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# Stein estimation of the intensity of a spatial homogeneous Poisson point process

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## Abstract

In this paper, we revisit the original ideas of Stein and propose an estimator of the intensity parameter of a homogeneous Poisson point process defined in  $\mathbb{R}^d$  and observed in a bounded window. The procedure is based on a new general integration by parts formula for Poisson point processes. We show that our Stein estimator outperforms the maximum likelihood estimator in terms of mean squared error. In particular, we show that in many practical situations we have a gain larger than 30%.

*Keywords:* Stein equation; Malliavin derivative; superefficient estimator; intensity estimation; spatial point process.

## 1 Introduction

Spatial point processes are stochastic processes modeling points at random locations in arbitrary domains. General references on this topic are Daley and Vere-Jones (2008); Stoyan et al. (1995); Møller and Waagepetersen (2004) who cover theoretical as well as practical aspects. Among all models, the reference is the Poisson point process, which models points without any interaction. When the Poisson point process has a probability measure invariant under translation, we say that it is stationary or homogeneous. In this paper, we consider, a homogeneous Poisson point process defined on  $\mathbb{R}^d$  and observed over a bounded window  $W \subset \mathbb{R}^d$ , characterized by the single intensity parameter  $\theta > 0$ , which is the mean number of points per unit volume. It is well-known that the maximum likelihood estimator of the parameter  $\theta$ , defined as the ratio of the number of points lying in  $W$  divided by its volume, is unbiased and efficient. In this work, we explain how to build superefficient and therefore biased estimators of  $\theta$  by revisiting the original ideas of Stein.

Based on the pioneering works (Stein, 1956; James and Stein, 1961), Stein (1981) explained how to design a whole collection of estimators for the mean of Gaussian random vectors by using the famous Stein formula for Normal random variables: for

any differentiable function  $g : \mathbb{R} \rightarrow \mathbb{R}$  such that  $\mathbb{E}(|g'(X)|) < +\infty$ , where  $X$  is a standard Normal random variable, the following integration by parts formula holds

$$\mathbb{E}(g'(X)) = \mathbb{E}(Xg(X)). \quad (1.1)$$

Stein suggested to consider estimators of the form  $X + \nabla \log f(X)$  for sufficiently smooth and positive functions  $f$ . For this class of estimators, he showed using (1.1) that the mean squared error is related to the expectation of  $\nabla^2 \sqrt{f(X)}/\sqrt{f(X)}$  thus providing an easy construction of estimators achieving a mean squared error smaller than the one of the maximum likelihood estimator.

A close look at the methodology developed by Stein reveals the key role played by the integration by parts formula (1.1), in which the involved differential operator is the classical notion of derivative. This remark proved to be of prime importance as these computations rely on the standard chain rule for the derivative operator related to the integration by parts formula. Hence, to extend this methodology to other frameworks, one first needs a derivative operator satisfying the classical chain rule and second an integration by parts formula for this operator. In the case of Gaussian processes, these objects are defined by the Malliavin calculus and Stein estimators have been proposed by Privault and Réveillac (2006), Privault and Réveillac (2008).

Let us focus on the Poisson case. An integration by parts formula already exists for functions of Poisson random variables. Let  $Y$  be a Poisson random variable with parameter  $\lambda$  and  $f$  a sufficiently integrable real valued function, then it is known from Chen (1975) that  $\mathbb{E}(Yf(Y)) = \lambda \mathbb{E}(f(Y + 1))$ . However, this formula involves a discrete derivative operator which does not satisfy the standard chain rule and which, therefore, cannot be used as the basement for designing new estimators. Privault and Réveillac (2009) tackled this problem in the case of a one-dimensional Poisson process but their derivative operator cannot be extended to spatial Poisson point processes. We aim at filling this gap in the present paper.

To develop the so-called Stein methodology on the Poisson space, we design, in Section 2, a derivative operator for functionals of a homogeneous Poisson point process, which satisfies the classical chain rule and leads to an integration by parts formula in Section 3. These two sections heavily rely on the theory of closable and adjoint operators, which makes some of the proofs become technical. We have decided to gather all these technicalities in Appendix to avoid being diverted from our main objective, namely devising superefficient estimators on the Poisson space. Based on this integration by parts formula and its related derivative operator, we propose in Section 4 a wide class of Stein estimators and study their mean squared errors. In Section 5, we lead a detailed numerical study of our Stein estimator in several realistic examples. In particular, we explain how to pick in practice the estimator with minimum mean squared error within a given class and in the one-dimensional case, we compare it to the estimator proposed by Privault and Réveillac (2009).

## 2 Background and notation

### 2.1 Some notation

Elements of  $\mathbb{R}^d$  are encoded as column vectors, i.e. if  $x \in \mathbb{R}^d$ ,  $x = (x_1, \dots, x_d)^\top$  and we denote their Euclidean norms by  $\|x\|^2 = x^\top x = \sum_{i=1}^d x_i^2$ . Let  $W$  be a bounded open set of  $\mathbb{R}^d$ . For any  $k \in \mathbb{N}$ , the set  $\mathcal{C}^k(W, \mathbb{R}^p)$  (resp.  $\mathcal{C}_c^k(W, \mathbb{R}^p)$ ) denotes the class of  $k$ -times continuously differentiable functions defined on  $W$  with values in  $\mathbb{R}^p$  (resp. in a compact subset of  $\mathbb{R}^p$ ). Let  $f : W \rightarrow \mathbb{R}$  be a locally integrable function. A function  $h$  is said to be the weak derivative on  $W$  of  $f$  w.r.t.  $x_i$  if for any  $\varphi \in \mathcal{C}_c^1(W, \mathbb{R})$ , we have

$$\int_W h(x)\varphi(x)dx = - \int_W f(x)\frac{\partial\varphi(x)}{\partial x_i}dx.$$

When such a function  $h$  exists, it is unique a.e. and we denote it by  $\partial f/\partial x_i$  in the sequel. When  $d = 1$ , we use the classical notation  $f'$  to denote the weak derivative of the function  $f$ . When all the weak partial derivatives of a real-valued and locally integrable function  $f$  defined on  $W$  exist, we can define its weak gradient on  $W$  as

$$\nabla f(x) = \left( \frac{\partial f}{\partial x_1}(x), \dots, \frac{\partial f}{\partial x_d}(x) \right)^\top, \quad \forall x \in \mathbb{R}^d. \quad (2.1)$$

For a locally integrable vector field  $V = (V_1, \dots, V_d)^\top$  defined from  $W$  into  $\mathbb{R}^d$  such that for all  $i$ ,  $V_i$  admits a weak partial derivative w.r.t. to  $x_i$ , we define the weak divergence of  $V$  on  $W$  as

$$\nabla \cdot V(x) = \sum_{i=1}^d \frac{\partial V_i}{\partial x_i}(x), \quad \forall x \in \mathbb{R}^d. \quad (2.2)$$

### 2.2 Poisson point processes on $\mathbb{R}^d$

For a countable subset  $\mathbf{x}$  of  $\mathbb{R}^d$ , we denote by  $n(\mathbf{x})$  the number of elements in  $\mathbf{x}$ . For any bounded Borel set  $B$  of  $\mathbb{R}^d$ ,  $\mathbf{x}_B$  stands for  $\mathbf{x} \cap B$ . We define the set of locally finite configurations of points by  $N_{lf} = \{\mathbf{x} \subset \mathbb{R}^d : n(\mathbf{x} \cap B) < \infty \text{ for all bounded sets } B \subset \mathbb{R}^d\}$ . We equip  $N_{lf}$  with the  $\sigma$ -algebra  $\mathcal{N}_{lf} = \sigma(\{\mathbf{x} \in N_{lf} : n(\mathbf{x}_B) = m\} : B \in \mathcal{B}_0, m \in \mathbb{N} \setminus \{0\})$  where  $\mathcal{B}_0$  is the class of bounded Borel sets of  $\mathbb{R}^d$ . Then, a spatial point process  $\mathbf{X}$  on  $\mathbb{R}^d$  is simply a measurable mapping on some probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and taking values in  $(N_{lf}, \mathcal{N}_{lf})$ .

Let  $W \subset \mathbb{R}^d$  be a compact set with positive Lebesgue measure  $|W|$  playing the role of the observation window of  $\mathbf{X}$ . Then, the number of points in  $\mathbf{X}_W$  is finite; we denote this number by  $N(W) = n(\mathbf{X}_W)$ ; a realization of  $\mathbf{X}_W$  is of the form  $\mathbf{x} = \{x_1, \dots, x_n\} \subset W$ , for some  $0 \leq n < \infty$ . If  $n = 0$ , then  $\mathbf{x} = \emptyset$  is the empty point pattern in  $W$ . For further background material and theoretical details on spatial point process, see e.g. Daley and Vere-Jones (2003, 2008) and Møller and Waagepetersen (2004). Given  $N(W) = n$ , we denote by  $X_1, \dots, X_n \in W$  the  $n$  location points.

In this paper,  $\mathbf{X}$  is a homogeneous Poisson point process, defined on  $\mathbb{R}^d$ , observed in  $W$  and with intensity parameter  $\theta > 0$ . Remember that the distribution of  $\mathbf{X}$  is entirely characterized by the void probabilities  $\mathbb{P}(\mathbf{X} \cap B = \emptyset) = e^{-\theta|B|}$  for any bounded  $B \subset \mathbb{R}^d$ . The more standard properties are: (i)  $N(B)$  follows a Poisson distribution with parameter  $\theta|B|$  for any bounded  $B$ . (ii) For  $B_1, B_2, \dots$  disjoint sets of  $\mathbb{R}^d$ ,  $N(B_1), N(B_2), \dots$  are independent random variables. As a consequence, we have for any  $F \subset N_{lf}$  and any bounded  $B \subset \mathbb{R}^d$

$$\mathbb{P}(X_B \in F) = \sum_{n \geq 0} \frac{\theta^n e^{-\theta|B|}}{n!} \int \dots \int 1(\{x_1, \dots, x_n\} \in F) dx_1 \dots dx_n.$$

### 2.3 Poisson functionals and Malliavin derivative

We introduce the space  $\mathcal{S}$  of Poisson functionals defined on  $\Omega$

$$\mathcal{S} = \left\{ F = f_0 1(N(W) = 0) + \sum_{n \geq 1} 1(N(W) = n) f_n(X_1, \dots, X_n), \right. \\ \left. \text{with } f_0 \in \mathbb{R}, \forall n \geq 1 f_n : W^n \longrightarrow \mathbb{R} \text{ are symmetric} \right\}. \quad (2.3)$$

The functions  $f_n$  are called the form functions of the Poisson functional  $F$ . Since  $\mathbf{X}$  is a Poisson point process, we have

$$\mathbb{E}[F] = e^{-\theta|W|} f_0 + e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \int_{W^n} f_n(z_1, \dots, z_n) dz_1 \dots dz_n. \quad (2.4)$$

In the following, we use the concise notation  $L^2(\Omega)$  to denote the space  $L^2(\Omega, \mathcal{F}, \mathbb{P})$ . With this definition,  $L^2(\Omega) = \{F \in \mathcal{S} : \forall n \geq 0, f_n \in L^2(W^n, \mathbb{R})\}$  and the  $L^2(\Omega)$ -norm writes for any  $F \in L^2(\Omega)$

$$\|F\|_{L^2(\Omega)} = \left( e^{-\theta|W|} f_0^2 + e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \int_{W^n} f_n^2(z_1, \dots, z_n) dz_1 \dots dz_n \right)^{1/2}.$$

In view of the expression of this norm, the convergence in  $L^2(\Omega)$  is linked to the convergence of the form functions.

**Lemma 2.1.** *Let  $\ell \geq 1$ ,  $F, F_\ell \in \mathcal{S}$  and  $(f_{n,\ell})$  (resp  $f_n$ ) be the form functions of the Poisson functionals  $F_\ell$  (resp  $F$ ). We have  $F_\ell \rightarrow F$  in  $L^2(\Omega)$  iff  $\forall n \geq 1, f_{n,\ell} \rightarrow f_n$  in  $L^2(W^n, \mathbb{R})$  as  $\ell \rightarrow \infty$ .*

The following subspace  $\mathcal{S}'$  of  $\mathcal{S}$  plays a crucial role in the sequel

$$\mathcal{S}' = \left\{ F \in \mathcal{S} : \forall n \geq 1, \forall i = 1, \dots, n, \right. \\ \left. z_i \in W \mapsto f_n(z_1, \dots, z_{i-1}, z_i, z_{i+1}, \dots, z_n) \in \mathcal{C}^1(W^n, \mathbb{R}) \right\}.$$

By Lemma 2.1 and since  $\mathcal{C}^1(W^n, \mathbb{R})$  is dense in  $L^2(W^n, \mathbb{R})$ ,  $\mathcal{S}'$  is also dense in  $L^2(\Omega)$ . We fix a real-valued function  $\pi$  defined on  $W^2$ , referred to as the weight function in the sequel. We assume that  $\pi$  is bounded on  $W^2$  and that for a.e.  $x \in W$ ,  $z \mapsto \pi(x, z)$

belongs to  $\mathcal{C}^1(W, \mathbb{R}^d)$ . For any  $x \in W$ , we denote by  $D_x^\pi$  the following differential operator defined for any  $F \in \mathcal{S}'$  by

$$D_x^\pi F = - \sum_{n \geq 1} 1(N(W) = n) \sum_{i=1}^n (\nabla_{x_i} f_n)(X_1, \dots, X_n) \pi(X_i, x) \quad (2.5)$$

where  $\nabla_{x_i} f_n$  stands for the gradient vector of  $x_i \mapsto f_n(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n)$ . The operator  $D^\pi$  is a Malliavin derivative satisfying the classical differentiation rules.

