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ScienceDirect
Journal of Multivariate Analysis 98 (2007) 194 – 208
Journal of Multivariate Analysis
www.elsevier.com/locate/jmva

Geometry and marginals

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Received 15 February 2005
Available online 21 November 2005

Abstract

It is known that observations of a real-valued random variable defined over a smooth manifold M can be used to make inferences about M, at least when M is a curve or surface. We refine and extend the underlying asymptotic results and remove the condition $\dim M \leqslant 2$. New examples of nonsmoothness in marginals are described in detail for $\dim M = 3, 4$, and methods are given for calculations in general.

AMS 1991 subject classification: primary 62A01; 62E10; 62E20; secondary 62G07; 44A12; 44A60

Keywords: Marginal distribution; Manifold; Morse function; Critical point

1. Introduction

First, we review the problem of making inferences about a random variable from observations of marginal distributions. The problem is not easy, indeed not even well-posed, without some simplifying assumptions. Depending on the assumptions, there are well-established mathematical subjects dealing with this kind of task.

For μ a countably additive measure on a measure space M, the *marginal* measure μ_f with respect to a measurable function $f : M \to V$ is given by

$$\mu_f(B) = \mu(f^{-1}(B)),$$

where V is another measure space, and B is measurable in V. We are particularly interested in cases where V is $\mathbb{R}$ with Borel measurable sets. It is well-known that μ is usually not determined by marginals of finitely many $f_j : M \to \mathbb{R}$, even when M and the f_j are given.

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0047-259X/$ - see front matter © 2005 Published by Elsevier Inc.
doi:10.1016/j.jmva.2005.09.009

Example 1. Let M be Euclidean m-space $\mathbb{E}^m$, with the sigma algebra of Borel subsets, and μ a signed measure given by a rapidly decreasing [11] density $\psi : \mathbb{E}^m \to \mathbb{R}$, namely $\mu(A) = \int_A \psi(x)\, dx$ for any $A \in \mathcal{S}$. If $f : \mathbb{E}^m \to V$ is the restriction of orthogonal projection onto a proper vector subspace V of $\mathbb{E}^m$, μ_f has density ψ_V where

$$\psi_V(y) \equiv \int_{f^{-1}(y)} \psi(x)\, dx.$$

Defining the Fourier transform $\hat{\psi} : \mathbb{E}^m \to \mathbb{C}$ of ψ by

$$\hat{\psi}(\xi) \equiv (2\pi)^{-m/2} \int_{\mathbb{E}^m} e^{-\mathbf{i}\langle \xi, x\rangle} \psi(x)\, dx,$$

the Fourier transform of ψ_V is proportional to the restriction of $\hat{\psi}$ to V. So marginals of μ with respect to $f_1, f_2, \ldots, f_k$, corresponding to proper subspaces $V_1, V_2, \ldots, V_k$, can be found from the restriction of $\hat{\psi}$ to $\cup_{j=1}^k V_j$. Perturbing $\hat{\psi}$ to another rapidly decreasing function with the same values on $\cup_{j=1}^k V_j$ gives another density with the same marginals. However, ψ can be found from the set of all marginals of projections onto lines, by inversion of the Radon transform [3]. In geometric tomography ψ is the characteristic function of a bounded open subset N of $\mathbb{E}^m$, and N cannot in general be determined from finitely many marginals with respect to projections on lines, even when N is known to be a bounded convex subset of the Euclidean plane $\mathbb{E}^2$. However, most convex bounded planar sets N are determined by marginals with respect to projections in any two nonparallel directions [2] Theorem 1.2.17.

Example 2. In Example 1 take ψ to be everywhere nonnegative and $\int_{\mathbb{E}^m} \psi(x)\, dx = 1$. By the Corollary to Theorem 2 of Gutmann et al. [5], there is a 2-valued density on $\mathbb{E}^m$ whose marginals with respect to $f_1, f_2, \ldots, f_k$ are also $\mu_{f_1}, \mu_{f_2}, \ldots, \mu_{f_k}$. For related results in probability and tomography, see [7–9,16].

A single marginal can be used to say more about M when μ arises geometrically as follows. Let M be a real C^∞ oriented m-manifold with a positive never-zero C^∞ integrable m-form ω_M. Define μ by

$$\mu(B_M) \equiv \int_{B_M} \omega_M \geqslant 0$$

for Borel-measurable B_M. If $f : M \to \mathbb{R}$ is C^∞ set

$$\Phi_{M,f}(w) \equiv \mu_f((-\infty, w]) = \int_{f^{-1}(-\infty, w]} \omega_M.$$

Then $\Phi_{M,f} : \mathbb{R} \to [0, \infty)$ is nonnegative, nondecreasing and bounded. We ask

Question 1. *Given $\Phi_{M,f}$ what can be said about M, ω_M and f?*

As it stands Question 1 is not well-posed, but we want to make geometrical inferences about random variables from numerical measurements. With this in mind, some additional hypotheses should make the task more manageable, but first some additional simple remarks:

- $\lim_{w\to\infty} \Phi_{M,f}(w) = \int_M \omega_M$,

- if $\Phi_{M,f}(v) = \Phi_{M,f}(w)$, where $v < w$ then $f^{-1}(v, w) = \emptyset$. So,
- $\Phi_{M,f}(v) = 0 \iff f(M) \subseteq [v, \infty)$ and $\Phi_{M,f}(w) = \int_M \omega_M \iff f(M) \subset (-\infty, w]$,
- if $v_i < w_i$ and $\Phi_{M,f}|(v_i, w_i)$ has constant value c_i for $1 \leqslant i \leqslant n$, with

$$0 < c_1 < c_2 < \ldots < c_n < \int_M \omega_M,$$

then M has at least $n + 1$ path-components.

Besides $\Phi_{M,f}$, additional information is needed to determine M, ω_M and f. As well as Examples 1, 2, consider

Example 3. Given M, ω_M and $n \geqslant 1$, write $\omega_M = \sum_{i=1}^{n} \omega_i$, where each m-form ω_i is positively oriented, never-zero and integrable. Define L as the disjoint union

$$M \times \{1\} \cup M \times \{2\} \cup \ldots \cup M \times \{n\}$$

with ω_L restricting to ω_i on $M \times \{i\}$. Given $f : M \to \mathbb{R}$ define $e : L \to \mathbb{R}$ to be f on each copy of M. Then $\Phi_{L,e} = \Phi_{M,f}$.

Example 4. If f is constant with value c then $\Phi_{M,f}(w)$ is 0 or $\int_M \omega_M$ according as $w < c$ or $w \geqslant c$. So all that can be determined from $\Phi_{M,f}$ is c and $\int_M \omega_M$. Nothing can be said about the number of components of M, its dimension or topological type.

