbb{R}$. Letting u_{α} denote the $(1 - \alpha)$ -quantile of this distribution, the test rejects H_0 at asymptotic level α if

$$V_n > n^{-1}(u_\alpha + \log n + \log \log n).$$

Nothing is known regarding the consistency of this test.

Since dealing with nearest neighbors in the square involves boundary effects (see, e.g., [7]), we initially employed both the Euclidean metric and the torus metric, i.e., the Euclidean metric on the 3d-torus, obtained as the quotient of the unit square by pasting opposite edges together via the identifications $(x, y) \sim (x + 1, y) \sim (x, y + 1)$. Because the power of the tests was in general somewhat higher for the torus metric than for the Euclidean metric, we decided to use the torus metric. It should be stressed that this choice conforms to the general set-up adopted in [23] so that Theorem 2.1 and Theorem 2.2 remain valid.

An empirical study of uniformity tests in several settings including the hypercube can be found in [24]. Guided by the simulation study in [4], we used a contamination and a clustering model as alternatives to the uniform distribution. The contamination model, denoted by CON, for the distribution of X_1 is the mixture

$$(1 - \varepsilon_1 - \varepsilon_2) \mathbf{U}[0, 1]^2 + \varepsilon_1 \mathbf{N}_2(c_1, \sigma_1^2) + \varepsilon_2 \mathbf{N}_2(c_2, \sigma_2^2),$$

conditionally on $X_1 \in [0,1]^2$. Here, $\varepsilon_1 = 0.135$, $\varepsilon_2 = 0.24$, $\sigma_1 = 0.09$, $\sigma_2 = 0.12$, $c_1 = (0.25, 0.25)$, $c_2 = (0.7, 0.7)$, U[0,1]² is the uniform distribution over $[0,1]^2$, and



Figure 1: Realization of the CON model (left) and the CLU model (right), n = 200

 $N_2(c_j, \sigma_j^2)$ stands for the bivariate normal distribution with expectation vector c_j and covariance matrix $\sigma_j^2 I_2$, where I_2 is the identity matrix of order 2. In other words, this model produces a uniform background noise and two radially symmetric point sources of data, centered at the points c_1 and c_2 . The additional specification "conditionally on $X_1 \in [0, 1]^{2n}$ " means that a realization was discarded whenever the generated point did not fall into the unit square.

The clustering alternative CLU (say) considers an alternative to H_0 in the non i.i.d. case, using a two step-technique. In a first step, one simulates $n_1 = 10$ i.i.d. random points with the uniform distribution U[0, 1]², which are then discarded but play the role of centers of clusters. In a second step, one generates, independently of each other, for each of those n_1 centers $n_2 = n/n_1$ points that are uniformly distributed in a disc of radius 0.05, the midpoint being the center. Similar to the CON alternative, each point was discarded if it fell outside $[0, 1]^2$, and the point was simulated according to U[0, 1]² to describe a small uniform noise effect. Figure 1 shows a realization of the CON (left) and the CLU (right) model.

Alt.	n	DB	MS	Alt.	n	DB	MS
	50	31	6		50	44	67
CON	100	58	14	CLU	100	44	85
	200	89	24		200	44	94

Table 1: Empirical rejection rates of DB and MS, unit square

Table 1 shows the percentages (out of 10000 replications) of rejections of H_0 of the distance to boundary test and the maximal spacing test, rounded to the nearest integer. Obviously, the latter test is sensitive to a cluster alternative, but much inferior to the distance to boundary test against the contamination alternative.