**Lemma 2.2.** *Let  $F, G \in \mathcal{S}'$  and  $g \in \mathcal{C}_b^1(\mathbb{R})$ . Then  $FG \in \mathcal{S}'$  and  $g(F) \in \mathcal{S}'$  and for any  $x \in W$*

$$D_x^\pi(FG) = (D_x^\pi F)G + F(D_x^\pi G) \quad \text{and} \quad D_x^\pi g(F) = g'(F)D_x^\pi F.$$

To have such rules, we had to consider a bespoke differential operator, which differs from the standard Malliavin derivative on the Poisson space (see e.g. Privault (1994)). Before establishing an integration by parts formula, we define the subset  $\text{Dom}(D^\pi)$  of  $\mathcal{S}'$  as

$$\text{Dom}(D^\pi) = \left\{ F \in \mathcal{S}' : \forall n \geq 1 \text{ and } z_1, \dots, z_n \in \mathbb{R}^d \right. \\ \left. f_{n+1}|_{z_{n+1} \in \partial W}(z_1, \dots, z_{n+1}) = f_n(z_1, \dots, z_n), f_1|_{z \in \partial W}(z) = f_0 \right\}. \quad (2.6)$$

and  $D^\pi F$  is the random field  $x \in W \mapsto D_x^\pi F$ . The operator  $D^\pi$  is defined from  $\text{Dom}(D^\pi) \subset \mathcal{S}'$  into  $L^2(\Omega, L^2(W, \mathbb{R}))$ , where  $L^2(\Omega, L^2(W, \mathbb{R}))$  is the space of random fields  $X$  defined on  $W$  such that  $\|X\|_{L^2(\Omega, L^2(W, \mathbb{R}))} = (\mathbb{E} [\int_W |X(x)|^2 dx])^{1/2} < \infty$ .

## 3 Integration by parts formula

### 3.1 Duality formula

In this section, we aim at extending the Malliavin derivative  $D^\pi$  to a larger class of Poisson functionals by using density arguments. We also prove an integration by parts formula for the Malliavin derivative, involving the extension  $\overline{D}^\pi$  of the operator  $D^\pi$  and its adjoint. We start with basic definitions of closable operators — i.e. operators which can be extended by density — and of the adjoint of a densely defined operator.

**Definition 3.1.** *Let  $H_1, H_2$  be two Hilbert spaces and  $T$  be a linear operator defined from  $\text{Dom}(T) \subset H_1 \rightarrow H_2$ . The operator  $T$  is said to be closable if and only if for any sequence  $(f_\ell) \subset \text{Dom}(T)$  such that  $f_\ell \rightarrow 0$  (in  $H_1$ ) and  $Tf_\ell \rightarrow g$  (in  $H_2$ ) then  $g = 0$ .*

The main point is that any closable operator  $T$  from  $\text{Dom}(T) \subset H_1 \rightarrow H_2$  can be extended by density. Set  $\text{Dom}(\overline{T}) = \{f \in H_1, \exists (f_\ell) \in \text{Dom}(T), f_\ell \rightarrow f \text{ in } H_1 \text{ and } (Tf_\ell) \text{ converges in } H_2\}$  and define for any  $f = \lim f_\ell \in \text{Dom}(\overline{T})$  with  $(f_\ell) \in \text{Dom}(T)$ ,  $\overline{T}f = \lim_{\ell \rightarrow \infty} Tf_\ell$ . Then, the operator  $\overline{T}$  is called the closure of  $T$ .

By the closability of  $T$ , the above limit does not depend on the chosen sequence  $(f_\ell)$ .

If we are given a linear operator  $T$  such that  $\overline{\text{Dom}(T)} = H_1$ , an element  $g$  of  $H_2$  is said to belong to  $\text{Dom}(T^*)$ , where  $T^*$  is the adjoint of  $T$ , if for any  $f \in \text{Dom}(T)$ , there exists some  $h \in H_1$  such that  $\langle Tf, g \rangle_{H_2} = \langle f, h \rangle_{H_1}$ . When such an  $h$  exists, the assumption  $\overline{\text{Dom}(T)} = H_1$  ensures it is unique and given by  $h = T^*g$ . The following duality relation between  $T$  and  $T^*$  holds:

$$\langle Tf, g \rangle_{H_2} = \langle f, T^*g \rangle_{H_1} \quad \forall (f, g) \in \text{Dom}(T) \times \text{Dom}(T^*). \quad (3.1)$$

In the case of the Malliavin derivative, this duality relation leads to an integration by parts formula.

**Theorem 3.2** (Duality relation). *The operator  $D^\pi$  is closable and admits a closable adjoint  $\delta^\pi$  from  $L^2(\Omega, L^2(W, \mathbb{R}^d))$  into  $L^2(\Omega)$  and the following duality relation holds:*

$$\mathbb{E} \left[ \int_W D_x^\pi F \cdot V(x) dx \right] = \mathbb{E} [F \delta^\pi(V)], \quad \forall F \in \text{Dom}(\overline{D^\pi}), \forall V \in \text{Dom}(\overline{\delta^\pi}). \quad (3.2)$$

If  $V \in L^\infty(W, \mathbb{R})$  then  $\mathcal{V} : W \rightarrow \mathbb{R}^d$ , defined by  $\mathcal{V}(u) = \int_W V(x) \pi(u, x) dx$ , is an element of  $\mathcal{C}^1(W, \mathbb{R}^d)$  and we have the following explicit expression for  $\delta^\pi$ :

$$\delta^\pi(V) = \sum_{u \in \mathbf{X}_W} \nabla \cdot \mathcal{V}(u) - \theta \int_W \nabla \cdot \mathcal{V}(u) du. \quad (3.3)$$

The proof of this result relies on the standard trace Theorem, recalled hereafter.

**Theorem 3.3.** *Let  $B$  be a bounded subset of  $\mathbb{R}^d$  with Lipschitz boundary and closure  $\overline{B}$ . Let  $\mathcal{V} = (\mathcal{V}_1, \dots, \mathcal{V}_d)^T \in \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}^d)$  be a vector field and  $g \in \mathcal{C}^1(\mathbb{R}^d, \mathbb{R})$  be a real-valued function. Then,*

$$\int_{\overline{B}} (\nabla g)(x) \cdot \mathcal{V}(x) dx = - \int_{\overline{B}} g(x) (\nabla \cdot \mathcal{V})(x) dx + \int_{\partial B} g(x) \mathcal{V}(x) \cdot \nu(dx) \quad (3.4)$$

where  $\nu$  stands for the outer normal to  $\partial B$ . When  $g \equiv 1$ , we get

$$\int_W \nabla \cdot \mathcal{V}(x) dx = \int_{\partial W} \mathcal{V}(x) \cdot \nu(dx). \quad (3.5)$$

*Proof of Theorem 3.2. Step 1 : weak duality relation.* Assume that  $F \in \mathcal{S}'$  and  $V \in L^\infty(W, \mathbb{R}^d)$ . Let us prove that (3.2) holds. Using standard results on Poisson processes, which are in particular justified by the fact that  $F \in \mathcal{S}'$ , we get

$$\begin{aligned} & \mathbb{E} \left[ \int_W D_x^\pi F \cdot V(x) dx \right] \\ &= -e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \sum_{i=1}^n \int_{W^n} \left( \int_W \nabla_{z_i} f_n(z_1, \dots, z_n) \cdot V(x) \pi(z_i, x) dx \right) dz_1 \dots dz_n \\ &= -e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \sum_{i=1}^n \int_{W^{n-1}} dz_1 \dots dz_{i-1} dz_{i+1} \dots dz_n \int_W \nabla_{z_i} f_n(z_1, \dots, z_n) \cdot \mathcal{V}(z_i) dz_i. \end{aligned}$$

Since  $\pi, V$  are both bounded on  $W$  and since for a.e.  $x \in W$ ,  $z \mapsto \pi(z, x)$  belongs to  $\mathcal{C}^1(W, \mathbb{R})$ , then  $\mathcal{V} \in \mathcal{C}^1(W, \mathbb{R})$ . Hence, we can apply Theorem 3.3. Using the compatibility conditions (2.6), we deduce that for  $i = 1, \dots, n$

$$\begin{aligned} & - \int_W \nabla_{z_i} f_n(z_1, \dots, z_n) \cdot \mathcal{V}(z_i) dz_i \\ &= \int_W f_n(z_1, \dots, z_n) \nabla \cdot \mathcal{V}(z_i) dz_i - \int_{\partial W} f_n(z_1, \dots, z_n) \mathcal{V}(z_i) d\nu_{z_i} \\ &= \int_W f_n(z_1, \dots, z_n) \nabla \cdot \mathcal{V}(z_i) dz_i - f_{n-1}(z_1, \dots, z_{n-1}) \int_W \nabla \cdot \mathcal{V}(u) du. \end{aligned}$$

The last equation comes from (3.5) and from the symmetry of the functions  $f_n$ . Therefore,

$$\begin{aligned} & \mathbb{E} \left[ \int_W D_x^\pi F \cdot V(x) dx \right] \\ &= e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \times \sum_{i=1}^n \int_{W^n} f_n(z_1, \dots, z_n) \nabla \cdot \mathcal{V}(z_i) dz_1 \dots dz_n \\ & \quad - e^{-\theta|W|} \sum_{n \geq 1} \frac{\theta^n}{n!} \times n \int_{W^{n-1}} f_{n-1}(z_1, \dots, z_{n-1}) \left( \int_W \nabla \cdot \mathcal{V}(u) du \right) dz_1 \dots dz_{n-1} \\ &= \mathbb{E} \left[ F \sum_{u \in \mathbf{X}_W} \nabla \cdot \mathcal{V}(u) \right] \\ & \quad - \theta e^{-\theta|W|} \left( \int_W \nabla \cdot \mathcal{V}(u) du \right) \sum_{n \geq 1} \frac{\theta^{n-1}}{(n-1)!} \int_{W^{n-1}} f_{n-1}(z_1, \dots, z_{n-1}) dz_1 \dots dz_{n-1}. \end{aligned}$$

The last equality ensues from the invariance of the functions  $f_n$  and the stability of the domain  $W^{n-1}$  by exchanging the coordinates. Then, we deduce the result.

*Step 2 : Extension of  $\delta^\pi$  on a dense subset of  $L^2(\Omega, L^2(W, \mathbb{R}^d))$ . Validity of (3.2) on this dense subset.* Remember that  $L^2(\Omega, L^2(W, \mathbb{R}^d)) = L^2(\Omega) \otimes L^2(W, \mathbb{R}^d)$ . Since  $\mathcal{S}'$  is a dense subset of  $L^2(\Omega)$  and  $L^\infty(W, \mathbb{R}^d)$  is a dense subset of  $L^2(W, \mathbb{R}^d)$ , we deduce that  $L^2(\Omega, L^2(W, \mathbb{R}^d)) = \overline{\mathcal{S}' \otimes L^\infty(W, \mathbb{R}^d)}$ . Now, we extend the operator  $\delta^\pi$  on  $\mathcal{S}' \otimes L^\infty(W, \mathbb{R}^d)$  and then prove (3.2) on this dense subset of  $L^2(\Omega, L^2(W, \mathbb{R}^d))$ . To this end, we consider  $G \in \mathcal{S}'$ ,  $V \in L^\infty(W, \mathbb{R}^d)$  and set

$$\delta^\pi(GV) = G\delta^\pi(V) - \int_{\mathbb{R}^d} D_x^\pi G \cdot V(x) dx.$$

Using the product rule, which is valid for any  $F, G \in \mathcal{S}'$ , we deduce that

$$\begin{aligned} \mathbb{E} \left[ G \int_W D_x^\pi F \cdot V(x) dx \right] &= \mathbb{E} \left[ \int_W D_x^\pi (FG) \cdot V(x) dx - F \int_W D_x^\pi G \cdot V(x) dx \right] \\ &= \mathbb{E} \left[ FG\delta^\pi(V) - F \int_W D_x^\pi G \cdot V(x) dx \right] \\ &= \mathbb{E} [F\delta^\pi(GV)]. \end{aligned}$$



The second equality comes from the duality relation (3.2) applied to  $FG$  as an element of  $\mathcal{S}'$  and  $V$  as an element of  $L^\infty(W, \mathbb{R}^d)$ , whereas the last equality comes directly from the definition of our extension of  $\delta^\pi$  to  $\mathcal{S}' \otimes L^\infty(W, \mathbb{R}^d)$ .

*Step 3 : closability of the operator  $D^\pi$  and extension of (3.2) to  $L^2(\Omega, L^2(W, \mathbb{R}^d))$ .* We extend (3.2) from  $\mathcal{S}' \otimes L^\infty(W, \mathbb{R}^d)$  to  $L^2(\Omega, L^2(W, \mathbb{R}^d))$  by proving that the operator  $D^\pi$  is closable. Since  $\mathcal{S}' \otimes L^\infty(W, \mathbb{R}^d)$  is dense in  $L^2(\Omega, L^2(W, \mathbb{R}^d))$ , Theorem 3.4 justifies the extension of the duality relation (3.2) to  $\text{Dom}(\overline{D^\pi}) \times \text{Dom}(\overline{\delta^\pi})$  as stated in Theorem 3.2.