Such cases are excluded by requiring M to be path-connected and f nonconstant.

Example 5. Let ψ be a probability density on $\mathbb{R}$ with finite mean μ and finite variance σ^2. Take $M = \mathbb{R}^m$ with

$$\omega_M = \psi(x_1)\psi(x_2)\ldots\psi(x_m)\, dx_1 \wedge dx_2 \wedge \ldots \wedge dx_m$$

and define $f : M \to \mathbb{R}$ by $f(x) = (\sum_{i=1}^{m} x_i/m)$. As m increases, the Central Limit Theorem says $\Phi_{M,f}$ approximates the cumulative normal distribution with mean μ and variance σ^2/m. So dim M, ω_M and f cannot in practice be inferred from $\Phi_{M,f}$.

Another simple ambiguity arises as follows. If $F : L \to M$ is a diffeomorphism of oriented Riemannian manifolds satisfying $F^*\omega_M = \omega_L$ then $\Phi_{L,f\circ F} = \Phi_{M,f}$. So

- M, ω_M and f are knowable at best up to diffeomorphism.
- M should be path-connected.
- f should have only isolated (maybe Morse) singularities.
- ω_M is essentially unknowable except perhaps near critical points of f.
- information about M may nonetheless be obtainable.

There is quite a lot of evidence for this last remark [12]. When $\dim M = 2$, $\Phi_{M,f}$ has an a.e. C^∞ density $\phi_{M,f}$; points w^* of nonsmoothness of $\phi_{M,f}$ are critical values of f and the corresponding critical points are classified by asymptotic expressions for $\phi_{M,f}$ near w^*. So the Euler characteristic of M is obtained, and then M up to diffeomorphism. For example, a histogram with two sharp spikes and two cliffs suggests M is a torus [12]. This 2-dimensional analysis extends to surfaces with boundary [14], and there are applications to dynamical systems [13]. There are statistical algorithms which use a phenomenon called *scalability* [15] to detect features of $\phi_{M,f}$. One might well ask what remains to be done.

One of the contributions of the present paper is a more careful analysis of $\phi_{M,f}$. Even when $\dim M = 2$, the normal forms of Theorems 1, 2 are sharper than the asymptotic estimates of [12]. We also remove the condition $\dim M \leqslant 2$ appearing in all prior work and, in so doing, give normal forms for singularities of $\Phi_{M,f}$ for any Morse function *f*. Explicit calculations are given for all such singularities when $m = 3, 4$ leading to essentially 5 new kinds of nonsmoothness for marginals (Proposition 5, Examples 10, 11).

Naturally, the nonsmooth features of $\phi_{M,f}$ revealing geometrical properties of *M* are degraded by standard methods of density estimation. Geometrical phenomena are also harder to detect as $\dim M$ increases (Proposition 3, Examples 8, 9, 10, 11). A first step towards dealing with this is the thesis of Roscoe [15] where for $\dim M \leqslant 2$ *scalability* of singularities in marginal densities is noted case-by-case, and exploited to give accurate density estimates. The present paper proves scalability of $\phi_{M,f}$ for a general class of singularities of *f*, including Morse singularities, without the condition $\dim M \leqslant 2$ (Proposition 4).

The layout is as follows:

- Proposition 1 shows $\Phi_{M,f}$ has a density $\phi_{M,f}$ that is C^∞ except at critical values of *f*.
- Proposition 2 relates products and densities by convolution.
- In §3, where *M* is Euclidean *m*-space $\mathbb{E}^m$, μ restricts to Lebesgue measure on an open neighbourhood *B* of $\mathbf{0}$, and $\mathbf{0}$ is the only critical point of *f*, results are proved on smoothness of $\phi_{B,f}$ (Propositions 3, 5) and scalability (Proposition 4).
- In §4, *f* is a nondegenerate quadratic form on $\mathbb{E}^m$ $(1 \leqslant m \leqslant 4)$ and Propositions 3, 4, 5 are illustrated by graphs of $\phi_{B,f}$.
- In §5 the study of $\phi_{M,f}$ near a point w^* of nonsmoothness reduces to the case where $M = \mathbb{E}^m$, $w^* = \mathbf{0}$ and $\omega_M = \psi\, dx_1 \wedge dx_2 \wedge \ldots \wedge dx_m$, where ψ is positive, C^∞ and integrable.
- Example 7 and Proposition 5 are strengthened to Theorems 1, 2.

2. Densities and critical values

Given C^∞ $f : M \to \mathbb{R}$, nonempty open $B \subseteq M$ and $w \in \mathbb{R}$, set

$$B_{f,w} \equiv \{x \in B : f(x) \leqslant w\}.$$

Defining $\Phi_{B,f} : \mathbb{R} \to [0, \infty)$ by $\Phi_{B,f}(w) = \int_{B_{f,w}} \omega_M$,

$$\Phi_{B,f}(-w) + \Phi_{B,-f}(w) = \int_B \omega_M + \int_{B \cap f^{-1}(-w)} \omega_M, \tag{1}$$

$$\Phi_{B,f}(a^{-1}w) = \Phi_{B,af}(w), \tag{2}$$

$$\Phi_{B\cup C,f} + \Phi_{B\cap C,f} = \Phi_{B,f} + \Phi_{C,f}, \tag{3}$$

where $a > 0$, and $C \subseteq M$ is also nonempty and open. If a diffeomorphism $F : L \to M$ satisfies $F^*\omega_M = \omega_L$ then $\Phi_{B,f} = \Phi_{F^{-1}B, f\circ F}$. Denote the set of critical points of $f|\bar{B}$ by $C_{B,f} \subset \bar{B}$ and the set of regular values by $R_{B,f} \subseteq \mathbb{R}$.