Alt.	α	$n \setminus J$	1	2	3	4	5	6	$\overline{7}$	8	9	10	15	20	25
		50	14	22	29	36	43	48	53	56	59	61	66	65	60
CON		100	19	27	36	45	53	60	66	71	76	79	90	93	94
	0.5	200	25	38	50	60	68	75	81	86	89	91	98	99	*
	0.0	50	*	*	*	*	*	*	*	*	*	*	*	*	*
CLU		100	*	*	*	*	*	*	*	*	*	*	*	*	*
		200	*	*	*	*	*	*	*	*	*	*	*	*	*
		50	11	11	9	6	4	3	2	2	1	1	0	0	1
CON		100	21	27	29	29	26	23	19	14	10	$\overline{7}$	1	0	0
	0	200	33	50	59	65	68	70	70	69	68	66	44	14	1
	2	50	39	40	36	29	22	16	12	8	6	5	9	12	13
CLU		100	54	52	43	33	24	17	12	8	5	4	6	10	13
		200	64	59	46	32	22	14	9	5	3	2	3	6	8
		50	13	18	19	20	20	19	17	15	14	12	10	11	13
CON		100	23	34	44	51	56	59	61	63	63	63	53	35	20
	F	200	36	58	74	83	89	92	94	96	97	97	98	98	98
	9	50	54	63	65	65	63	61	59	57	55	61	64	61	56
CLU		100	78	87	88	86	85	83	80	77	74	76	83	81	81
		200	93	98	97	97	96	95	93	91	89	89	94	92	92

Table 2: Empirical rejection rates of the test based on $T_{n,J}^{(\alpha)}$, unit square

Table 2 exhibits the corresponding percentages of the test based on $T_{n,J}^{(\alpha)}$. An asterisk denotes power 100%. As was to be expected, rejection rates depend crucially on the power α and the number of neighbors J taken into account. In each row, the maximum rejection rates have been highlighted using boldface ciphers. The beginning

of a sequence of asterisks has also been emphasized, thus indicating the smallest value of J for which the maximum power is attained. A comparison with Table 1 shows the choice $\alpha = 0.5$ yields a very strong test against cluster alternatives, even for J = 1. Likewise, taking $\alpha = 5$ and any $J \leq 15$, the test based on $T_{n,J}^{(\alpha)}$ outperforms both DBand MS.

3.2 The circle S^1

A good overview of tests for uniformity on the circle is presented in the monograph [14]. We considered the following classical procedures.

 (i) The modified Rayleigh Test, suggested in [17] and denoted by Ra in what follows, is based on the statistic

$$Ra_n := \left(1 - \frac{1}{2n} + \frac{T_n}{8n}\right) T_n. \tag{3.1}$$

Here, $T_n := 2n |\overline{X}_n|^2$, and $\overline{X}_n = n^{-1} \sum_{j=1}^n X_j$ is the sample mean vector. Under H_0 , the limit distribution of Ra_n as $n \to \infty$ is the χ_3^2 -distribution.

(ii) Kuiper's test (see [19]), denoted by Ku, uses a transformation of X_1, \ldots, X_n to normed radial data U_1, \ldots, U_n , as described in [14], p. 153. Writing $0 \le U_{(1)} \le \cdots \le U_{(n)} \le 1$ for the order statistics of U_1, \ldots, U_n , Kuiper's test is a Kolmogorov-Smirnov type test using the statistic

$$Ku_n := \sqrt{n} \left(\max_{1 \le j \le n} \left(U_{(j)} - \frac{j-1}{n} \right) + \max_{1 \le j \le n} \left(\frac{j}{n} - U_{(j)} \right) \right)$$

(see [14], p. 153).

(iii) Using the same radial data transformation as in (ii), Watson's test (see [30]), denoted by Wa, employs the statistic (see [14], p. 156)

$$Wa_n := \sum_{j=1}^n \left(U_{(j)} - \frac{2j-1}{2n} - \frac{1}{n} \sum_{\ell=1}^n U_\ell + \frac{1}{2} \right)^2 + \frac{1}{12n}$$

The implementation and critical values of the Kuiper (ii) and the Watson (iii) test were taken from the R-package Directional, as provided by [27]. As alternative distributions on the circle we considered the von Mises-Fisher (MF) and the Bimodal von Mises-Fisher (BMF) distributions, see [14], Section 2.3 and [20], Section 9.3. Note that a unit random vector has the (d-1)-dimensional von Mises-Fisher distribution if its probability density function with respect to the uniform distribution is

$$f_{\mu,\kappa}(x) = \left(\frac{\kappa}{2}\right)^{\frac{d}{2}-1} \frac{1}{\Gamma\left(\frac{d}{2}\right) I_{\frac{d}{2}-1}(\kappa)} \exp\left(\kappa \mu' x\right), \quad |x| = 1.$$
(3.2)

Here, $\kappa > 0$ is a concentration parameter, the unit vector μ denotes the mean direction, I_{ν} is the modified Bessel function of the first kind and order ν , and the prime stands for transpose. For the simulations in Tables 3 and 4 we chose $\mu = (1,0)'$ and $\kappa = 0.5$. The Bimodal von Mises-Fisher distribution is a mixture of a von Mises-Fisher distribution with $\mu = (1,0)'$ and $\mu = (-1,0)'$ with the same concentration parameter $\kappa = 1$.