To prove that  $D^\pi$  is closable, we consider  $(F_\ell) \subset \mathcal{S}'$  such that  $F_\ell \rightarrow 0$  in  $L^2(\Omega)$ . Assume also that  $D^\pi F_\ell \rightarrow U$  for some  $U$  in  $L^2(\Omega, L^2(W, \mathbb{R}^d))$ . Then, we need to prove that  $U = 0$ , which is done using the following computations for any  $G \in \mathcal{S}'$  and any  $V \in L^\infty(W, \mathbb{R}^d)$

$$\begin{aligned}
& \left| \mathbb{E} \left[ \int_W U(x)GV(x)dx \right] \right| \\
& \leq \left| \mathbb{E} [F_\ell \delta^\pi(GV)] - \mathbb{E} \left[ \int_{\mathbb{R}^d} U(x)GV(x)dx \right] \right| + |\mathbb{E} [F_\ell \delta^\pi(GV)]| \\
& \leq \left| \mathbb{E} \left[ G \int_W D_x^\pi F_\ell \cdot V(x)dx \right] - \mathbb{E} \left[ G \int_W U(x)V(x)dx \right] \right| + |\mathbb{E} [F_\ell \delta^\pi(GV)]| \\
& \leq \|G\|_{L^2(\Omega)} \left\| \int_W (D_x^\pi F_\ell - U(x)) \cdot V(x)dx \right\|_{L^2(\Omega)} + \|F_\ell\|_{L^2(\Omega)} \|\delta^\pi(GV)\|_{L^2(\Omega)} \\
& \leq \|G\|_{L^2(\Omega)} \|V\|_{L^2(W, \mathbb{R}^d)} \|D_x^\pi F_\ell - U(x)\|_{L^2(\Omega, L^2(W, \mathbb{R}^d))} + \|F_\ell\|_{L^2(\Omega)} \|\delta^\pi(GV)\|_{L^2(\Omega)}.
\end{aligned}$$

The conclusion ensues from Theorem 7 of Chapter 2 of Birman and Solomjak (1987), which is rephrased in Theorem 3.4 for the sake of completeness. Equation (3.2) is recovered by applying Theorem 3.4 with  $T^* = \delta^\pi$ ,  $T = D^\pi$ ,  $H_1 = L^2(\Omega, L^2(W, \mathbb{R}))$  and  $H_2 = L^2(\Omega)$ .  $\square$

**Theorem 3.4.** *Let  $H_1, H_2$  be two Hilbert spaces and  $T$  be a linear operator defined from  $\text{Dom}(T) \subset H_1 \rightarrow H_2$ . Assume that  $\overline{\text{Dom}(T)} = H_1$ . Then,  $\overline{\text{Dom}(T^*)} = H_2$  if and only if  $T$  is closable. In this case,  $T^{**}$  exists and coincides with  $\overline{T}$ . Then, Relation (3.1) can be extended as follows:  $\langle f, T^*g \rangle_{H_1} = \langle \overline{T}f, g \rangle_{H_2}$ ,  $\forall (f, g) \in \text{Dom}(\overline{T}) \times \text{Dom}(T^*)$ .*

For any  $F \in \text{Dom}(D^\pi)$  and any  $V \in L^2(\Omega, L^2(W, \mathbb{R}^d))$ , we define the operator  $\nabla^{\pi, V} : \text{Dom}(D^\pi) \rightarrow \mathbb{R}$  by

$$\nabla^{\pi, V} F = \int_W D_x^\pi F \cdot V(x)dx = - \sum_{n \geq 1} 1(N(W) = n) \sum_{i=1}^n \nabla_{x_i} f_n(X_1, \dots, X_n) \cdot \mathcal{V}(X_i). \tag{3.6}$$

Note that the closability of  $D^\pi$  implies the one of the operator  $\nabla^{\pi, V}$ .

## 3.2 A specific choice for $\pi$ and $V$

In this section, we focus on a specific choice of functions  $\pi$  and  $V$  leading to a specific definition of the gradient of a Poisson functional. This choice is guided by

two important remarks. First, Lemma 3.5 will underline that the key-ingredient to derive a superefficient estimator is to define a gradient  $\nabla^{\pi, V}$  such that

$$\mathbb{E}[\nabla^{\pi, V} F] = \mathbb{E}[F(N(W) - \theta|W|)]. \quad (3.7)$$

From (3.6) and Theorem 3.2, this is achieved if  $\nabla \cdot \mathcal{V} \equiv 1$ . Second, to agree with the isotropic nature of the homogeneous Poisson point process, it is natural to define a Stein estimator being also isotropic. As pointed out by Proposition 4.2, this can be achieved by defining a Malliavin derivative which transforms an isotropic Poisson functional into an isotropic Poisson functional at any point. We do not want to go into these details right now but Lemma 4.4 suggests to require that both  $\pi$  and  $V$  be isotropic. Now, we explicit a pair of functions  $(\pi, V)$  satisfying the above requirements.

**Proposition 3.5.** *For  $m \in \{1, \dots, d\}$ , let  $V_m : W \rightarrow \mathbb{R}$  be bounded functions satisfying the following two relations*

$$\begin{aligned} \int_W V_m^2(x) dx &= 1, \quad \forall m \in \{1, \dots, d\} \\ V_m V_{m'} &\equiv 0, \quad \forall (m, m') \in \{1, \dots, d\}^2 \text{ such that } m \neq m'. \end{aligned}$$

For any  $x, y \in \mathbb{R}^d$ , set  $V(x) = d^{-1/2}(V_1(x), \dots, V_d(x))^\top$  and  $\pi(y, x) = y^\top V(x)$ . Then,  $\mathcal{V}(y) = y/d$ , which implies that  $\nabla \cdot \mathcal{V} \equiv 1$ . With the above choices, we simply denote  $D = D^\pi$ ,  $\nabla = \nabla^{\pi, V}$ . From (3.6), we deduce that

$$\nabla F = -\frac{1}{d} \sum_{n \geq 1} 1(N(W) = n) \sum_{i=1}^n \nabla_{x_i} f_n(X_1, \dots, X_n) \cdot X_i \quad (3.8)$$

where the gradient of a real-valued function is given by (2.1). Finally, for any  $F \in \text{Dom}(\overline{D})$ , (3.7) holds.

*Proof.* By definition, we have for any  $y = (y_1, \dots, y_d)^\top \in \mathbb{R}^d$  and any  $m \in \{1, \dots, d\}$

$$\begin{aligned} \mathcal{V}_m(y) &= \int_{\mathbb{R}^d} V_m(x) \pi(y, x) dx = d^{-1} \int_W \left( \sum_{m'} y_{m'} V_{m'}(x) \right) V_m(x) dx \\ &= d^{-1} \int_W \left( \sum_{m'} y_{m'} V_{m'}(x) V_m(x) \right) dx = d^{-1} \int_W y_m V_m^2(x) dx = y_m/d. \end{aligned}$$

Plugging this result in Equation (3.6) yields (3.8). Equation (3.7) can be extended to  $\text{Dom}(\overline{D})$  using the closability of the operator  $\nabla$ , which follows from the one of  $\nabla^{\pi, V}$  in the general case.  $\square$

Again, we want to stress the fact that other choices of pairs of functions  $(\pi, V)$  may lead to (3.7) like the simple choice  $V(x) = (d|W|)^{-1/2}(1, \dots, 1)^\top 1(x \in W)$  and  $\pi(y, x) = y^\top V(x)$ . However, the gradient derived from this choice would not preserve the isotropy of an isotropic Poisson functional anymore and would lead to technical difficulties especially in the formulation of (4.13) in Lemma 4.4, which should take into account the jumps involved by the discontinuity of the form functions.

## 4 Stein estimator

### 4.1 Main results

In this section, we present a Stein estimator of the intensity  $\theta$  of a spatial Poisson point process. In particular, we investigate modifications of the maximum likelihood estimator of the form

$$\hat{\theta} = \hat{\theta}_{\text{MLE}} + \frac{1}{|W|}\zeta = \frac{1}{|W|}(N(W) + \zeta) \quad (4.1)$$

where the choice of the isotropic Poisson functional  $\zeta$  is discussed below. We aim at building an estimator with smaller mean squared error than the maximum likelihood estimator. By applying Proposition 3.5, we can link the mean squared errors of these two estimators.

**Lemma 4.1.** *Let  $\zeta \in \text{Dom}(\overline{D})$ . Consider  $\hat{\theta}$  defined by (4.1). Then,*

$$\text{MSE}(\hat{\theta}) = \text{MSE}(\hat{\theta}_{\text{MLE}}) + \frac{1}{|W|^2} (\mathbb{E}[\zeta^2] + 2\mathbb{E}[\nabla\zeta]). \quad (4.2)$$

*Proof.* By definition,

$$\begin{aligned} \text{MSE}(\hat{\theta}) &= \mathbb{E} \left[ \left( \hat{\theta}_{\text{MLE}} + \frac{1}{|W|}\zeta - \theta \right)^2 \right] \\ &= \text{MSE}(\hat{\theta}_{\text{MLE}}) + \frac{1}{|W|^2} (\mathbb{E}[\zeta^2] + 2\mathbb{E}[\zeta(N(W) - \theta|W|)]). \end{aligned}$$

Since  $\zeta \in \text{Dom}(\overline{D})$ , we can apply (3.7) with  $F = \zeta$  to deduce (4.2).  $\square$

Now, we consider a random variable  $\zeta$  written as  $\zeta = \zeta_0 1(N(W) = 0) + \nabla \log(F)$  where  $\zeta_0$  is a constant (possibly zero) and  $F$  an almost surely positive Poisson functional belonging to  $\mathcal{S}$ . Both  $\zeta_0$  and  $F$  are adjusted such that  $\zeta \in \text{Dom}(\overline{D})$ . Using Lemma 2.2, we can follow the initial calculations of Stein (1981), also used in Privault and Réveillac (2009), to deduce that  $\nabla \log F = \nabla F/F$  and  $\nabla \sqrt{F} = \nabla F/2\sqrt{F}$ . Using Lemma 2.2, we establish the key relations

$$\nabla \nabla \log F = \frac{F \nabla \nabla F - (\nabla F)^2}{F^2} \quad \text{and} \quad \nabla \nabla \sqrt{F} = \frac{2\sqrt{F} \nabla \nabla F - (\nabla F)^2/\sqrt{F}}{4F}$$

leading to

$$2\nabla \nabla \log F + \left( \frac{\nabla F}{F} \right)^2 = 4 \frac{\nabla \nabla \sqrt{F}}{\sqrt{F}}. \quad (4.3)$$

By combining (4.2) and (4.3), we obtain the following result.

**Proposition 4.2.** *Let  $\zeta_0 \in \mathbb{R}$  and  $F$  be an almost surely positive Poisson functional such that  $F$ ,  $\nabla F$  and  $\zeta = \zeta_0 1(N(W) = 0) + \nabla \log(F) \in \text{Dom}(\overline{D})$ . Then, the estimator  $\hat{\theta}$  defined from  $\zeta$  by (4.1) satisfies*

$$\text{MSE}(\hat{\theta}) = \text{MSE}(\hat{\theta}_{\text{MLE}}) + \frac{1}{|W|^2} \left( \zeta_0^2 e^{-\theta|W|} + 4\mathbb{E} \left( \frac{\nabla \nabla \sqrt{F}}{\sqrt{F}} \right) \right). \quad (4.4)$$

Proposition 4.2 gives a similar result to Privault and Réveillac (2009, Proposition 4.1) for one-dimensional Poisson point processes. As a consequence of Proposition 4.2, the Stein estimator given by (4.1) will be more efficient than the maximum likelihood estimator if we manage to find  $F$  and  $\zeta_0$  satisfying the conditions of Proposition 4.2 and such that  $\zeta_0^2 e^{-\theta|W|} + 4 \mathbb{E}(\nabla \nabla \sqrt{F} / \sqrt{F}) < 0$ . This is investigated in the next section.

## 4.2 A class of Stein estimators on the $d$ -dimensional Euclidean ball

In this section, we focus on the case where  $W$  is the  $d$ -dimensional Euclidean closed ball with center 0 and radius  $w$ , denoted  $\overline{B}(0, w)$  in the following. Without loss of generality, we can restrict to the case  $w = 1$ . We combine Proposition 4.2 and the isotropic Malliavin derivative defined in Section 2 to build a large class of isotropic Stein estimators. We need some additional notation. Let  $n \geq 1$ ,  $1 \leq k \leq n$  and let  $x_1, \dots, x_n \in W$ , we define  $x_{(k),n}$  by induction as follows

$$\begin{aligned} x_{(1),n} &= \operatorname{argmin}_{u \in \{x_1, \dots, x_n\}} \|u\|^2 \\ x_{(k),n} &= \operatorname{argmin}_{u \in \{x_1, \dots, x_n\} \setminus \{x_{(1),n}, \dots, x_{(k-1),n}\}} \|u\|^2. \end{aligned}$$

The point  $x_{(k),n}$  is the  $k$ -th closest point of  $\{x_1, \dots, x_n\}$  to zero. Similarly, we denote by  $X_{(k)}$  the  $k$ -th closest point of  $\mathbf{X}$  to zero. Note that, the point  $X_{(k)}$  may lie outside  $W$  depending on the value of  $N(W)$  for the given realization. We are also given some function  $\varphi \in \mathcal{C}^2([0, 1], \mathbb{R}^+)$  satisfying the two following additional properties

$$\inf_{t \in [0, 1]} \varphi(t) > 0 \text{ and } \varphi'(1) = 0. \quad (\mathcal{P})$$

Then, the Poisson functional involved in the definition of our Stein estimator writes

$$\sqrt{F}_k = \sum_{n \geq k} 1(N(W) = n) g_{k,n}(X_1, \dots, X_n) + \varphi(1) 1(N(W) < k) \quad (4.5)$$

where for  $x_1, \dots, x_n \in W$  and  $n \geq k \geq 1$

$$g_{k,n}(x_1, \dots, x_n) = \varphi(\|x_{(k),n}\|^2) \quad (4.6)$$

for a function  $\varphi$  satisfying  $(\mathcal{P})$ . In other words, we focus on functionals  $F \in \mathcal{S}'$  such that

$$\sqrt{F}_k = \sum_{n \geq k} 1(N(W) = n) \varphi(\|X_{(k),n}\|^2) + \varphi(1) 1(N(W) < k) \quad (4.7)$$

from which we build our main result.