Lemma 1. *For $C_{B,f}$ compact, $\Phi_{B,f}|R_{B,f}$ is C^∞.*

Proof. For $w \in R_{B,f}$, $\Phi_{B,f}(w) = \int_{f^{-1}(-\infty,w]} \chi_B \omega_M$ where the C^∞ m-manifold with boundary $f^{-1}(-\infty, w]$ depends smoothly on w. Indeed,

$$\Phi'_{B,f}(w) = \int_{B\cap f^{-1}(w)} \frac{1}{\|\nabla f\|}\omega_{f^{-1}(w)} \geqslant 0,$$

where $\|\nabla f\|$ is bounded away from 0 because $C_{B,f}$ is compact. □

Lemma 2. *Let $U \subset B$ be any open neighbourhood of $C_{B,f}$, where $C_{B,f}$ is compact. Then $\Phi_{B,f} - \Phi_{U,f}$ is C^∞.*

Proof. By (3) $\Phi_{B,f} - \Phi_{U,f} = \Phi_{B-\bar{U},f}$, and by Lemma 1 $\Phi_{B-\bar{U},f}$ is C^∞. □

Corollary 1. *Let $C_{B,f}$ be compact. Then modulo C^∞ functions $\Phi_{M,f}$ depends only on the germs of ω_M and of f at $C_{B,f}$. If f has only finitely many critical values $w_1, w_2, \ldots w_k$ then, for any open neighbourhoods U_j of w_j,*

$$\Phi_{M,f} - \sum_{j=1}^{k} \Phi_{U_j,f} : \mathbb{R} \to [0,\infty) \quad \text{is} \quad C^\infty.$$

Proposition 1. *Let $C_{B,f}$ be compact of measure* 0. *For some $\phi_{B,f} \in L^1(\mathbb{R})$, $\phi_{B,f}|R_{B,f}$ is C^∞ and*

$$\Phi_{B,f}(w) = \int_{-\infty}^{w} \phi_{B,f}(v)\,dv \quad \textit{for all} \quad w \in \mathbb{R}.$$

Proof. Given $p \in \mathbb{Z}_+$, let $U^{(p)}$ be an open neighbourhood of $C_{B,f}$ of measure less than $\frac{1}{p}$. Any $w \in \mathbb{R}$ is a regular value of $f|B - U^{(p)}$, and so

$$\Phi_{B-U^{(p)},f}(w) = \int_{-\infty}^{w} \phi_{B-U^{(p)},f}(v)\,dv,$$

where $\phi_{B-U^{(p)},f}$ is nonnegative and C^∞. Without loss $U^{(p+1)} \subset U^{(p)}$ for every p. Since $\phi_{B-U^{(p)},f} : \mathbb{R} \to \mathbb{R}$ increases pointwise with p and $\int_{\mathbb{R}} \phi_{B-U^{(p)},f}(w)\,dw \leqslant \int_B \omega$, the pointwise limit $\phi_{B,f}$ of $\phi_{B-U^{(p)},f}$ is integrable [6, §27, Theorem B] over every interval $(-\infty, w]$ and

$$\lim_{p\to\infty} \Phi_{B-U^{(p)},f}(w) = \lim_{p\to\infty} \int_{-\infty}^{w} \phi_{B-U^{(p)},f}(v)\,dv = \int_{-\infty}^{w} \phi_{B,f}(v)\,dv.$$

$$\text{Also} \quad \Phi_{B-U^{(p)},f}(w) \leqslant \Phi_{B,f}(w) \leqslant \Phi_{B-U^{(p)},f}(w) + \frac{1}{p}.$$

Taking limits $\int_{-\infty}^{w} \phi_{B,f}(v)\,dv = \Phi_{B,f}(w)$. Notice $\phi_{B-U^{(p)},f}$ is C^∞ and agrees with $\phi_{B,f}$ on $\mathbb{R} - f(U^{(p)})$. Since $R_{B,f}$ is covered by a countable set of open intervals the $U^{(p)}$ can be chosen so that $\cap_{p\geqslant 1} U^{(p)} = C_{B,f}$. Then $\cup_{p\geqslant 1}(\mathbb{R} - f(U^{(p)})) = R_{B,f}$ and $\phi_{B,f}|R_{B,f}$ is C^∞. □

In Proposition 1, $\phi_{B,f}|R_{B,f}$ is unique and $\phi_{B,f} \in L^1(\mathbb{R})$ is called the *density* of $\Phi_{B,f}$ (there is no density when f is constant). Since the second term on the right-hand side of (1) vanishes when $C_{B,f}$ has measure 0,

$$\phi_{B,f}(w) = \phi_{B,-f}(-w). \tag{4}$$

Let N be a real C^∞ oriented Riemannian n-manifold with ω_N integrable, and set $\omega_{M\times N} = \omega_M \wedge \omega_N$. Given C^∞ $g : N \to \mathbb{R}$ define

$$f \oplus g : M \times N \to \mathbb{R} \quad \text{by} \quad (f \oplus g)(b, c) = f(b) + g(c)$$

and the *convolution* $\phi * \psi$ of $\phi, \psi \in L^1(\mathbb{R})$ according to the convention

$$(\phi * \psi)(w) = \int_{\mathbb{R}} \phi(v)\psi(w - v)\, dv = \int_{\mathbb{R}} \phi(w - v)\psi(v)\, dv.$$

Let C be a nonempty open subset of N.

Proposition 2. *Suppose $C_{B,f}$ and $C_{C,g}$ are compact of measure* 0 *in M and N respectively. Then*

$$\phi_{B\times C, f\oplus g} = \phi_{B,f} * \phi_{C,g}.$$

Proof. $(B \times C)_{f\oplus g,w} = \cup_{y\in B}(\{y\} \times C \cap g^{-1}(-\infty, w - f(y)])$. By Fubini's Theorem,

$$\begin{aligned}
\Phi_{B\times C,f\oplus g}(w) &= \int_B \left(\int_{C\cap g^{-1}(-\infty,w-f(y)]} \omega_N \right) \omega_M = \int_B \Phi_{C,g}(w - f(y))\omega_M \\
&= \int_B \int_{-\infty}^{w-f(y)} \phi_{C,g}(v)\, dv\omega_M \\
&= \int_{-\infty}^{\infty} \left(\phi_{C,g}(v) \int_{B\cap f^{-1}(w-v)} \omega_M \right) dv \\
&= \int_{-\infty}^{\infty} \phi_{C,g}(v)\Phi_{B,f}(w - v)\, dv. \qquad \square
\end{aligned}$$

Corollary 2. *Suppose $C_{B,f}$ and $C_{C,g}$ are compact of measure* 0 *in M and N, respectively, that $\phi_{B,f}$ is C^p and $\phi_{C,g}$ is C^q. Then $\phi_{B\times C,f\oplus g}$ is at least C^{p+q}.*

3. Euclidean singularities

Now we are going to look at singularities of marginal densities and scalability in the special case where ψ is locally constant. The asymptotic expressions in [12] follow from the analysis in such a case where $\dim\, M = 2$. Our present more general arguments work without the dimension restriction.