Alt.	n	Ra	Ku	Wa	Alt.	n	Ra	Ku	Wa
	50	58	53	58		50	6	63	61
MF	100	88	84	88	BMF	100	6	97	99
	200	*	99	*		200	6	*	*

Table 3: Empirical rejection rates of the tests based on Ra, Ku and Wa, circle

A comparison of Table 3 and Table 4 shows that, among the values of α taken into account, the choice $\alpha = 0.05$ and J = 25 yields the highest power of the new tests against the von Mises-Fisher distribution. This power is comparable with that of Ra, Ku and Wa if n = 50, but the latter tests are superior if n = 100 or n = 200. Against the bimodal von Mises-Fisher distribution, the choice $\alpha = 0.5$ and J = 20 results in a test that outperforms Ku and Wa for n = 50 and is at least as powerful as these tests if n = 100 or n = 200. Against this alternative, the Rayleigh test is not competitive.

3.3 Sphere S^2

We now treat the case of testing for uniformity on a sphere in \mathbb{R}^3 , for which many tests have been proposed. A good overview, also for the corresponding testing problems in higher dimensions, is given in [9, 20]. We considered the following procedures.

Alt.	α	$n \backslash J$	1	2	3	4	5	6	7	8	9	10	15	20	25
		50	8	9	10	12	13	15	16	18	19	21	32	42	50
MF		100	10	12	13	15	17	19	20	21	23	25	34	43	53
	0.5	200	12	15	18	20	23	25	27	30	31	33	43	54	63
	0.5	50	28	44	56	67	76	82	87	90	93	95	98	98	97
BMF		100	37	56	71	80	87	92	95	97	98	99	*	*	*
		200	55	77	88	94	97	98	99	*	*	*	*	*	*
		50	17	24	29	32	34	36	36	35	33	31	11	1	0
MF		100	22	33	42	48	53	57	60	63	64	66	67	64	50
	0	200	30	46	58	66	72	77	80	83	85	87	92	94	95
		50	36	41	37	28	16	8	3	1	0	0	0	0	0
BMF		100	64	79	83	83	81	77	71	63	53	42	3	0	0
		200	86	96	99	99	99	99	99	99	99	99	94	73	28
		50	19	27	33	37	41	44	46	48	50	51	50	39	15
MF		100	24	36	46	52	59	63	67	70	72	75	82	85	86
	F	200	32	50	62	71	78	83	86	89	91	92	96	97	98
	9	50	48	61	66	66	61	52	41	28	16	8	2	6	18
BMF.		100	75	91	96	98	99	99	99	99	99	98	92	51	4
		200	92	99	*	*	*	*	*	*	*	*	*	*	*

Table 4: Empirical rejection rates of the test based on $T_{n,J}^{(\alpha)}$, circle

 (i) The Rayleigh Test (see [17]), denoted by *Ra*, rejects the hypothesis of uniformity for large values of

$$\widetilde{Ra}_n := \left(1 - \frac{1}{2n} + \frac{T_n}{16n}\right) T_n,$$

where $T_n := 2n |\overline{X}_n|^2$. Under H_0 , the limit distribution of \widetilde{Ra}_n as $n \to \infty$ is χ_3^2 .