**Proposition 4.3.** *Let  $k \geq 1$ . Let  $\varphi \in \mathcal{C}^2([0, 1], \mathbb{R}^+)$  satisfying  $(\mathcal{P})$ . Define  $F_k$  from  $\varphi$  as in (4.7). Then  $\zeta_k = \nabla \log F_k$  is an element of  $\operatorname{Dom}(\overline{D})$ . Moreover, the Stein*

estimator, its mean-squared error and its gain with respect to the maximum likelihood estimator are given by

$$\widehat{\theta}_k = \widehat{\theta}_{\text{MLE}} - \frac{4}{d|W|} \frac{Y_{(k)} \varphi'(Y_{(k)})}{\varphi(Y_{(k)})} \quad (4.8)$$

$$\text{MSE}(\widehat{\theta}_k) = \text{MSE}(\widehat{\theta}_{\text{MLE}}) - \frac{16}{d^2|W|^2} \mathbb{E} [\mathcal{G}(Y_{(k)})] \quad (4.9)$$

$$\text{Gain}(\widehat{\theta}_k) = \frac{\text{MSE}(\widehat{\theta}_{\text{MLE}}) - \text{MSE}(\widehat{\theta}_k)}{\text{MSE}(\widehat{\theta}_{\text{MLE}})} = \frac{16}{\theta d^2|W|} \mathbb{E} [\mathcal{G}(Y_{(k)})] \quad (4.10)$$

where

$$Y_{(k)} = 1 + (\|X_{(k)}\|^2 - 1)1(\|X_{(k)}\| \leq 1) = \begin{cases} \|X_{(k)}\|^2 & \text{if } \|X_{(k)}\| \leq 1 \\ 1 & \text{otherwise} \end{cases} \quad (4.11)$$

and  $\mathcal{G}(t) = -t \frac{\varphi'(t) + t\varphi''(t)}{\varphi(t)}$ .

Proposition 4.3 reveals the interest of the Poisson functional  $F_k$  given by (4.7). We obtain isotropic estimators of  $\theta$  depending only on  $\|X_{(k)}\|^2$ . It is worth mentioning that the distribution of  $\|X_{(k)}\|^2$  is well-known for a homogeneous Poisson point process (see Lemma 5.1). This allows us to derive efficient and fast estimates of  $\mathbb{E}[\mathcal{G}(Y_{(k)})]$  which can then be optimized w.r.t. the different parameters. This is studied in more details in Section 5.

The proof of Proposition 4.3 requires first to compute the gradient of the functions  $g_{k,n}$  given by (4.6) and second to ensure that  $\sqrt{F_k}$  belongs to  $\text{Dom}(\overline{D})$ . To this end, we use the following lemma.

**Lemma 4.4.** *Let  $\Psi$  be a function belonging to  $H^1([0, 1], \mathbb{R})$ . Then,*

$$G_k = \sum_{n \geq k} 1(N(W) = n) \Psi(\|X_{(k),n}\|^2) + \Psi(1)1(N(W) < k) \in \text{Dom}(\overline{D}) \quad (4.12)$$

and

$$\overline{\nabla} G_k = -\frac{2}{d} \sum_{n \geq k} 1(N(W) = n) \|X_{(k),n}\|^2 \Psi'(\|X_{(k),n}\|^2). \quad (4.13)$$

The proof of Lemma 4.4 being quite technical, we postpone it to Appendix B. Here, we only present the key ideas sustaining it.

*Sketch of the proof of Lemma 4.4.* Let  $n \geq k$  and  $x_{n+1} \in \partial W$ , i.e.  $\|x_{n+1}\| = 1$ , we have  $x_{(k),n+1} = x_{(k),n}$  and  $\Psi(\|x_{(k),n+1}\|^2) = \Psi(\|x_{(k),n}\|^2)$ , which is exactly the compatibility condition which has to be satisfied for  $n \geq k$  by the form functions of Poisson functionals belonging to  $\mathcal{S}'$ . When  $n = k - 1$  and  $x_{n+1} = x_k \in \partial W$ , i.e.  $\|x_k\| = 1$ , we still have  $x_{(k),k} = x_k$  and  $\Psi(\|x_{(k),k}\|^2) = \Psi(1)$ . Since for  $n < k$ , the forms functions are all equal to the constant function  $\Psi(1)$ , the compatibility conditions also hold for  $n = k - 1$  and  $n < k - 1$ .

At any point  $(x_1, \dots, x_n)$  such that  $(x_1, \dots, x_n) \mapsto \|x_{(k),n}\|^2$  is differentiable, the definition of the Malliavin derivative and the usual chain rule easily lead to (4.13).

Note that that even if  $\Psi \in \mathcal{C}^1(W, \mathbb{R})$ , the functional  $G_k$  may not belong to  $\text{Dom}(D)$  since its form functions are not differentiable everywhere. Indeed for any  $n \geq 1$ ,  $(x_1, \dots, x_n) \mapsto \|x_{(k),n}\|^2$  is not differentiable at any point  $(x_1, \dots, x_n)$  such that for some  $i \neq j$ ,  $\|x_i\| = \|x_j\| = \|x_{(k),n}\|$ . In Lemma 4.4, we prove a weaker assertion, namely that  $G_k \in \text{Dom}(\overline{D})$ , which means that  $G_k$  can be obtained as the limit of Poisson functionals of  $\text{Dom}(D)$ . Then, the proof of Lemma 4.4 relies on density results stated in Appendix C.

*Proof of Proposition 4.3.* By definition,

$$\log F_k = 2 \sum_{n \geq k} 1(N(W) = n) \log \varphi(\|X_{(k),n}\|^2) + \log \varphi(1) 1(N(W) < k).$$

Since  $\varphi$  is a continuously differentiable function, we can easily check that  $\Psi \in H^1([0, 1])$ . So Lemma 4.4 can be applied to  $\Psi = \log \varphi$  and  $G_k = \log(F_k)$ . Hence,  $\log F_k \in \text{Dom}(\overline{D})$  and

$$\zeta_k = \overline{\nabla} \log F_k = -\frac{4}{d} \sum_{n \geq k} 1(N(W) = n) \|X_{(k),n}\|^2 \frac{\varphi'(\|X_{(k),n}\|^2)}{\varphi(\|X_{(k),n}\|^2)}.$$

Then, we derive the explicit expression of  $\widehat{\theta}_k$  given by (4.8). We also deduce that  $\zeta_k = \nabla \log F_k \in \text{Dom}(\overline{D})$  by applying once more Lemma 4.4 with  $\Psi(t) = t\varphi'(t)/\varphi(t)$ , which also satisfies the required properties thanks to the smoothness of  $\varphi'$ . In view of Proposition 4.2, we estimate  $\nabla \nabla \sqrt{F_k}/\sqrt{F_k}$  to derive (4.9). From (4.5) and (4.6),  $\sqrt{F_k}$  also satisfies the assumptions of Lemma 4.4 with  $\Psi = \varphi$ . Hence  $\sqrt{F_k} \in \text{Dom}(\overline{D})$  and

$$\nabla \sqrt{F_k} = -\frac{2}{d} \sum_{n \geq k} 1(N(W) = n) \|X_{(k),n}\|^2 \varphi'(\|X_{(k),n}\|^2).$$

The conclusion ensues by applying Lemma 4.4 to  $G_k = \nabla \sqrt{F_k}$  with  $\Psi(t) = -2t\varphi'(t)/d$  and we obtain the following formulae.

$$\begin{aligned} \nabla \nabla \sqrt{F_k} &= \frac{4}{d^2} \sum_{n \geq k} 1(N(W) = n) [\|X_{(k),n}\|^2 \varphi'(\|X_{(k),n}\|^2) + \|X_{(k),n}\|^4 \varphi''(\|X_{(k),n}\|^2)] \\ \frac{\nabla \nabla \sqrt{F_k}}{\sqrt{F_k}} &= \frac{4}{d^2} \sum_{n \geq k} 1(N(W) = n) \frac{[\|X_{(k),n}\|^2 \varphi'(\|X_{(k),n}\|^2) + \|X_{(k),n}\|^4 \varphi''(\|X_{(k),n}\|^2)]}{\varphi(\|X_{(k),n}\|^2)}. \end{aligned}$$

Then (4.9) follows from the last equality, while (4.10) is directly deduced from (4.9).  $\square$

## 5 Numerical experiments

We underline that it is impossible to find a function  $\varphi$  satisfying  $(\mathcal{P})$  and such that  $\mathcal{G}(t)$  defined by (4.10) is positive for any  $t \in [0, 1]$ . In this section, we analyze two examples for which we can obtain positive gain even though  $\mathcal{G}$  is not positive everywhere. Then, we conduct a numerical and simulation study where, in particular, we show that in many practical situations we can get a gain larger than 30%.

Before this, we should notice that the mean squared error and the gain of our new estimators  $\widehat{\theta}_k$  only depend on the distribution of  $\|X_{(k)}\|^2$ . The following result shows that expectations involving this random variable can be computed directly without sampling a Poisson point process, which speeds up the simulations a lot.

**Lemma 5.1.** *Let  $k \geq 1$ , then the density of  $\|X_{(k)}\|^2$  is given by*

$$f_{\|X_{(k)}\|^2}(t) = \frac{d}{2} v_d \theta t^{-1} e^{v_d \theta t^{d/2}} \frac{(v_d \theta t^{d/2})^{k-1}}{(k-1)!} 1(t \geq 0)$$

where  $v_d = \pi^{d/2} \Gamma(d/2 + 1) w^d$  is the volume of  $\overline{B}(0, w)$ . Moreover, for any positive measurable function  $h : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ , we have  $\mathbb{E}(h(\|X_{(k)}\|^2)) = \mathbb{E}(h(Z^{2/d}))$  where  $Z$  is a real valued random variable following a Gamma distribution with shape  $k$  and rate  $v_d \theta$ .

## 5.1 First example

Let  $\kappa > 0$  and  $\gamma \in (0, 1/2)$ , we define for  $t \in [0, 1]$

$$\varphi(t) = (1-t)(\chi_{[0, 1-\gamma]} * \psi)(t) + \kappa \quad (5.1)$$

where, for any measurable set  $A$ ,  $\chi_A = 1(t \in A)$  denotes the characteristic function of the set  $A$  and the star  $*$  stands for the convolution product. The Schwarz function (see e.g. Hörmander (2003))  $\psi : [-1, 1] \rightarrow \mathbb{R}^+$ , defined by

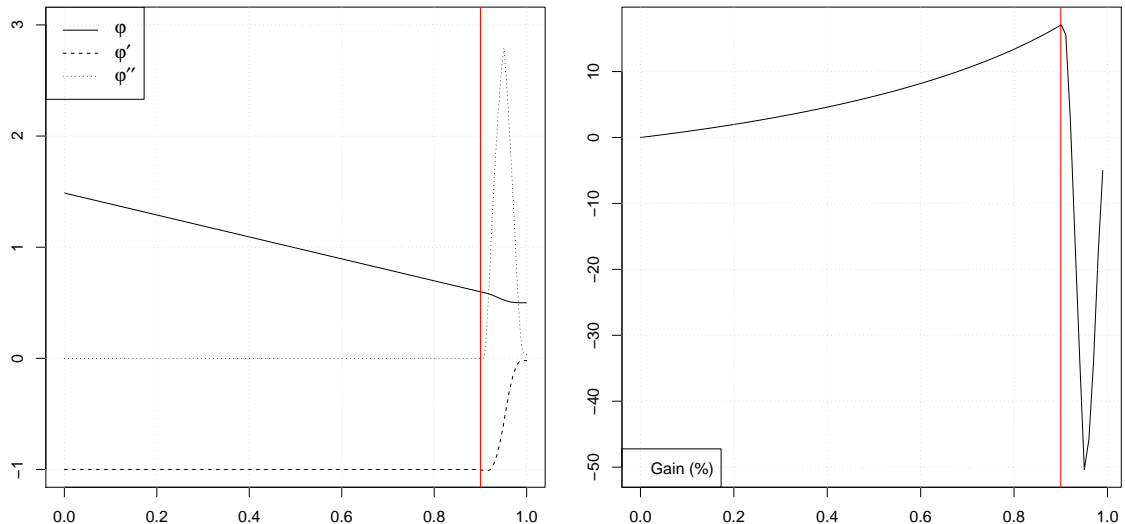
$$\psi(t) = c \exp\left(-\frac{1}{1-|t|}\right) \text{ with } c \text{ such that } \int_0^1 \psi(t) dt = 1$$

satisfies  $\psi \geq 0$  and  $\psi^{(m)}(\pm 1) = 0$  for any  $m \geq 0$ , which implies that  $\varphi$  satisfies  $(\mathcal{P})$ . The main interest of this function is that for any  $t \in [0, 1 - 2\gamma]$ ,  $\varphi(t) = 1 - t + \kappa$ ,  $\varphi'(t) = -1$  and  $\varphi''(t) = 0$  which leads to  $\mathcal{G}(t) = t/(1-t+\kappa) \geq 0$  for any  $t \in [0, 1 - 2\gamma]$ . Figure 1 illustrates this function  $\varphi$  with  $\kappa = 0.5$  and  $\gamma = 0.05$ . We can observe that  $\mathcal{G}(t) \geq 0$  for  $t \leq 0.9$  but  $\mathcal{G}(t)$  can be highly negative for  $t > 0.9$ . Note also that the smaller  $\gamma$ , the more negative  $\mathcal{G}$ . This highlights the danger of Example 1. From a practical point of view, the best choice would be to tune the integer  $k$  such that  $\|X_{(k)}\|^2$  often lies in a region in which  $\mathcal{G}$  is high, however this region is quite small and the function  $\mathcal{G}$  decreases quickly outside of it and takes highly negative values, which may yield to negative gains in the end. On the contrary, if reasonable values are chosen for  $\gamma$  and  $k$  is small then there is hardly no chance that  $\|X_{(k)}\|^2 > 1 - 2\gamma$  but the corresponding gain value remains very small. This first example shares some similarities with the estimator proposed by Privault and Réveillac (2009) in the case  $d = 1$ , see Section 5.4.