Let M be Euclidean m-space $\mathbb{E}^m$, with Euclidean norm $\| \|_m$ and m-dimensional Lebesgue measure λ_m. For λ_m-integrable $\psi : \mathbb{E}^m \to (0, \infty)$ identically 1 on some open neighbourhood U of $\mathbf{0}$ containing the open ball $B = B^m(\delta)$ of radius $\delta > 0$ and centre $\mathbf{0}$, set $\omega_M(x) = \psi(x)\, dx_1 \wedge dx_2 \wedge \ldots \wedge dx_m$. Then

$$\lambda_m(B^m(\delta)) = \kappa_m \delta^m, \quad \text{where} \quad \kappa_m \equiv \frac{\pi^{\frac{m}{2}}}{\Gamma(1 + \frac{m}{2})}.$$

For $w \in \mathbb{R}$, and nonsingular linear $T : \mathbb{E}^m \to \mathbb{E}^m$ satisfying $T^{-1}B \subset U$, we have

$$\Phi_{T^{-1}B, f\circ T}(w) = |\det\, T|^{-m}\Phi_{B,f}(w). \tag{5}$$

Example 6. Take $m = 1$ and $f(x) = x^q$, where $q \in \mathbb{Z}_+$. For $w \notin (-\delta^q, \delta^q)$, $\phi_{(-\delta,\delta),f}(w) = 0$. For q even and $w \in (-\delta^q, 0)$, $\phi_{(-\delta,\delta),f}(w) = 0$. For q even and $w \in (0, \delta^q)$, $\Phi_{(-\delta,\delta),f}(w) = 2w^{\frac{1}{q}}$. For q odd and $w \in (-\delta^q, \delta^q)$, $\Phi_{(-\delta,\delta),f}(w) = w^{\frac{1}{q}} + \delta$. For $q \geqslant 2$, $\phi_{(-\delta,\delta),f}$ is unbounded in any neighbourhood of 0.

Example 7. For $m \geqslant 1$ let $f(x) = \|x\|_m^2$. Then $\Phi_{B,f}(w) = \kappa_m w_+^{\frac{m}{2}}$, where $w_+ \equiv \max\{w, 0\}$. So $\phi_{B,f}$ is $C^{[\frac{m}{2}]-1}$. By Lemma 2 this holds even if B is not contained in U. Define $g : \mathbb{E}^n \to \mathbb{R}$ by $g(z) = -\|z\|_n^2$. Then $\phi_{C,g}$ is $C^{[\frac{n}{2}]-1}$ for an open neighbourhood C of $\mathbf{0}$ in $\mathbb{E}^n$. By Corollary 2 $\phi_{B\times C, f\oplus g}$ is $C^{[\frac{m}{2}]+[\frac{n}{2}]-2}$. By Lemma 2 $\phi_{D,f\oplus g}$ is also $C^{[\frac{m}{2}]+[\frac{n}{2}]-2}$, where D is an open neighbourhood of $\mathbf{0}$ in $\mathbb{E}^{m+n} \cong \mathbb{E}^m \times \mathbb{E}^n$.

Proposition 3. *Let $f : \mathbb{E}^m \to \mathbb{R}$ be a nondegenerate quadratic form of index $0 \leqslant n \leqslant m$, where $f(\mathbf{0}) = 0$. Then $\phi_{B,f}(w)$ has at least $[\frac{m-n}{2}] + [\frac{n}{2}] - 2$ and at most $[\frac{m}{2}]$ continuous derivatives at $w = 0$.*

Proof. By (5) and Lemma 2 there is no loss of generality in supposing f is represented by a diagonal matrix with entries ± 1 with respect to the standard basis of $\mathbb{E}^m$. Then the lower bound on numbers of derivatives follows from Example 7. For the upper bound, consider first the case where $m = 1$ and $n = 0$, namely $f(x) = x^2$. Example 7 also deals with this simple situation, but a closer look will be useful:

Let $\kappa : \mathbb{R} \to [0, \infty)$ be C^∞, identically 1 on $[-\delta, \delta]$, and with support in $[-2\delta, 2\delta]$. The Fourier transform of $\phi^* \equiv \kappa\phi_{(-\delta,\delta),f}$ is given by

$$\sqrt{2\pi}\tilde{\phi}^*(\xi) = \int_0^\delta x^{-1/2} e^{-\mathbf{i}x\xi}\, dy + \int_\delta^{2\delta} \phi^*(x) e^{-\mathbf{i}x\xi}\, dy.$$

For $\xi > 0$, on substituting $v = \sqrt{x\xi}$ and integration by parts, the right-hand side is

$$\begin{aligned}
&2\xi^{-\frac{1}{2}} \int_0^{\sqrt{\delta\xi}} e^{-\mathbf{i}v^2}\, dv + \frac{1}{\mathbf{i}\xi}\left(\phi^*(\delta)e^{-\mathbf{i}\xi} + \int_\delta^{2\delta} \phi^{*\prime}(x) e^{-\mathbf{i}x\xi}\, dx\right) \\
&= 2\xi^{-\frac{1}{2}}\sqrt{\frac{\pi}{2}}(1-\mathbf{i}) + \frac{1}{\mathbf{i}\xi}\left(\delta^{-\frac{1}{2}} e^{-\mathbf{i}\xi} + \int_\delta^{2\delta} \phi^{*\prime}(x) e^{-\mathbf{i}x\xi}\, dx\right) \\
&= 2\sqrt{\frac{\pi}{2}}(1-\mathbf{i})\xi^{-\frac{1}{2}} + O\left(\frac{1}{\xi}\right)
\end{aligned}$$

as $\xi \to \infty$. Arguing similarly, as $\xi \to -\infty$,

$$\sqrt{2\pi}\tilde{\kappa} * \tilde{\phi}_{(-\delta,\delta),f} = |\tilde{\phi}^*(\xi)| = |\xi|^{-\frac{1}{2}} + O(|\xi|^{-1}) \quad \text{as} \quad |\xi| \to \infty. \tag{6}$$

By (4), (6) is unaltered when f is replaced by $-f$.