(ii) The data-driven Sobolev test for uniformity applied to the sphere, here called the Jupp test and denoted by JT (see [16]), computes

$$B_n(k) = S_n(k) - k(k+2) \log n,$$

where

$$S_n(k) = \frac{2k+1}{n} \sum_{j,\ell=1}^n P_k(X'_j X_\ell),$$

and P_k is the Legendre polynomial of order k. The test statistic is then $JT_n := S_n(\hat{k})$, where

$$\widehat{k} = \widehat{k}(n) = \inf \left\{ k \in \mathbb{N} : B_n(k) = \sup_{m \in \mathbb{N}} B_n(m) \right\}.$$
(3.3)

As suggested in [16], p. 1250, a suitable approximation of the supremum in (3.3) can be done by considering $\sup_{1 \le m \le 5} B_n(m)$ instead. Critical values may be obtained from the χ_3^2 -distribution, since $JT_n \xrightarrow{\mathcal{D}} \chi_3^2$ as $n \to \infty$ under the hypothesis H_0 of uniformity.

As alternatives we considered the von Mises-Fisher distribution as in (3.2) with concentration parameter $\kappa = 0.5$ and mean direction to $\mu = (1, 0, 0)'$. A second alternative is the Kent distribution, see [20], p. 176, with density

$$f_{\mu,\kappa,\beta}(x) = \frac{1}{c(\beta,\kappa)} \exp(\kappa \mu' x + \beta x' (\tau_1 \tau_1' - \tau_2 \tau_2') x), \quad |x| = 1.$$

Here, $c(\beta, \kappa)$ is a normalizing constant, and τ_1, τ_2 and μ are mutually orthogonal vectors. The references to the Kent distribution in Tables 5 and 6 use $\kappa = 0.25, \mu = (1, 0, 0)'$ and $\beta = 2$.

The results of the simulation study are given in Tables 5 and 6. The presented procedure is competitive for sample sizes $n \ge 100$ to the other tests and outperforms the modified Rayleigh test for the Kent distribution.

Alt.	n	\widetilde{Ra}	JT	Alt.	n	\widetilde{Ra}	JT
	50	36	36		50	10	99
MF	100	66	66	Kent	100	13	*
	200	94	94		200	22	*

Table 5: Empirical rejection rates of \widetilde{Ra} and JT, sphere.

4 Conclusions and open problems

We have introduced a new, flexible class of universally consistent goodness-of-fit tests based on sums of powers of volumes of weighted kth nearest neighbor balls. Under fixed alternatives, scaled versions of the test statistics converge to the α -entropy between probability distributions. The approach is fairly general, since it covers both goodnessof-fit testing for distributions with a compact, 'full-dimensional' support in \mathbb{R}^d , but also on lower-dimensional manifolds embedded in \mathbb{R}^d . Our approach requires J, the

Alt.	α	$n \backslash J$	1	2	3	4	5	6	7	8	9	10	15	20	25
		50	7	8	9	10	11	13	14	15	16	17	23	27	31
MF.		100	8	9	10	11	12	13	15	16	17	18	25	32	39
	05	200	9	11	13	14	16	17	19	20	22	24	31	39	47
	0.5	50	66	87	95	98	99	99	*	*	*	*	*	*	*
Kent		100	83	97	99	*	*	*	*	*	*	*	*	*	*
		200	96	*	*	*	*	*	*	*	*	*	*	*	*
		50	10	12	13	13	13	13	12	11	10	8	3	2	1
MF.		100	13	17	19	22	24	25	26	26	25	25	20	14	6
	9	200	17	24	30	36	40	43	46	48	50	51	55	54	50
		50	14	9	4	1	0	0	0	0	0	0	0	0	0
Kent		100	41	42	36	27	18	10	5	2	0	0	0	0	0
		200	77	87	88	86	83	78	71	62	51	41	4	0	0
		50	12	15	18	21	23	25	26	27	27	27	26	20	11
MF.		100	15	22	28	33	38	42	44	48	50	51	57	59	59
	Б	200	19	31	41	50	57	63	67	71	74	76	84	87	90
	9	50	29	35	34	30	25	18	12	7	4	2	2	8	29
Kent		100	63	79	86	88	88	87	86	83	80	76	40	1	0
		200	91	99	*	*	*	*	*	*	*	*	*	97	96

Table 6: Empirical rejection rates of the test based on $T_{n,J}^{(\alpha)}$, sphere

maximum number of neighbors taken into account, to remain fixed as $n \to \infty$. It would be desirable to obtain limit theorems also for the case that J = J(n) tends to infinity with the sample size n. Another problem is to generalize the theory to cover testing for a parametric family $\{f(\cdot; \vartheta) : \vartheta \in \Theta\}$ of densities. This could be done by substituting $f(X_i; \widehat{\vartheta}_n)$ for the weight $f_0(X_i)$, where $\widehat{\vartheta}_n$ is a suitable estimator of ϑ , based on X_1, \ldots, X_n .