## 5.2 Second example

Let  $\kappa \geq 2$  and  $\gamma \in \mathbb{R}$ , we define for  $t \in [0, 1]$

$$\varphi(t) = \exp(\gamma(1-t)^\kappa). \quad (5.2)$$



**Figure 1:** Plots of  $\varphi, \varphi', \varphi''$  and  $\mathcal{G}$  for the function  $\varphi$  defined by (5.1) with  $\kappa = 0.5$  and  $\gamma = 0.05$ . The vertical line indicates the value  $1 - 2\gamma = 0.9$  before which the function  $\varphi$  is linear.

We can easily check that the property  $(\mathcal{P})$  holds for any  $\kappa \geq 2$ . The main advantage of this function is that the gain function has a “power” shape. For instance, when  $\kappa = 2$ ,  $\mathcal{G}(t) = 2\gamma t(1 - 2t - 2\gamma t(1 - t)^2)$ . For any value of  $\kappa$ , we can show that there exists a unique  $t_0 \in (0, 1)$  such that  $\mathcal{G}(t_0) = 0$  and such that  $\text{sign}(\mathcal{G}) = \text{sign}(\gamma)$  for  $t \in [0, t_0)$  and  $\text{sign}(\mathcal{G}) = \text{sign}(-\gamma)$  for  $t \in (t_0, 1]$ . Figure 2 illustrates this function. The top-right figure reveals the interest of Example 2. It shows that when  $k$  is chosen large enough, then  $\|X_{(k)}\|^2 > t_0$  very often and therefore  $\mathcal{G}(t)$  is quite large.

The latter comment is the main reason why among these two examples (and many others we have tried) the exponential function (5.2) produces the best and the most stable empirical results. Thus, we only focus on this case in the following. With this choice for the function  $\varphi$ , the Stein estimator writes

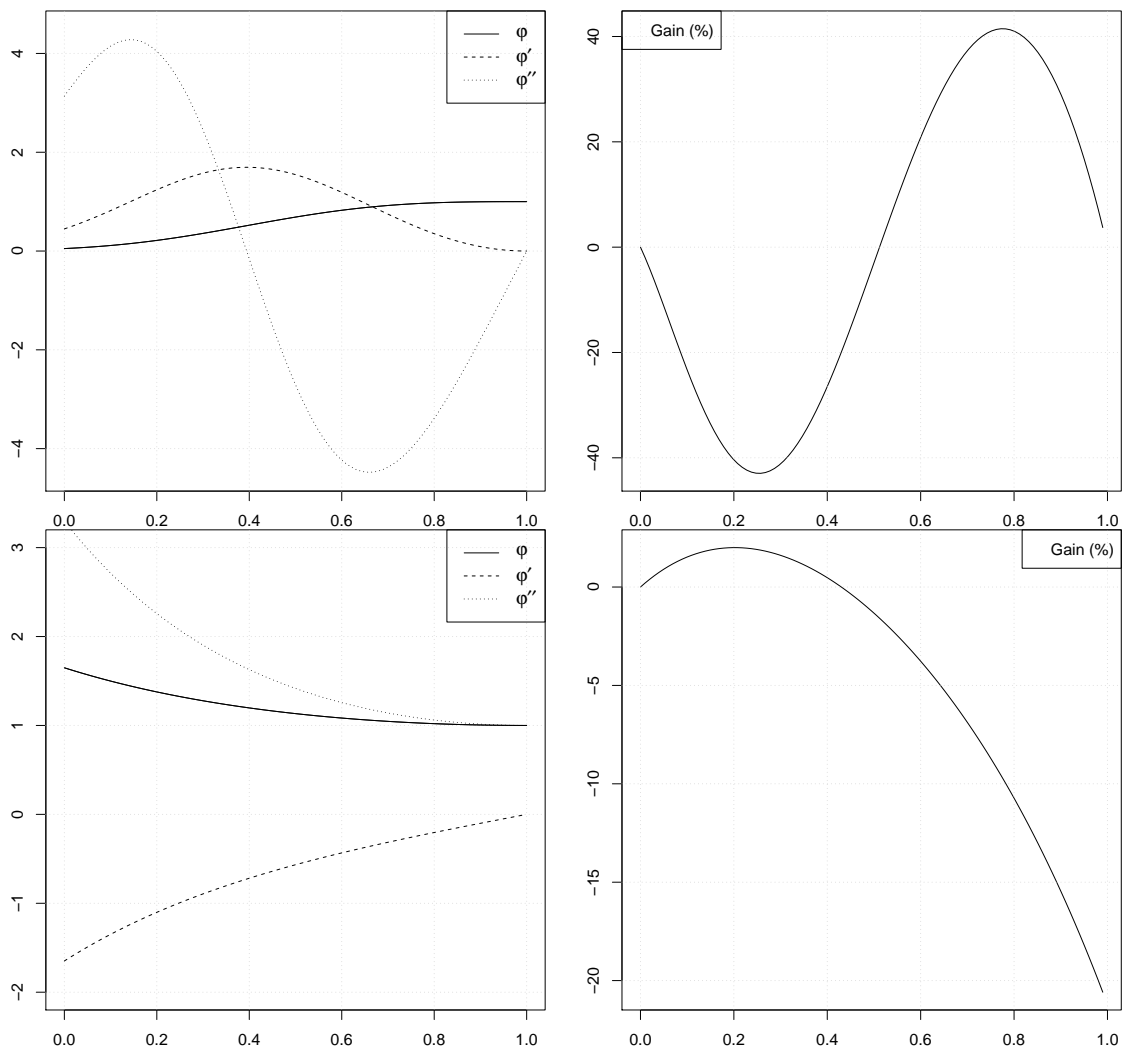
$$\hat{\theta}_k = \hat{\theta}_{\text{MLE}} + \frac{4d}{|W|} \gamma \kappa Y_{(k)} (1 - Y_{(k)})^{\kappa-1} \quad (5.3)$$

where  $Y_{(k)}$  is given by (4.11).

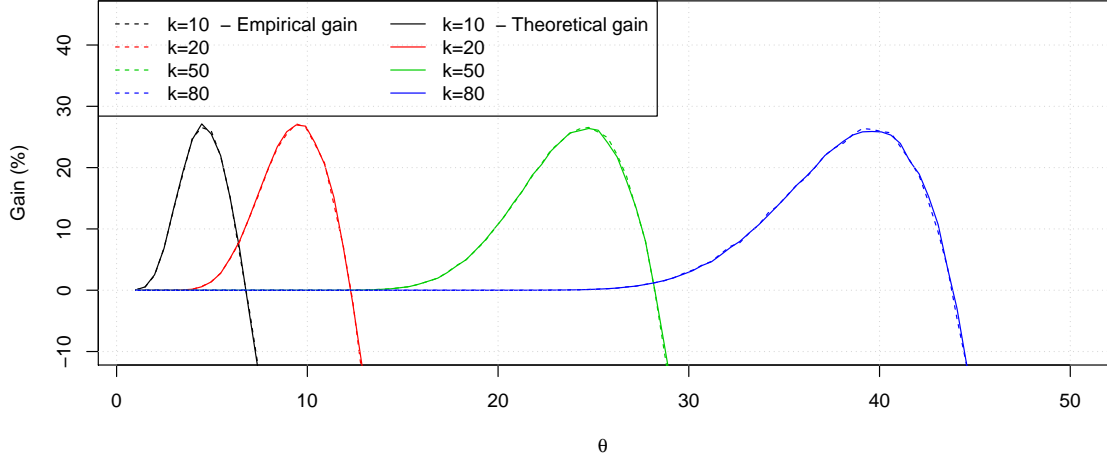
### 5.3 Optimization of the gain and a first simulation study

Before optimizing the parameters  $k, \kappa$  and  $\gamma$ , we first want to check the integration by parts formula. For  $k = 10, 20, 50$  and  $80$  (and for specific parameters  $\kappa$  and  $\gamma$  we do not comment upon for now), we represent in Figure 3 the empirical and theoretical gains computed by the Monte-Carlo approximation of (4.10) based on 50000 replications of Poisson point processes in the 2-dimensional Euclidean ball. We clearly observe that the empirical gain perfectly fits the one computed from (4.10). The second observation is that  $k, \kappa$  and  $\gamma$  need appropriate tuning, otherwise the gain can become highly negative. For instance, when  $k = 20$  and  $\theta = 20$  (and  $\kappa, \gamma$  chosen as specified in the caption of Figure 3) the gain reaches the value -200%.





**Figure 2:** Plots of  $\varphi, \varphi', \varphi''$  and  $\mathcal{G}$  for the function  $\varphi$  defined by (5.2). The parameters  $\kappa$  and  $\gamma$  are equal to 3 and  $-3$  for the top figures and to 2 and 0.5 respectively for the bottom figures.



**Figure 3:** Empirical and Monte-Carlo approximations of the theoretical gain in terms of  $\theta$  for the exponential family (5.2). For  $k = 10, 20, 50, 80$ , the parameters  $\kappa$  and  $\gamma$  are chosen to optimize the theoretical gain for  $\theta = 5, 10, 25, 40$  respectively. The results are based on  $m = 50000$  replications of Poisson point processes in the 2-dimensional euclidean ball  $\overline{B}(0, 1)$ . The Monte-Carlo approximation of (5.4) is also based on  $m = 500000$  samples.

For the exponential function  $\varphi$  given by (5.2), the gain function writes

$$\mathcal{G}(t; \kappa; \gamma) = \gamma \kappa t (1 - t)^{\kappa-1} - \gamma^2 \kappa^2 t^2 (1 - t)^{2(\kappa-1)} - t^2 \gamma \kappa (\kappa - 1) (1 - t)^{\kappa-2}.$$

Now, we explain how we can compute  $\arg \max_{(k, \gamma, \kappa)} \mathbb{E}(\mathcal{G}(Y_k; \kappa; \gamma))$ . First, note that solving the equation  $\frac{\partial}{\partial \gamma} \mathcal{G}(t; \kappa; \gamma) = 0$  leads to an explicit formula for the optimal choice of the parameter  $\gamma$

$$\gamma^* = \frac{\mathbb{E} \left( Y_{(k)} (1 - Y_{(k)})^{\kappa-1} - Y_{(k)}^2 (\kappa - 1) (1 - Y_{(k)})^{\kappa-2} \right)}{\mathbb{E} \left( 2\kappa Y_{(k)}^2 (1 - Y_{(k)})^{2(\kappa-1)} \right)}.$$

Plugging this value back in the formula of the gain leads to

$$\mathbb{E}(\mathcal{G}(Y_{(k)}; \kappa; \gamma^*)) = \frac{\mathbb{E} \left( Y_{(k)} (1 - Y_{(k)})^{\kappa-2} (1 - \kappa Y_{(k)}) \right)}{\mathbb{E} \left( Y_{(k)}^2 (1 - Y_{(k)})^{2(\kappa-1)} \right)}. \quad (5.4)$$

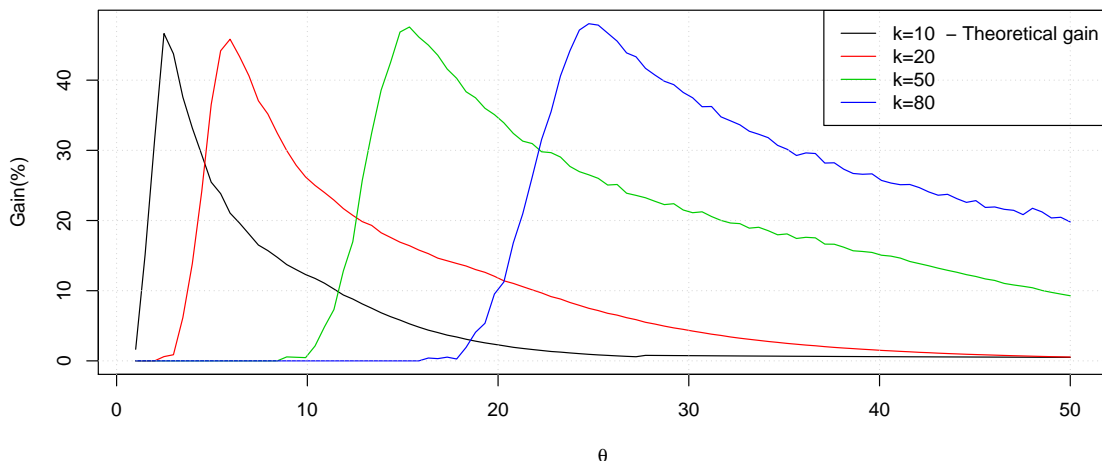
Second, we compute numerically  $\arg \max_{\kappa} \mathbb{E}(\mathcal{G}(Y_{(k)}; \kappa; \gamma^*))$ . To do so, we rely on deterministic optimization techniques after replacing the expectation by a sample average; we refer the reader to Rubinstein and Shapiro (1993) for a review of on sample average approximation. Note that the random variable  $Y_{(k)}$  can be sampled very efficiently by using Lemma 5.1 and (4.11).