In general, by Proposition 2, $\phi_{B,f} = \phi_1 * \phi_2 * \ldots * \phi_m$ where $\phi_i = \phi_{(-\delta,\delta),\pm g}$ and $g(x) = \pm x^2$. Setting $\bar{\phi} \equiv \lambda\phi_{(-\delta,\delta)^m,f}$ with $\lambda \equiv \kappa^m$, we have $(2\pi)^{\frac{m}{2}}\tilde{\bar{\phi}} =$

$$\begin{aligned}
(2\pi)^{\frac{m-1}{2}}\tilde{\lambda} * \tilde{\phi}_{(-\delta,\delta)^m,f} &= \tilde{\kappa} * \tilde{\kappa} * \ldots * \tilde{\kappa} * \tilde{\phi}_{(-\delta,\delta)^m,f} = (2\pi)^{\frac{m-1}{2}}|\xi|^{-\frac{m}{2}} \\
&\quad + O(|\xi|^{-\frac{m}{2}-1})
\end{aligned}$$

by (6). So $\lambda\phi_{(-\delta,\delta)^m,f} = \bar{\phi}$ has at most $[\frac{m}{2}]$ continuous derivatives. Write

$$\phi_{(-\delta,\delta)^m,f} = \lambda\phi_{(-\delta,\delta)^m,f} + (1-\lambda)\phi_{(-\delta,\delta)^m,f}.$$

By Lemma 1, $\phi_{(-\delta,\delta)^m,f}$ is C^∞ except at $w = 0$. Since $\lambda|(-\delta,\delta)$ is identically 1, $\phi_{(-\delta,\delta)^m,f}$ is at most $C^{[\frac{m}{2}]}$. So $\phi_{B,f}$ is at most $C^{[\frac{m}{2}]}$, by Lemma 2. $\square$

Definition 1. A function $\Phi : \mathbb{R} \to \mathbb{R}$ is *scalable* of order σ at $c \in \mathbb{R}$ when, for any $a > 0$,

$$\Phi(aw + (1-a)c) - a^\sigma \Phi(w)$$

is C^∞ in $w \in \mathbb{R}$.

If Φ is C^r and scalable of order σ at c, then $r \leqslant \sigma$ and $\Phi^{(r)}$ is scalable of order $\sigma - r$ at c. Scalability is used in algorithms of Roscoe [15] for detection of geometrical features: singular histograms are identified up to smooth local changes of coordinates, by calculating covariances of observed and ideal marginal distributions. Scalability permits the use of one ideal marginal at any convenient scale, for each kind of singularity being investigated.

Lemma 3. *Let $f : \mathbb{E}^m \to \mathbb{R}$ and $g : \mathbb{E}^n \to \mathbb{R}$ have $\mathbf{0}$ as the only critical point. If $\phi_{B,f}$ is scalable of order σ at $c \equiv f(\mathbf{0})$, and $\phi_{C,g}$ is scalable of order μ at $d \equiv g(\mathbf{0})$, then $\phi_{B\times C, f\oplus g}$ is scalable of order $\sigma + \mu + 1$ at $c + d$.*

Proof. By Proposition 2, $\phi_{B\times C,f\oplus g} = \phi_{B,f} * \phi_{C,g}$. So for $a > 0$,

$$\begin{aligned}
&\phi_{B\times C,f\oplus g}(aw + (1-a)(c+d)) \\
&\quad = \int_{\mathbb{R}} \phi_{B,f}(v)\phi_{C,g}(aw + (1-a)(c+d) - v)\, dv \\
&\quad = a\int_{\mathbb{R}} \phi_{B,f}(au + (1-a)c)\phi_{C,g}(a(w-u) + (1-a)d)\, du \\
&\quad = a\int_{\mathbb{R}} (a^\sigma \phi_{B,f}(u) + \psi_B(u))(a^\mu \phi_{C,g}(w-u) + \psi_C(w-u))\, du,
\end{aligned}$$

where ψ_B and ψ_C are C^∞. The right-hand side is

$$\begin{aligned}
&a^{\sigma+\mu+1}(\phi_{B,f} * \phi_{C,g})(w) + a^{\mu+1}(\psi_B * \phi_{C,g})(w) + a^{\sigma+1}(\phi_{B,f} * \psi_C)(w) \\
&\quad + a(\psi_B * \psi_C)(w),
\end{aligned}$$

where the last three terms are C^∞ in w. $\square$

Lemma 4. *If $f : \mathbb{E}^m \to \mathbb{R}$ is positively homogeneous of degree $q > 0$, $\Phi_{B,f}$ is scalable of order $\frac{m}{q}$ at 0.*

Proof. By homogeneity, $x \in B^m(\delta) \cap f^{-1}(-\infty, w]$ when, for any $a > 1$,

$$a^{\frac{1}{q}} x \in B^m(a^{\frac{1}{q}}\delta) \cap f^{-1}(-\infty, aw].$$

So

$$\begin{aligned}
\Phi_{B,f}(w) &= \lambda_m(B^m(\delta) \cap f^{-1}(-\infty, w]) = a^{-\frac{m}{q}} \lambda_m(B^m(a^{\frac{1}{q}}\delta) \cap f^{-1}(-\infty, aw]) \\
&= a^{-\frac{m}{q}}(\Phi_{B,f}(aw) + \Phi_{C,f}(aw)), \quad \text{where } C \equiv B^m(a^{\frac{1}{q}}\delta) - B^m(\delta).
\end{aligned}$$

Since $f|C$ has no critical points, $\Phi_{C,f}$ is C^∞, by Lemma 1. So $\Phi_{B,f}(aw) - a^{\frac{m}{q}}\Phi_{B,f}(w)$ is C^∞ for $a > 1$. The same holds for $a \in (0,1)$ on replacing a by a^{-1}, and the identity is trivial when $a = 1$. □

Comparing Lemmas 3, 4, we obtain

Proposition 4. *For $i = 1, 2, \ldots, r$ let $f_i : \mathbb{E}^{m_i} \to \mathbb{R}$ be positively homogeneous of degree $q_i > 0$ with $\mathbf{0}$ the only critical point. Setting $m \equiv \sum_{i=1}^r m_i$,*

$$f \equiv f_1 \oplus f_2 \oplus \ldots \oplus f_r : \mathbb{E}^{m_1} \times \mathbb{E}^{m_2} \times \ldots \times \mathbb{E}^{m_r} \cong \mathbb{E}^m \to \mathbb{R}$$

for any bounded neighbourhood B of $\mathbf{0} \in \mathbb{E}^m$, $\phi_{B,f}$ is scalable at 0 of order

$$\sum_{i=1}^r \frac{m_i}{q_i} + r - 1.$$

Our definition of scalability is a little different (and Proposition 4 establishes the property in greater generality) than in [15].