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α	$n \backslash J$	1	2	3	4	5	6	7	8	9	10	15
	50	0.78	2.02	3.58	5.43	7.52	9.82	12.32	15.01	17.88	20.91	38.24
0.5^{*}	100	0.81	2.07	3.67	5.54	7.66	9.99	12.52	15.23	18.12	21.18	38.67
	200	0.83	2.12	3.73	5.62	7.76	10.11	12.66	15.40	18.31	21.38	38.97
	50	1.74	5.59	12.10	21.70	34.70	51.48	72.29	97.46	127.19	161.76	414.95
1.5	100	1.63	5.33	11.67	21.04	33.80	50.30	70.84	95.67	125.04	159.20	409.94
	200	1.54	5.14	11.33	20.53	33.11	49.37	69.63	94.19	123.27	157.12	405.75
	50	2.90	10.18	24.03	46.44	79.42	124.97	185.22	262.12	357.71	473.86	1435.79
2	100	2.65	9.62	23.06	45.02	77.52	122.63	182.27	258.48	353.32	468.77	1425.60
	200	2.47	9.17	22.25	43.72	75.65	120.05	178.89	254.30	348.28	462.78	1413.86
	50	11.03	44.74	121.28	266.69	511.32	891.65	1449.73	2233.59	3295.24	4692.49	19245.32
3	100	9.94	41.83	116.04	258.27	501.19	882.49	1445.57	2240.49	3324.52	4754.26	19656.36
	200	8.87	38.72	109.44	246.81	482.75	855.10	1409.72	2193.28	3264.21	4685.00	19603.93
	50	54.72	257.57	788.16	1930.49	4070.50	7751.35	13650.51	22653.06	35839.35	54392.65	291880.50
4	100	50.79	242.73	758.58	1880.32	4024.20	7785.46	13870.01	23246.64	37053.41	56712.60	311282.60
	200	45.04	222.23	704.17	1776.53	3848.90	7489.95	13461.61	22687.94	36382.98	55935.54	312608.60
	50	312.65	1734.80	6015.97	16205.09	37517.20	77431.40	147116.35	260944.95	439900.80	707981.50	4871049.50
5	100	306.50	1698.35	5908.46	16242.55	37930.64	79553.08	153602.30	276095.80	471859.40	768763.70	5476554.00
	200	281.05	1570.43	5554.40	15449.12	36579.58	77266.56	149773.42	271403.80	465433.00	763477.00	5557572.00

Table 7: Empirical 95% (*: 5%) quantiles of $n^{-1}T_{n,J}^{(\alpha)}$, unit square