In Figure 4, we chose different values of  $k$  and optimized, w.r.t  $\kappa$  and  $\gamma$  for every value of  $\theta$ , the theoretical gain (4.10) computed by Monte-Carlo approximations. The plots are presented in terms of  $\theta$  (when  $d = 2$ ). For a fixed value of  $k$ , we observe that when  $\gamma$  and  $\kappa$  are correctly adjusted the gain is always positive for any  $\theta$ . Still, the choice of  $k$  is very sensitive to the value of  $\theta$  and also needs to be optimized to reach the highest gain. This has been done in Table 1, in which we

present a first simulation study. We investigate the gains for different values of  $d$  and  $\theta$ . For any,  $\theta$  and  $d$ , we chose

$$(k^*, \gamma^*, \kappa^*) = \operatorname{argmax}_{(k, \gamma, \kappa)} \operatorname{Gain}(\hat{\theta}_k).$$

Our experience is that interesting choices for  $k$  are values close to the number of points, say  $n$ . Therefore, the optimization has been done for  $k \in \{\lfloor .75n \rfloor, \dots, \lfloor 1.2n \rfloor\}$ . Such an optimization is extremely fast. Using 50000 samples to approximate (4.10) with the help of Lemma 5.1, it takes less than two seconds to find the optimal parameters when  $d = 3$  and  $\theta = 40$ . The empirical results presented in Table 1 are based on 50000 replications. We report the empirical means, standard deviations, MSE for both the MLE and the "optimized" Stein estimator and finally the empirical gain. The average number of points in  $\overline{B}(0, 1)$  equals to  $\theta|W|$  with  $|W| = 2, 3.14, 4.19$  approximately. The first three columns allow us to recover that the MLE is unbiased with variance (and thus MSE) equal to  $\theta/|W|$ . Then, we observe that our Stein estimator is always negatively biased. This can be seen from (5.3) since the optimal value  $\gamma^*$  is always negative. We point out that the standard deviation is considerably reduced which enables us to obtain empirical gain of between 43% and 48% for the cases considered in the simulation.



**Figure 4:** Monte-Carlo approximation of the theoretical gain for the exponential family (5.2). For each value of  $k$  and  $\theta$ , the parameters  $\kappa$  and  $\gamma$  are chosen to optimize the theoretical gain. The Monte-Carlo approximations of (5.4) are based on  $m = 50000$  replications of Poisson point processes in the 2-dimensional euclidean ball  $\overline{B}(0, 1)$ .

#### 5.4 Comparison with Privault-Réveillac's estimator in the case $d = 1$

In this section, we focus on the case  $d = 1$  and we aim at comparing the performance of our estimator with the one proposed by Privault and Réveillac (2009) and denoted  $\hat{\theta}_{\text{PR}}$  for the sake of conciseness. As underlined previously,  $\hat{\theta}_{\text{PR}}$  shares some similarities with our first example. The main difference comes from the fact that, even in the case  $d = 1$ , the integration by parts formula obtained by Privault and Réveillac

	MLE			STEIN				Gain (%)
	mean	sd	mse	$k^*$	mean	sd	mse	
$\theta = 5, d = 1$	5	1.6	2.52	11	4.4	1.0	1.44	43.0
$d = 2$	5	1.3	1.58	18	4.6	0.8	0.86	45.6
$d = 3$	5	1.1	1.19	22	4.6	0.7	0.64	46.1
$\theta = 10, d = 1$	10	2.2	5.03	22	9.2	1.4	2.73	45.8
$d = 2$	10	1.8	3.18	34	9.4	1.2	1.72	46.0
$d = 3$	10	1.5	2.37	44	9.5	1.0	1.27	46.3
$\theta = 20, d = 1$	20	3.1	9.91	42	18.8	2.0	5.31	46.4
$d = 2$	20	2.5	6.38	66	19.1	1.6	3.41	46.5
$d = 3$	20	2.2	4.72	84	19.1	1.3	2.47	47.5
$\theta = 40, d = 1$	40	4.5	20.09	84	38.5	2.9	10.61	47.2
$d = 2$	40	3.6	12.79	125	38.6	2.2	6.78	46.9
$d = 3$	40	3.1	9.58	169	38.8	1.9	4.95	48.3

**Table 1:** Empirical means, standard deviations (sd), mean squared errors (mse) of MLE estimators and STEIN estimators of the intensity parameter of Poisson point processes observed in the  $d$ -dimensional euclidean ball  $\overline{B}(0, 1)$ . The results are based on  $m = 50000$  replications. The Stein estimator is based on the exponential function. For each  $\theta$  and  $d$ , the parameters  $\kappa$ ,  $\gamma$  and the  $k$ -th nearest-neighbor are optimized to maximize the theoretical gain. The column  $k^*$  reports the optimal nearest-neighbour. Finally, the last column reports the gain of mse in percentage of the Stein estimator with respect to the MLE.

(2009, Proposition 3.3) differs from ours (see Theorem 3.2). Since our framework was to work with  $d$ -dimensional Poisson point processes for any  $d \geq 1$ , we had to impose different compatibility conditions. To ease the comparison with our estimator based on  $\mathbf{X}$  defined on  $\mathbb{R}$  and observed on  $W = [-1, 1]$ , we define  $\widehat{\theta}_{\text{PR}}$  based on the observation of  $\mathbf{X}$  on  $\widetilde{W} = [0, 2]$ . Note that by stationarity,  $(\mathbf{X}_W + 1) \stackrel{d}{=} \mathbf{X}_{\widetilde{W}}$  so both estimators are based on the same amount of information. Let  $X_1$  be the point of  $\mathbf{X}$  closest to 0, then  $\widehat{\theta}_{\text{PR}}$  is defined for some  $\kappa > 0$  by

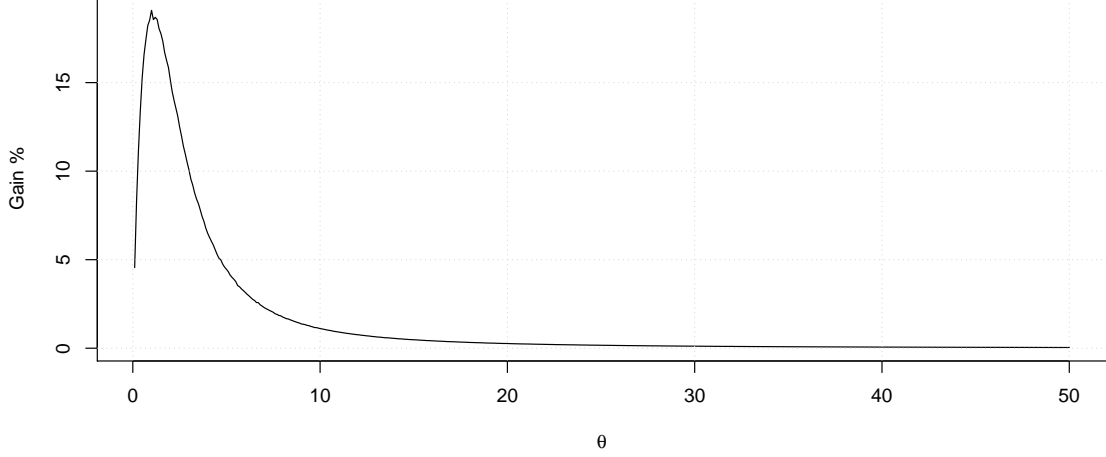
$$\widehat{\theta}_{\text{PR}} = \widehat{\theta}_{\text{MLE}} + \frac{2}{\kappa} 1(N(\widetilde{W}) = 0) + \frac{2X_1}{2(1 + \kappa) - X_1} 1(0 < X_1 \leq 2).$$

The mean squared error and the corresponding gain are given by

$$\begin{aligned} \text{MSE}(\widehat{\theta}_{\text{PR}}) &= \text{MSE}(\widehat{\theta}_{\text{MLE}}) + \frac{1}{\kappa^2} \exp(-2\theta) - \mathbb{E} \left( \frac{X_1}{2(1 + \kappa) - X_1} 1(0 < X_1 \leq 2) \right) \\ \text{Gain}(\widehat{\theta}_{\text{PR}}) &= \frac{2}{\theta \kappa^2} \exp(-2\theta) - \frac{2}{\theta} \mathbb{E} \left( \frac{X_1}{2(1 + \kappa) - X_1} 1(X_1 \leq 2) \right). \end{aligned} \quad (5.5)$$

Note that  $X_1 \sim \mathcal{E}(\theta)$ . We took the same point of view as in the previous section and optimized the gain w.r.t.  $\kappa$ . The optimal gain reached by  $\widehat{\theta}_{\text{PR}}$  is presented in Figure 5. As a summary of this curve, the optimal gain for  $\theta = 5, 10, 20$  and  $40$  is equal to 4.4%, 1.1%, 0.2% and 0.06% respectively. The results are clear. Our Stein estimator,

based on the exponential function and on the idea of picking the  $k$ -th closest point to 0 instead of just the first one, considerably outperforms the estimator proposed by Privault and Réveillac (2009).



**Figure 5:** Monte-Carlo approximation of the theoretical gain (5.5) optimized in terms of  $\kappa$  of the Stein estimator  $\hat{\theta}_{\text{PR}}$  in terms of  $\theta$ .

## 5.5 Data-driven Stein estimator

Table 1 is somehow a theoretical table since the optimal parameters  $k^*$ ,  $\gamma^*$  and  $\kappa^*$  are searched for given the value of  $\theta$ , which is useless in practice since  $\theta$  is unknown. A natural idea consists in first estimating the MLE and then look for the optimal parameters given  $\hat{\theta}_{\text{MLE}}$ . Preliminary experiments have shown us that this procedure can be quite varying when  $d$  or  $\theta$  are large. We think that this is essentially due to the high variance of the MLE. To explain how we can reduce this, let  $f_{k,\gamma,\kappa}(\theta) = 16 \mathbb{E} \mathcal{G}(Y_{(k)}) / (\theta d^2 |W|)$ . Instead of maximizing  $f_{k,\gamma,\kappa}(\hat{\theta}_{\text{MLE}})$ , we suggest to maximize the average gain for a range of values of  $\theta$  and we fix this range as a factor of the standard deviation of the MLE. More specifically, let

$$\Theta(\theta, \rho) = \left[ \theta - \rho \sqrt{\theta / |W|}, \theta + \rho \sqrt{\theta / |W|} \right].$$

When  $\rho = 1$  (resp.  $\rho = 1.6449$ ,  $\rho = 1.96$ ),  $\Theta(\hat{\theta}_{\text{MLE}}, \rho)$  corresponds to the confidence interval of  $\theta$  based on  $\hat{\theta}_{\text{MLE}}$  with confidence level 68.3% (resp. 90% and 95%). Then, we suggest to maximize

$$\int_{\Theta(\hat{\theta}_{\text{MLE}}, \rho)} f_{k,\gamma,\kappa}(\theta) d\theta = \frac{16}{d^2 |W|} \mathbb{E} \int_{\Theta(\hat{\theta}_{\text{MLE}}, \rho)} \frac{\mathcal{G}(Y_{(k)})}{\theta} d\theta. \quad (5.6)$$

In the following, we may write  $Y_{(k)}(\theta)$  to emphasize that the distribution of the random variable  $Y_{(k)}$  depends on the parameter  $\theta$ . Thus, we can rewrite (5.6) as

$$\int_{\Theta(\hat{\theta}_{\text{MLE}}, \rho)} f_{k,\gamma,\kappa}(\theta) d\theta = \frac{16}{d^2 |W|} 2\rho \sqrt{\hat{\theta}_{\text{MLE}} / |W|} \mathbb{E} \left( \frac{\mathcal{G}(Y_{(k)}(U))}{U} \right),$$

where  $U$  is a random variable independent of  $Y_{(k)}$  with uniform distribution over  $\Theta(\widehat{\theta}_{\text{MLE}}, \rho)$ . Sampling  $Y_{(k)}(U)$  is performed in two steps: first, sample  $U$  and second sample a Gamma distributed random variable as explained in Lemma 5.1, in which the value of  $\theta$  is replaced by the current sample of  $U$ . Hence, optimizing this new criteria basically boils down to the same kind of computations as for a fixed value of  $\theta$  without bringing in any extra computations.

Table 2 reports the empirical results regarding this suggestion. As the optimization procedure needs to be conducted for each replication, we only considered 5000 replications. We report the results of the empirical gains of the previous procedure for  $\rho = 0, 1, 1.6449$  and  $1.96$ , the value 0 meaning that we simply maximize  $f_{k,\gamma,\kappa}(\widehat{\theta}_{\text{MLE}})$ . Globally, the empirical gains are slightly smaller than the ones obtained in Table 1. Yet, the results remain pretty impressive. When  $\theta$  is equal to 5 or 10, optimizing (5.6) with  $\rho = 1$  leads to similar results as the previous ones. The value  $\rho = 1$  seems again to be a good choice when  $\theta = 20$  while  $\rho = 1.6449$  is a good compromise when  $\theta = 40$ .