For $m, n \geqslant 0$ let $S_{m,n} : \mathbb{E}^m \times \mathbb{E}^n \to \mathbb{E}^{m+n}$ be the standard identification:

$$S_{m,n}(y, z) = (y_1, y_2, \ldots, y_m, z_1, z_2, \ldots, z_n).$$

Define $f_{m,n} : \mathbb{E}^{m+n} \to \mathbb{R}$ by $f_{m,n}(x) = \|y\|_m^2 - \|z\|_n^2$, where $x = S_{m,n}(y, z)$. (The significance of $f_{m,n}$ is due to the Morse Lemma, which says that, near a nondegenerate critical point, a smooth function can be written in the form $f_{m,n}$ after suitable C^∞ reparameterization.) We have

$$\Phi_{B,f_{m,n}}(w) = \lambda_{m+n}((f_{m,n}^{-1}[-\delta^2, w]) \cap B),$$

where $B \equiv B^{m+n}(\delta)$ and $\delta > 0$. By Lemma 1 $\Phi_{B,f_{m,n}}$ is C^∞ except at $w = 0$. The coordinate-switch $\sigma : \mathbb{E}^m \times \mathbb{E}^n \to \mathbb{E}^n \times \mathbb{E}^m$ induces an orthogonal transformation

$$T_{m,n} \equiv S_{n,m} \circ \sigma \circ S_{m,n}^{-1} : \mathbb{E}^{m+n} \to \mathbb{E}^{m+n}.$$

As in Example 7, $\Phi_{B,f_{m,0}}(w) = \kappa_m w_+^{\frac{m}{2}}$. For $t > 0$ and integers $m, n \geqslant 1$, define

$$I_{m,n}(t) \equiv \int_0^t \cosh^{m-1} s \sinh^{n-1} s\, ds = \frac{1}{2^{m+n-2}} \int_0^t (e^s + e^{-s})^{m-1}(e^s - e^{-s})^{n-1}\, ds.$$

Proposition 5. *For $m, n \geqslant 1$, and $|w| < \delta^2$ set $I^* \equiv I_{m,n}(t^*)$ or $I_{n,m}(t^*)$ according as $w \geqslant 0$ or $w \leqslant 0$, where $t^* \equiv -\frac{1}{2}\ln 2|w| + \ln(\sqrt{\delta^2 + w} + \sqrt{\delta^2 - w})$. Then $\Phi_{B,f_{m,n}}$ has density*

$$\phi_{B,f_{m,n}}(w) = \frac{mn\kappa_m\kappa_n}{2}|w|^{\frac{m+n}{2}-1} I^*.$$

Proof. For $w > 0$, $S_{m,n}(y,z) \in B \cap f_{m,n}^{-1}[-\delta^2, w]$ when

$$z \in Z_y \equiv \{z : (\|y\|_m^2 - w)_+ \leqslant \|z\|_n^2 \leqslant \delta^2 - \|y\|_m^2\} \subset \mathbb{E}^n.$$

Then $\lambda_n(Z_y) = \kappa_n((\delta^2 - \|y\|_m^2)^{\frac{n}{2}} - (\|y\|_m^2 - w)_+^{\frac{n}{2}})$. By Fubini's Theorem,

$$\Phi_{B,f_{m,n}}(w) = m\kappa_m\kappa_n \left(\int_{\sqrt{w}}^{\sqrt{\frac{w+\delta^2}{2}}} ((\delta^2 - r^2)^{\frac{n}{2}} - (r^2 - w)^{\frac{n}{2}}) r^{m-1}\, dr \right.$$

$$\left. + \int_0^{\sqrt{w}} (\delta^2 - r^2)^{\frac{n}{2}} r^{m-1}\, dr \right).$$

It follows that $\Phi'_{B,f_{m,n}}(w)$ is

$$\frac{mn\kappa_m\kappa_n}{2} \int_{\sqrt{w}}^{\sqrt{\frac{w+\delta^2}{2}}} (r^2 - w)^{\frac{n}{2}-1} r^{m-1} dr$$

$$= \frac{mn\kappa_m\kappa_n}{2} w^{\frac{m+n}{2}-1} I_{m,n} \left(-\frac{1}{2}\ln 2w + \ln\left(\sqrt{\delta^2 + w} + \sqrt{\delta^2 - w}\right)\right).$$

For $w < 0$, by (4), $\Phi'_{B,f_{m,n}}(w) = \Phi'_{B,f_{n,m}}(-w)$ and the result follows. $\square$

In accordance with (4), $\phi_{B,f_{m,n}}(w) = \phi_{B,f_{n,m}}(-w)$ for $w \neq 0$. In particular $\phi_{B,f_{m,m}}$ is even.

4. Euclidean examples

In the following examples take $|w| < \delta^2$.

Example 8. $\Phi_{B,f_{1,0}}(w) = 2w_+^{1/2}$ and $\Phi_{B,f_{0,1}}(w) = 2\delta - 2((-w)_+)^{1/2}$ (Fig. 1).

Example 9. $\Phi_{B,f_{2,0}}(w) = \pi w_+$, and $\Phi_{B,f_{0,2}}(w) = \pi\delta^2 - \Phi_{B,f_{0,2}}(-w)$ (Fig. 2). For $f_{1,1}$ the density spikes at $w = 0$ (Fig. 3):

$$\phi_{B,f_{1,1}}(w) = -\ln(2|w|) + 2\ln\left(\sqrt{\delta^2 + w} + \sqrt{\delta^2 - w}\right).$$

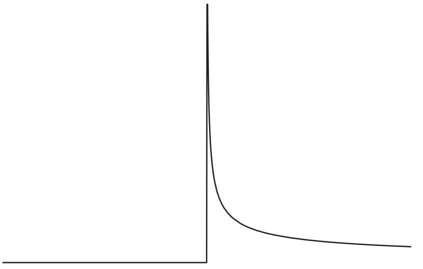

Fig. 1. Graph of $\phi_{B,f_{1,0}}$ in Example 8.

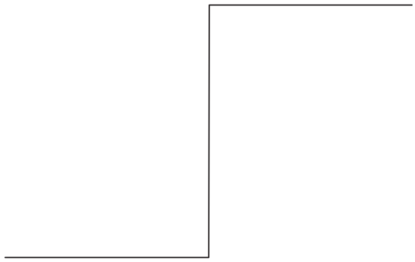

Fig. 2. Graph of $\phi_{B,f_{2,0}}$ (cliff) in Example 9.

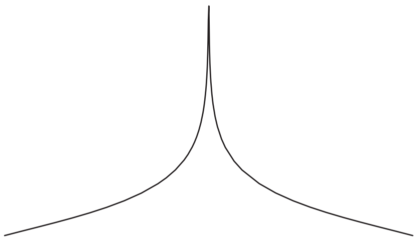

Fig. 3. Graph of $\phi_{B,f_{1,1}}$ (spike) in Example 9.

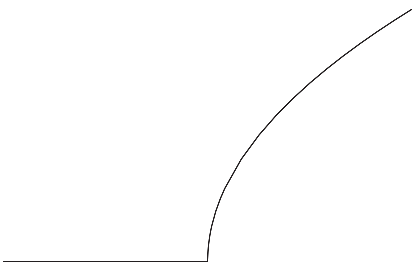

Fig. 4. Graph of $\phi_{B,f_{3,0}}$ in Example 10.