α	$n \backslash J$	1	2	3	4	5	6	7	8	9	10	15
	50	0.79	2.03	3.60	5.45	7.54	9.84	12.33	15.01	17.86	20.86	37.98
0.5^{*}	100	0.81	2.08	3.68	5.56	7.68	10.02	12.55	15.27	18.16	21.21	38.66
	200	0.84	2.12	3.74	5.64	7.77	10.13	12.69	15.42	18.34	21.42	39.01
	50	1.68	5.38	11.69	20.98	33.58	49.76	69.79	93.90	122.32	155.15	390.82
1.5	200	1.58	5.21	11.42	20.63	33.18	49.41	69.59	93.96	122.79	156.32	401.12
	100	1.51	5.06	11.18	20.28	32.72	48.84	68.92	93.23	122.03	155.58	401.79
	50	2.76	9.75	23.12	44.77	76.69	120.49	178.17	251.15	341.35	450.18	1319.84
2	100	2.57	9.36	22.56	44.17	76.19	120.63	179.35	254.37	347.56	460.84	1391.83
	200	2.41	9.02	21.93	43.20	74.85	118.92	177.36	252.23	345.50	459.05	1401.71
	50	10.60	43.34	118.42	261.50	501.48	873.17	1414.22	2164.48	3171.86	4477.84	17233.30
3	100	9.58	41.12	114.99	257.73	501.28	884.43	1447.28	2241.43	3320.23	4740.78	19363.40
	200	8.70	38.47	109.41	247.74	485.79	861.66	1420.44	2211.10	3291.23	4721.69	19694.42
	50	52.85	250.52	773.08	1900.67	4007.25	7624.74	13366.61	21984.31	34446.25	51695.70	254726.46
4	100	49.10	239.95	762.58	1905.83	4108.24	7956.09	14162.64	23708.80	37708.27	57628.95	309717.34
	200	44.64	222.63	715.20	1821.47	3969.98	7720.87	13872.85	23382.36	37446.71	57560.69	318814.82
	50	298.41	1675.10	5838.66	15867.96	36735.05	75663.47	142943.40	250659.04	417322.93	662873.89	4100114.35
5	100	297.07	1704.63	6065.70	16774.09	39537.66	83076.29	160282.91	287664.48	489264.08	791912.14	5477284.59
	200	278.18	1595.17	5727.94	15994.55	38089.13	80827.49	156752.23	284457.16	487537.46	797292.10	5757879.69

Table 8: Empirical 95% (*: 5%) quantiles of $n^{-1}T_{n,J}^{(\alpha)}$, circle.

α	$n \backslash J$	1	2	3	4	5	6	7	8	9	10	15
	50	0.78	2.01	3.58	5.43	7.51	9.82	12.33	15.02	17.88	20.92	38.28
0.5^{*}	100	0.81	2.07	3.67	5.54	7.66	9.99	12.52	15.24	18.13	21.19	38.68
	200	0.83	2.12	3.73	5.62	7.76	10.11	12.66	15.40	18.31	21.39	38.97
	50	1.74	5.57	12.07	21.64	34.62	51.35	72.12	97.19	126.83	161.28	413.52
1.5	100	1.63	5.33	11.66	21.04	33.81	50.29	70.78	95.60	124.97	159.14	409.60
	200	1.54	5.14	11.34	20.54	33.11	49.37	69.63	94.16	123.21	157.03	405.72
	50	2.89	10.15	23.98	46.38	79.42	125.09	185.38	262.19	357.62	473.44	1429.69
2	100	2.65	9.63	23.07	45.00	77.51	122.55	182.25	258.53	353.50	469.04	1425.90
	200	2.46	9.18	22.24	43.71	75.61	119.96	178.79	254.13	348.09	462.50	1413.42
	50	11.05	44.70	121.62	267.35	514.39	899.85	1465.00	2259.71	3334.17	4753.49	19354.84
3	100	9.88	41.61	115.67	258.08	501.29	882.86	1446.89	2243.22	3329.77	4766.78	19759.49
	200	8.89	38.78	109.53	247.04	483.45	856.25	1409.95	2195.31	3266.71	4688.33	19641.06
	50	55.17	257.13	789.21	1934.64	4099.03	7841.76	13896.74	23139.96	36671.41	55854.21	298772.54
4	100	50.44	241.42	756.21	1882.42	4046.14	7822.84	13949.15	23382.01	37302.88	57241.48	315602.34
	200	45.06	221.64	706.06	1778.94	3853.76	7503.19	13470.18	22738.34	36479.18	56091.39	313949.22
	50	312.86	1751.03	6086.85	16525.35	38243.32	79307.62	151325.83	270378.36	456890.66	738839.85	5085970.95
5	100	304.65	1690.91	5915.53	16290.68	38389.23	80548.51	155432.36	279993.35	478289.61	780194.53	5581455.18
_	200	285.05	1578.28	5582.39	15450.00	36521.11	77144.17	149839.80	272028.17	466294.26	763822.88	5578854.38

Table 9: Empirical 95% (*: 5%) quantiles of $n^{-1}T_{n,J}^{(\alpha)}$, sphere.