	Gain (%)			
	$\rho = 0$	$\rho = 1$	$\rho = 1.6449$	$\rho = 1.96$
$\theta = 5, d = 1$	48.8	47.9	36.4	30.1
$d = 2$	38.6	42.4	37.1	31.4
$d = 3$	39.4	42.6	37.0	31.7
$\theta = 10, d = 1$	40.3	43.8	36.7	30.1
$d = 2$	36.2	38.8	33.7	27.9
$d = 3$	31.6	36.6	32.0	28.3
$\theta = 20, d = 1$	37.3	38.6	34.5	28.0
$d = 2$	27.3	33.1	31.0	26.5
$d = 3$	20.8	28.6	28.1	23.8
$\theta = 40, d = 1$	22.3	30.8	29.2	23.9
$d = 2$	16.3	24.0	28.2	24.4
$d = 3$	12.7	19.0	24.5	22.0

**Table 2:** Empirical gain of Stein estimators of the intensity parameter of Poisson point processes observed in the  $d$ -dimensional euclidean ball  $\overline{B}(0,1)$ . The results are based on  $m = 5000$  replications. The Stein estimator is based on the exponential function. For each replication, the parameters  $k, \gamma$  and  $\kappa$  maximize (5.6) for different values of  $\rho$ .

## A Notation

We introduce some additional notation required in the proofs. Let  $m$  be a fixed integer. We denote by  $\mathcal{D}(\mathcal{O}, \mathbb{R})$  the space of compactly supported functions which are infinitely differentiable on an open subset  $\mathcal{O}$  of  $\mathbb{R}^m$ . If  $\overline{\mathcal{O}}$  is a closed subset of  $\mathbb{R}^m$ , we let

$$\mathcal{D}(\overline{\mathcal{O}}, \mathbb{R}) = \{g : \exists \tilde{g} \in \mathcal{D}(\mathbb{R}^m, \mathbb{R}) \text{ such that } g = \tilde{g}|_{\overline{\mathcal{O}}}\}.$$

The Sobolev spaces on an open subset  $\mathcal{O}$  of  $\mathbb{R}^m$  are defined by

$$H^1(\mathcal{O}, \mathbb{R}) = \left\{ f \in L^2(\mathcal{O}, \mathbb{R}) : \forall 1 \leq i \leq m, \frac{\partial f}{\partial x_i} \in L^2(\mathcal{O}, \mathbb{R}) \right\}$$

with the norm defined for any  $g \in H^1(\mathcal{O}, \mathbb{R})$  by

$$\|g\|_{H^1(\mathcal{O}, \mathbb{R})} = \|g\|_{L^2(\mathcal{O}, \mathbb{R})} + \sqrt{\sum_{i=1}^m \left\| \frac{\partial g}{\partial x_i} \right\|_{L^2(\mathcal{O}, \mathbb{R})}^2}$$

where the partial derivatives have to be understood in the weak sense. The Sobolev spaces can also be defined on a closed subset  $\overline{\mathcal{O}}$  of  $\mathbb{R}^m$  as

$$H^1(\overline{\mathcal{O}}, \mathbb{R}) = \{f \in L^2(\overline{\mathcal{O}}, \mathbb{R}) : \exists g \in H^1(\mathbb{R}^m, \mathbb{R}) \text{ such that } g|_{\overline{\mathcal{O}}} = f\}.$$

## B Proof of Lemma 4.4

### B.1 An explicit formula for the weak gradient of $\Psi(\|x_{(k),n}\|^2)$

In this section, we consider form functions defined by  $f_n(x_1, \dots, x_n) \mapsto \Psi(\|x_{(k),n}\|^2)$ . Even if  $\Psi \in \mathcal{C}^1(\mathbb{R}, \mathbb{R})$ , the function  $f_n$  may not be differentiable everywhere since the function  $(x_1, \dots, x_n) \mapsto \|x_{(k),n}\|^2$  is non-differentiable at points  $(x_1, \dots, x_n)$  for which  $\|x_i\| = \|x_j\| = \|x_{(k),n}\|$  for some  $i \neq j$ . Nevertheless,  $(x_1, \dots, x_n) \mapsto \|x_{(k),n}\|^2$  is continuous on  $(\mathbb{R}^d)^n$  and so is  $f_n$ . Then, we deduce in this section that  $f_n$  admits partial weak derivatives (see Lemma B.3). Our result is based on the following classical result concerning the existence of weak derivatives for continuous functions (see e.g. Zuily (2002, Proposition 2.4 of Chapter 3)).

**Lemma B.1.** *Let  $(a_n)_{n \in \mathbb{N}}$  be an increasing sequence of real numbers such that  $a_n \rightarrow \infty$  as  $n \rightarrow \infty$ . Set  $a_0 = -\infty$ . For any  $j \geq 0$ , let  $f_j : [a_j, a_{j+1}] \rightarrow \mathbb{R}$  be such that  $f_j \in \mathcal{C}^1((a_j, a_{j+1}), \mathbb{R})$ ,  $f'_j \in L^1((a_j, a_{j+1}), \mathbb{R})$  and define  $f$  by  $f = \sum_{j \in \mathbb{N}} f_j 1_{[a_j, a_{j+1})}$ . If the function  $f$  is continuous on  $\mathbb{R}$ , then it admits a weak derivative, denoted  $f'$ , defined as the locally integrable function  $f' = \sum_j f'_j 1_{(a_j, a_{j+1})}$ .*

**Remark B.2.** The continuity assumption on  $f$  is crucial since if  $f$  were discontinuous at some points  $a_i$ ,  $f$  would not admit a weak derivative. Indeed, in this case the usual jump discontinuity formula (see again Zuily (2002, Proposition 2.4 of Chapter 3)) would imply that the derivative of  $f$ , in the sense of distributions, would be the sum of a locally integrable function and some Dirac masses.

We deduce the following result from Lemma B.1.

**Lemma B.3.** *Let  $n \geq k \geq 1$  and let  $\Psi : \mathbb{R} \rightarrow \mathbb{R}$  be a continuously differentiable function defined on  $\mathbb{R}$ . For any  $j$ ,  $f_n$  admits a weak gradient  $\nabla_{x_j} f_n(x_1, \dots, x_n)$  w.r.t.  $x_j$  and the following equality holds*

$$\sum_{j=1}^n \nabla_{x_j} f_n(x_1, \dots, x_n) \cdot x_j = 2\|x_{(k),n}\|^2 \Psi'(\|x_{(k),n}\|^2), \text{ a.e.} \quad (\text{B.1})$$

In addition, if  $\Psi$  is compactly supported in  $[-\sqrt{a}, \sqrt{a}]$  for some  $a > 0$ , the function  $f_n$  belongs to  $H^1(\overline{B}(0, a)^n, \mathbb{R})$ .

*Proof.* Define for any  $j \in \{1, \dots, n\}$ , the following set

$$A_j = \{(x_1, \dots, x_n) \in (\mathbb{R}^d)^n : x_{(k),n} = x_j \text{ and } \|x_j\| \neq \|x_i\| \text{ for } j \neq i\}.$$

Observe that on  $\bigcup_j A_j$

$$f_n(x_1, \dots, x_n) = \sum_j \Psi(\|x_j\|^2) 1_{A_j}(x_1, \dots, x_n).$$

Hence, the everywhere differentiability of  $\Psi$  implies that the function  $f_n$  is differentiable on  $\bigcup_j A_j$ . In addition, the usual differentiability rules lead to

$$\begin{aligned} \nabla_{x_i} f_n(x_1, \dots, x_n) &= \sum_{j=1}^n \nabla_{x_i} [\Psi(\|x_j\|^2) 1_{A_j}(x_1, \dots, x_n)] \\ &= \nabla_{x_i} [\Psi(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n)] \\ &= 2x_i \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n) \end{aligned}$$

for any  $i \in \{1, \dots, n\}$ . By using Lemma B.1, we prove that  $f_n$  admits a weak gradient w.r.t.  $x_i$ . In the following, we denote the coordinates of elements  $x_i \in \mathbb{R}^d$  by  $x_i = (x_i^{(1)}, \dots, x_i^{(d)})^\top$ . For any  $\ell = 1, \dots, d$ , define

$$f_{i,n}^{(\ell)}(x_i^{(\ell)}) = f(x_1, \dots, x_{i-1}, (x_i^{(1)}, \dots, x_i^{(\ell)}, \dots, x_i^{(d)}), \dots, x_n).$$

Then, we deduce from the differentiability of  $f_n$  on  $\bigcup_j A_j$  that the function  $f_{i,n}^{(\ell)}$  is differentiable at any point  $x_i^{(\ell)} \in \mathbb{R}$ , such that  $\|x_i\| \neq \|x_j\|$  for all  $j \neq i$ . Since in addition  $f_{i,n}^{(\ell)}$  is continuous on  $\mathbb{R}$ , we can apply Lemma B.1 to deduce that  $f_{i,n}^{(\ell)}$  admits a weak derivative defined as

$$[f_{i,n}^{(\ell)}]'(x_i^{(\ell)}) = \frac{\partial}{\partial x_i^{(\ell)}} [\Psi(\|x_i\|^2)] 1_{A_i}(x_1, \dots, x_n) = 2x_i^{(\ell)} \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n)$$

which also means that for any  $(i, \ell)$ ,  $f_n$  admits a weak partial derivative w.r.t.  $x_i^{(\ell)}$  defined by

$$\frac{\partial f_n}{\partial x_i^{(\ell)}} = \frac{\partial}{\partial x_i^{(\ell)}} [\Psi(\|x_i\|^2)] 1_{A_i}(x_1, \dots, x_n) = 2x_i^{(\ell)} \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n). \quad (\text{B.2})$$

We also deduce that

$$\sum_{\ell=1}^d \frac{\partial f_n}{\partial x_i^{(\ell)}} x_i^\ell = 2 \sum_{\ell=1}^d [x_i^{(\ell)}]^2 \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n) = 2\|x_i\|^2 \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n),$$

which, once combined with the definition of  $\nabla_{x_i} f_n$ , yields

$$\sum_{i=1}^n \nabla_{x_i} f_n(x_1, \dots, x_n) \cdot x_i = \sum_{i=1}^n \sum_{\ell=1}^d \frac{\partial f_n}{\partial x_i^{(\ell)}} x_i^{(\ell)} = 2 \sum_{i=1}^n \|x_i\|^2 \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n). \quad (\text{B.3})$$



For any  $i$  and any  $(x_1, \dots, x_n) \in A_i$ ,  $\|x_{(k),n}\|^2 \Psi'(\|x_{(k),n}\|^2) = \|x_i\|^2 \Psi'(\|x_i\|^2)$ . So on  $\cup_j A_j$  (which is a set of full measure)

$$\|x_{(k),n}\|^2 \Psi'(\|x_{(k),n}\|^2) = \sum_{i=1}^n \|x_i\|^2 \Psi'(\|x_i\|^2) 1_{A_i}(x_1, \dots, x_n).$$

Equation (B.1) of Lemma B.3 follows from the last equation and from (B.3). Furthermore, if  $\Psi$  is compactly supported in  $[-\sqrt{a}, \sqrt{a}]$  then  $f_n$  coincides with  $\tilde{f}_n(x_1, \dots, x_n) = \Psi(\|x_{(k),n}\|)u(x_1, \dots, x_n)$  on  $(\overline{B}(0, a))^n$  where  $u$  is a compactly supported and infinitely differentiable function such that  $u \equiv 1$  on  $(\overline{B}(0, a))^n$  and  $u \equiv 0$  on  $(\mathbb{R}^d)^n \setminus (\overline{B}(0, 2a))^n$ . Using the smoothness of  $u$  and the continuity of  $\tilde{f}_n$ , we deduce that  $\tilde{f}_n$  is also continuous on  $(\mathbb{R}^d)^n$ . Then, we get in particular that  $\tilde{f}_n \in L^2((\mathbb{R}^d)^n, \mathbb{R})$ . In addition  $\Psi'$  is also compactly supported and by the smoothness of  $u$ , we have for any  $i, \ell$

$$\frac{\partial \tilde{f}_n}{\partial x_i^{(\ell)}} = u \frac{\partial f_n}{\partial x_i^{(\ell)}} + f_n \frac{\partial u}{\partial x_i^{(\ell)}}$$

in the sense of weak partial derivatives. Using once more (B.2), we deduce that for any  $(i, \ell)$ ,  $\frac{\partial \tilde{f}_n}{\partial x_i^{(\ell)}}$  also belongs to  $L^2((\mathbb{R}^d)^n)$ . Hence  $\tilde{f}_n \in H^1((\mathbb{R}^d)^n)$ .

Since, on  $(\overline{B}(0, a))^n$   $f_n$  coincides with the function  $\tilde{f}_n$ , which belongs to  $H^1((\mathbb{R}^d)^n, \mathbb{R})$ , we deduce that  $f_n \in H^1((\overline{B}(0, a))^n, \mathbb{R})$ .  $\square$

## B.2 A density result for the form functions considered in Lemma 4.4

In the following lemma, we state a useful density result to approximate the form functions  $f_n$  defined in Lemma 4.4.

**Lemma B.4.** *Let  $k \geq 1$  be a fixed integer and let  $\Psi$  be a function belonging to  $H^1([0, 1], \mathbb{R})$ . Define  $\Psi_n(x_1, \dots, x_n) = \Psi(1)1(n < k) + \Psi(\|x_{(k),n}\|^2)1(n \geq k)$ . Then, there exists a sequence  $(f_{\ell,n})$  of symmetric functions of  $\mathcal{C}^1(W^n, \mathbb{R})$  such that*

- (i) *For any  $n, \ell \geq 0$ ,  $f_{\ell,n+1}|_{x_{n+1} \in \partial W} \equiv f_{\ell,n}$ .*
- (ii) *For any  $n \geq 0$ ,  $f_{\ell,n} \rightarrow \Psi_n$  in  $H^1(W^n, \mathbb{R})$  as  $\ell \rightarrow \infty$ .*

**Remark B.5.** The notation  $\Psi(1)$  makes sense if  $\Psi \in H^1([0, 1], \mathbb{R})$  since the usual Sobolev injection yields that  $H^1([0, 1], \mathbb{R}) \hookrightarrow \mathcal{C}^0([0, 1], \mathbb{R})$ .