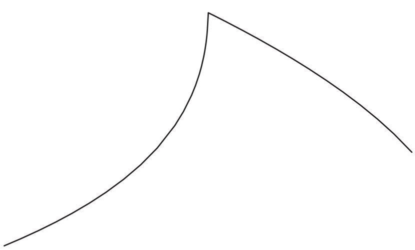

Fig. 5. Graph of $\phi_{B,f_{2,1}}$ (shark tooth) in Example 10.

Example 10. $\phi_{B,f_{3,0}}(w) = 2\pi w_+^{1/2}$ and $\phi_{B,f_{0,3}}(w) = \phi_{B,f_{3,0}}(-w)$. $\phi_{B,f_{2,1}}(w) = \pi\sqrt{2(\delta^2 - w)}$ $-2\pi\sqrt{(-w)_+}$ (Fig. 4). The graph of $\phi_{B,f_{2,1}}$ in Fig. 5 has the appearance of a shark tooth: reflection in the vertical axis gives the graph of $\phi_{B,f_{1,2}}$.

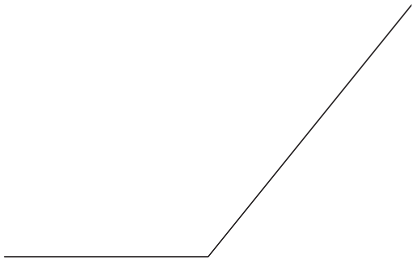

Fig. 6. Graph of $\phi_{B,f_{4,0}}$ in Example 11.

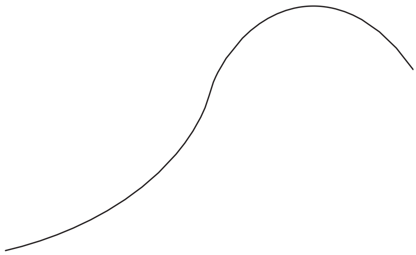

Fig. 7. Graph of $\phi_{B,f_{3,1}}$ in Example 11.

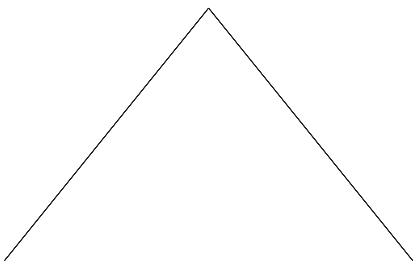

Fig. 8. Graph of $\phi_{B,f_{2,2}}$ in Example 11.

Example 11. $\phi_{B,f_{4,0}}(w) = \pi^2 w_+$, and $\phi_{B,f_{0,4}}(w) = \phi_{B,f_{4,0}}(-w)$ (Fig. 6). For $\phi_{B,f_{3,1}}(w)$, where $w \neq 0$ we obtain

$$\pi\left(\sqrt{\delta^4 - w^2} - w \ln\left(\frac{|w|}{\delta^2 + \sqrt{\delta^4 - w^2}}\right)\right)$$

whose graph is shown in Fig. 7, and then $\phi_{B,f_{1,3}}$ is obtained by reflection (Fig. 8). For $w \neq 0$,

$$\phi_{B,f_{2,2}}(w) = \frac{\pi^2}{2}(\delta^2 - |w|).$$

5. Riemannian singularities

The examples in §4 show singularities of $\phi_{M,f}$ when ψ is locally constant. In general, when ψ is not locally constant, we can replace the nonzero density ψ by $\psi(w^*)$ in some neighbourhood of a critical point w^* of f. This approach, taken in [12], is sufficient for some asymptotic results. The present section goes further, giving normal forms for $\phi_{M,f}$ near points of nonsmoothness.

By the Morse Lemma [10, Lemma 2.2] near a nondegenerate critical point of f we can take $M = \mathbb{R}^m$ and $f = f_{n,m-n} : \mathbb{E}^m \cong \mathbb{R}^m \to \mathbb{R}$ where $0 \leqslant n \leqslant m$. Also

$$\omega_M = \psi dx_1 \wedge dx_2 \wedge \ldots \wedge dx_m,$$

where $\psi : \mathbb{R}^m \to (0, \infty)$ is C^∞ and integrable. Let $O_{n,m-n}$ be the space of linear transformations of $\mathbb{R}^m$ of determinant ± 1 preserving the quadratic form $f_{n,m-n}$. For $T \in O_{n,m-n}$ $\Phi_{B,f_{n,m-n}} = \Phi_{T^{-1}B, f_{n,m-n}\circ T}$. For convenience we include a proof of the following well-known result [4, p. 248 Lemma 2.1]:

Lemma 5. *Let $\alpha : (-\delta, \delta) \to \mathbb{R}$ be C^∞ and even. For some C^∞ $\beta : (-\delta^2, \delta^2) \to \mathbb{R}$,*

$$\alpha(v) = \beta(v^2) \quad \textit{for all } v \in (-\delta, \delta).$$

Proof. By Hadamard's Lemma [10, Lemma 2.1] $\alpha(v) - \alpha(0) = v\alpha^1(v)$ where $\alpha^1 : (-\delta, \delta) \to \mathbb{R}$ is C^∞ and odd. Again by Hadamard's Lemma, since $\alpha^1(0) = 0$, $\alpha(v) - \alpha(0) = v^2\alpha_2(v)$ where $\alpha_2 : (-\delta, \delta) \to \mathbb{R}$ is C^∞ and even. Continuing in this way, for any integer $k \geqslant 1$,

$$\alpha(v) = \sum_{j=0}^{k-1} v^{2j}\alpha_{2j}(0) + v^{2k}\alpha_{2k}(v),$$

where $\alpha_0 \equiv \alpha$, and each $\alpha_{2j} : (-\delta, \delta) \to \mathbb{R}$ is C^∞ and even. Define $\beta_0 : [0, \delta^2) \to \mathbb{R}$ by $\beta_0(u) = \sum_{j=0}^{k-1} u^j \alpha_{2j}(0) + u^k \alpha_{2k}(\sqrt{u})$. For $1 \leqslant l \leqslant k-1$, $\lim_{u\to 0^+} \beta_0^{(l)}(u) = l!\alpha_{2l}(0)$. Denoting the continuous extension of $\beta_0^{(l)} : (0, \delta^2) \to \mathbb{R}$ to $[0, \delta^2)$ by β_l,

$$\beta_0(u) = \sum_{j=0}^{k-1} \frac{1}{j!} \beta_j(0) u^j + u^k \alpha_{2k}(\sqrt{u}).$$

Writing $m = k - l$, $\beta_l(u) = \sum_{i=0}^{m-1} \frac{1}{i!}\beta_{l+i}(0)u^i + O(u^m)$. So by the Whitney Extension Theorem [11, Theorem 1.5.6] β_0 extends from $[0, \delta^2)$ to a C^∞ function β defined on $(-\delta^2, \delta^2)$. $\square$

Theorem 1. *Let $B = B^m(\delta)$. For $w < 0$, $\phi_{B,f_{m,0}}(w) = 0$. For $0 < w < \delta^2$,*

$$\phi_{B,f_{m,0}}(w) = \frac{m}{2}\kappa_m \beta(w) w^{\frac{m}{2}-1},$$

where $\beta : (-\delta^2, \delta^2) \to (0, \infty)$ is C^∞. For $w \in (0, \delta^2)$ and any $x \in \mathbb{E}^m$ with $\|x\| = \sqrt{w}$,

$$\beta(\|x\|) = \int_{O_m} \psi(Tx)\, dT,$$

where integration is with respect to normalized Haar measure on the orthogonal group O_m.

Proof of Theorem 1. $O_m \equiv O_{m,0}$ is compact and leaves B invariant. Because $f_{m,0}$ is O_m-invariant ψ can be replaced in the integral for $\Phi_{B,f_{m,0}}(w)$ by its O_m-average $\psi_{\text{av}} : \mathbb{R}^m \to (0, \infty)$. Because ψ_{av} is O_m-invariant $\psi_{\text{av}}(x) = \bar{\psi}(\|x\|)$ where $\bar{\psi} \equiv \psi_{\text{av}}|\mathbb{R} \times \{\mathbf{0}\} \cong \mathbb{R} \to (0, \infty)$ is C^∞ and even. For $w \in (-\delta^2, 0)$ evidently $\Phi_{B,f_{m,0}}(w) = 0$. For $0 \leqslant w < \delta^2$

$$\Phi_{B,f_{m,0}}(w) = m\kappa_m \int_0^{\sqrt{w}} u^{m-1}\bar{\psi}(u)\, du.$$

So for $0 < w < \delta^2$ $\phi_{B,f_{m,0}}(w) = \frac{m}{2}\kappa_m w^{\frac{m}{2}-1}\bar{\psi}(\sqrt{w})$ and the formula for $\phi_{B,f_{m,0}}$ follows from Lemma 5 (with a little care β remains positive). $\square$

By (4) $\phi_{B,f_{0,m}}(w) = \phi_{B,f_{m,0}}(-w)$. So it remains only to investigate $\phi_{B,f_{n,m-n}}$ when $0 < n < m$. For $T \in O_{n,m-n}$ and any open neighbourhood B of $\mathbf{0}$

$$\begin{aligned}\Phi_{B,f_{n,m-n}} &= \Phi_{T^{-1}B,f_{n,m-n}\circ T} = \Phi_{B,f_{n,m-n}\circ T} + \Phi_{T^{-1}B-B,f_{n,m-n}\circ T}\\ &\quad -\Phi_{B-T^{-1}B,f_{n,m-n}\circ T},\end{aligned}$$

where the last two terms on the right are C^∞ by Lemma 2. So $\Phi_{B,f_{n,m-n}} - \Phi_{B,f_{n,m-n}\circ T}$ is C^∞. Suppose ψ is rapidly decreasing [1, X.6]: by Lemma 2 this can be enforced at the expense of adding a C^∞ function to $\Phi_{B,f}$. Define C^∞ $O_{n,m-n}$-invariant (but not rapidly decreasing) $\psi_{\text{av},n,m-n} : \mathbb{R}^m \to (0, \infty)$ by taking $\psi_{\text{av},n,m-n} \circ S_{n,m-n}(y, z)$ as

$$\frac{\int_{-\infty}^{\infty}\int_{O_n}\int_{O_{m-n}} \psi \circ S_{n,m-n}(T(y)\cosh s + U(z)\sinh s, T(y)\sinh s + U(z)\cosh s)\, dT\, dU\, ds}{\int_{\mathbb{R}^m} \psi(x)\, d\lambda_m},$$

where integration over $T \in O_n$ and $U \in O_{m-n}$ is with respect to normalized Haar measures. Notice $\psi_{\text{av},n,m-n} = \psi_{\text{av},m-n,m}$. Then $\bar{\psi}_{n,m-n} \equiv \psi_{\text{av},n,m-n} \circ S_{n,m-n}|\mathbb{R} \times \{\mathbf{0}\} \times \mathbb{E}^{m-n} \cong \mathbb{R} \to (0, \infty)$ is C^∞ even and integrable. So by Lemma 5 $\bar{\psi}_{n,m-n}(v) = \beta_{n,m-n}(v^2)$ where $\beta_{n,m-n} : \mathbb{R} \to \mathbb{R}$ is C^∞ and $\beta_{n,m-n} = \beta_{m-n,n}$.

Theorem 2. *For $0 < n < m$, let B be the unbounded open neighbourhood $f_{n,m-n}^{-1}(-\delta^2, \delta^2)$ of $\mathbf{0}$ in $\mathbb{R}^m$. Let $B_E \subset B$ be the open Euclidean ball in $\mathbb{E}^m$ with centre $\mathbf{0}$ and radius δ. For $0 < |w| < \delta^2$,*

$$\begin{aligned}\phi_{B,f_{n,m-n}}(w) &= \phi_{B-B_E,f_{n,m-n}}(w) + \beta_{n,m-n}\left(\sqrt{|w|}\right)\frac{n(m-n)\kappa_n\kappa_{m-n}}{2}\\ &\quad \times|w|^{\frac{m}{2}-1}I_{n,m-n}(t_*),\end{aligned}$$

where $t^* \equiv -\frac{1}{2}\ln 2|w| + \ln(\sqrt{\delta^2 + w} + \sqrt{\delta^2 - w})$ and $I_{n,m-n}$ is defined for Proposition 5.

Proof of Theorem 2. Because $f_{n,m-n}$ and B are $O_{n,m-n}$-invariant ψ can be replaced by $\psi_{\text{av},n,m-n}$ in the integral for $\Phi_{B,f_{n,m-n}}(w)$. Now compare with Proposition 5 (where ψ is constant). $\square$

Note that by Lemma 2 $\phi_{B-B_E,f_{n,m-n}}$ is C^∞.

Acknowledgements

I want to thank two anonymous referees for their very careful readings and many constructive comments.

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