*Proof.* The case  $d = 1$  would deserve a particular treatment, but as it can be easily adapted from the case  $d \geq 2$ , we only handle the latter one. For any  $n \geq 1$ , and any  $(r_1, \dots, r_n) \in (0, 1)^n$  define by induction

$$\begin{aligned} r_{(1),n} &= \min(r_1, \dots, r_n) \\ r_{(k),n} &= \min\{r \in \{r_1, \dots, r_n\} \setminus \{r_{(1),n}, \dots, r_{(k-1),n}\}\} \text{ for } 2 \leq k \leq n. \end{aligned}$$

Then fix  $k \geq 1$  and define the following functions  $\Phi_n$  on  $[0, 1]^n$  for any  $n \geq 0$  by  $\Phi_n(r_1, \dots, r_n) = (\Psi(r_{(k),n}) - \Psi(1)) 1(n \geq k)$ . In particular  $\Phi_0 \equiv 0$ . We observe that

$$\Psi_n(x_1, \dots, x_n) = \Phi_n(\|x_1\|^2, \dots, \|x_n\|^2) + \Psi(1) \text{ on } W^n.$$

If we approximate  $\Phi_n$  by density using Proposition C.4, Lemma B.4 will be deduced using a change of variables in polar coordinates justified in the sequel.

Since Proposition C.4 applies to a sequence of functions defined on  $\mathbb{R}^n$ , we need at first to extend each function  $\Phi_n$  on  $\mathbb{R}^n$  into a function  $\tilde{\Phi}_n$  belonging to  $H^1(\mathbb{R}^n, \mathbb{R})$ . This will be possible since for any  $n$ ,  $\Phi_n \in H^1((0, 1)^n, \mathbb{R})$ . Hereafter, we prove that the new sequence  $(\tilde{\Phi}_n)$  satisfies the assumptions (a)–(c) of Proposition C.4 with  $a = 1$ .

*Step 1 : we prove that for any  $n$ ,  $\Phi_n \in H^1((0, 1)^n, \mathbb{R})$ .* We focus on the case  $n \geq k$  as the case  $n < k$  is obvious. Since  $\Psi \in H^1((0, 1), \mathbb{R}) \subset L^2((0, 1), \mathbb{R})$

$$\begin{aligned} \int_{(0,1)^n} |\Phi_n(r_1, \dots, r_n)|^2 dr_1 \dots dr_n &= \int_{(0,1)^n} |\Psi(r_{(k),n}) - \Psi(1)|^2 dr_1 \dots dr_n \\ &= \sum_{i=1}^n \int_{\substack{(r_1, \dots, r_n) \in (0,1)^n \\ r_i = r_{(k),n}}} |\Psi(r_i) - \Psi(1)|^2 dr_1 \dots dr_n \\ &\leq 2 \left[ \sum_{i=1}^n \int_0^1 (|\Psi(r_i)|^2 + |\Psi(1)|^2) dr_i \right] \\ &\quad \times \int_{(r_1, \dots, r_{i-1}, r_{i+1}, \dots, r_n) \in (0,1)^{n-1}} dr_1 \dots dr_{i-1} dr_{i+1} \dots dr_n \\ &\leq 2n(\|\Psi\|_{L^2}^2 + |\Psi(1)|^2) < \infty \end{aligned}$$

whereby we deduce that  $\Phi_n \in L^2((0, 1)^n, \mathbb{R})$  for any  $n \geq 0$ .

To deduce that each  $\Phi_n$  belongs to  $H^1((0, 1)^n, \mathbb{R})$ , we prove that for any  $n \geq 0$ ,  $\Phi_n \in L^2((0, 1)^n, \mathbb{R})$  admits partial derivatives w.r.t.  $r_i$  for any  $i$  and that these partial derivatives are all square integrable. Since  $\Psi \in H^1((0, 1), \mathbb{R})$ ,  $\Psi$  is continuous on  $[0, 1]$  as well as  $(r_1, \dots, r_n) \mapsto r_{(k),n}$ . Hence,  $\Phi_n$  is continuous on  $W^n$ . Applying Lemma B.1 to the functions  $\Phi_n^{(i)} : r_i \mapsto \Phi_n(r_1, \dots, r_i, \dots, r_n)$ , we deduce that for any  $(n, i)$ ,  $\Phi_n$  admits a weak derivative w.r.t.  $r_i$  and that for a.e.  $(r_1, \dots, r_n)$

$$\frac{\partial \Phi_n(r_1, \dots, r_n)}{\partial r_i} = 2r_{(k),n} \Psi'(r_{(k),n}) 1_{r_{(k),n} = r_i}(r_1, \dots, r_n).$$

Since  $\Psi \in H^1((0, 1), \mathbb{R})$  we have for any  $i \in \{1, \dots, n\}$

$$\begin{aligned} \int_{(0,1)^n} \left| \frac{\partial \Phi_n(r_1, \dots, r_n)}{\partial r_i} \right|^2 dr_1 \dots dr_n &\leq \sum_{i=1}^n \int_0^1 \left| \frac{\partial \Psi(r_i)}{\partial r_i} \right|^2 \times 2r_i dr_i \\ &\leq 2 \sum_{i=1}^n \int_0^1 \left| \frac{\partial \Psi(r_i)}{\partial r_i} \right|^2 dr_i < \infty, \end{aligned}$$

which shows that  $\Phi_n \in H^1((0, 1)^n, \mathbb{R})$ .

*Step 2: extension of  $\tilde{\Phi}_n$  and properties.* Let us define the sequence  $\tilde{\Phi}_n$  as follows

$$\tilde{\Phi}_n = \begin{cases} \tilde{\Phi}_n(r_1, \dots, r_n) = \Phi_n(|r_1|, \dots, |r_n|) & \text{if } (r_1, \dots, r_n) \in (-1, 1)^n \\ \tilde{\Phi}_n(r_1, \dots, r_n) = 0 & \text{otherwise.} \end{cases}$$

We prove that this sequence satisfies the assumptions of Proposition C.4. First, Assumption (a) is clearly satisfied. Second, since by Step 1,  $\Phi_n \in H^1((0, 1)^n, \mathbb{R})$  for any  $n$  and is symmetric, it is also clear from the definition of the sequence  $\tilde{\Phi}_n$  that these functions all belong to  $H^1(\mathbb{R}^n, \mathbb{R})$  and are also symmetric. This proves Assumption (b). Third, we can check that Assumption (c) is satisfied for the functions  $(\Phi_n)$ . If  $r_{n+1} = 1$  and  $(r_1, \dots, r_n) \in (0, 1)^n$ ,  $r_{(k),n+1} = r_{(k),n}$ , which implies that for any  $n$   $\Phi_{n+1}|_{r_{n+1}=1} \equiv \Phi_n$ . The case  $n < k - 1$  is also clear. When  $n = k - 1$ ,  $r_k = 1$  so  $r_{(k),k} = 1$  and  $\Psi(r_{(k),k}) - \Psi(1) = 0$ . Then, we deduce that Assumption (c) is satisfied by the sequence  $(\Phi_n)$ . By definition of the sequence  $\tilde{\Phi}_n$ , it is obvious that Assumption (c) is also satisfied for the functions  $\tilde{\Phi}_n$ .

*Step 3 : construction of the sequences  $(f_{\ell,n})$  which approximate the functions  $\Phi_n$ .* By Step 2, Proposition C.4 can be applied to the sequence  $(\tilde{\Phi}_n)$  with  $a = 1$ . We deduce the existence of a sequence  $g_{\ell,n}$  of symmetric functions on  $\mathbb{R}^n$  satisfying (A)-(D) of Proposition C.4. To conclude, we define the sequence of symmetric functions  $f_{\ell,n}$  on  $W^n$  by  $f_{\ell,n}(x_1, \dots, x_n) = g_{\ell,n}(\|x_1\|^2, \dots, \|x_n\|^2) + \Psi(1)$  and check that the desired result holds. The compatibility relations are clearly satisfied. Furthermore, since for any  $(\ell, n)$ ,  $g_{\ell,n} \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ , then  $f_{\ell,n} \in \mathcal{C}^1(W^n, \mathbb{R})$ . To achieve the proof of Lemma B.4, we prove that  $(f_{\ell,n}) \rightarrow \Psi_n$  in  $H^1((0, 1)^n)$  as  $\ell \rightarrow \infty$ . For any  $i$  and any  $x_i \in W$ , let  $r_i = \|x_i\|$ ,  $\Theta_i = x_i/\|x_i\|$ ,  $u_i = r_i^2$  and  $\mathbb{S}^{d-1} = \{x \in \mathbb{R}^d, \|x\| = 1\}$ . We have

$$\begin{aligned} & \int_{W^n} |f_{\ell,n}(x_1, \dots, x_n) - \Psi_n(x_1, \dots, x_n)|^2 dx_1 \dots dx_n \\ &= \left[ \int_{(0,1)^n} |g_{\ell,n}(u_1, \dots, u_n) - \Phi_n(u_1, \dots, u_n)|^2 \prod_{i=1}^n (u_i)^{(d-1)/2-1/2} du_1 \dots du_n \right] \\ & \quad \times \left[ \int_{(\mathbb{S}^{d-1})^n} d\Theta_1 \dots d\Theta_n \right]. \end{aligned}$$

Since  $d \geq 2$  and  $g_{\ell,n} \rightarrow \Phi_n$  in  $H^1((0, 1)^n, \mathbb{R}) \hookrightarrow L^2((0, 1)^n, \mathbb{R})$ ,

$$\begin{aligned} & \int_{(0,1)^n} |g_{\ell,n}(u_1, \dots, u_n) - \Phi_n(u_1, \dots, u_n)|^2 \prod_{i=1}^n (u_i)^{(d-1)/2-1/2} du_1 \dots du_n \\ &= \int_{(0,1)^n} |g_{\ell,n}(u_1, \dots, u_n) - \Phi_n(u_1, \dots, u_n)|^2 \prod_{i=1}^n (u_i)^{d/2-1} du_1 \dots du_n \\ &\leq \int_{(0,1)^n} |g_{\ell,n}(u_1, \dots, u_n) - \Phi_n(u_1, \dots, u_n)|^2 du_1 \dots du_n \end{aligned}$$

which tends to 0 as  $\ell \rightarrow \infty$ , the last display coming from the fact that  $d/2 - 1 \geq 0$ . It implies that  $f_{\ell,n} \rightarrow \Phi_n$  in  $L^2(W^n, \mathbb{R})$ . We also note that for any  $i$  and any  $(x_1, \dots, x_n) \in W^n$ ,  $\nabla_{x_i} f(x_1, \dots, x_n) = 2x_i \cdot g(\|x_1\|^2, \dots, \|x_n\|^2)$ . The same change of variables as above and the convergence of  $\nabla_{r_i} g_{\ell,n} \rightarrow \nabla_{r_i} \Phi_n$  in  $L^2((0, 1)^n, \mathbb{R})$  yield that  $\nabla_{x_i} f_{\ell,n} \in L^2(W^n, \mathbb{R}) \rightarrow \nabla_{x_i} \Psi_n$ . The convergence of  $(f_{\ell,n})$  to  $\Psi_n$  in  $H^1((0, 1)^n)$  is therefore deduced.  $\square$

### B.3 Proof of Lemma 4.4

Following Section 3.1, we extend the closable operator  $\nabla : \text{Dom}(D) \rightarrow L^2(\Omega)$  to

$$\text{Dom}(\overline{D}) = \{F \in L^2(\Omega) : \exists(F_\ell) \in \text{Dom}(D), \nabla F_\ell \text{ converges in } L^2(\Omega)\}.$$

Now, we apply Lemma B.4 and choose a sequence  $(f_{\ell,n}) \in \mathcal{C}^1(W^n, \mathbb{R})$  satisfying the compatibility relations and converging to  $\Phi_n$  in  $H^1((0,1)^n, \mathbb{R})$  as  $\ell \rightarrow \infty$ . Let us define the sequence  $(F_\ell) \subset L^2(\Omega)$ , which admits  $(f_{\ell,n})$  as form functions and check that this sequence satisfies the following properties: (i) For any  $\ell$ ,  $F_\ell \in \text{Dom}(D)$ ; (ii)  $F_\ell \rightarrow F$  in  $L^2(\Omega)$ ; (iii)  $\nabla F_\ell$  converges in  $L^2(\Omega)$  to some  $G_k$ .

(i) is deduced from the compatibility relations since  $(f_{\ell,n}) \in \mathcal{C}^1(W^n, \mathbb{R})$ . (ii) For any  $n \geq 1$ ,  $f_{\ell,n} \rightarrow \Phi_n$  in  $L^2(W^n)$  which implies by Lemma 2.1 that  $F_\ell \rightarrow F$  in  $L^2(\Omega)$ . (iii) Since the functions  $(f_{\ell,n})$  given by Lemma B.4 converge to  $\Psi_n$  in  $H^1((0,1)^n, \mathbb{R})$ , we also have  $\nabla_{x_i} f_{\ell,n} \rightarrow \nabla_{x_i} \Phi_n$  in  $L^2(W^n)$  and

$$\sum_{i=1}^n \nabla_{x_i} f_{\ell,n} \cdot x_i \rightarrow \sum_{i=1}^n \nabla_{x_i} \Phi_n \cdot x_i \text{ in } L^2(W^n).$$

Hence, in view of Lemma 2.1 and of the definition of  $\nabla F_\ell$ , we have  $\nabla F_\ell \rightarrow G_k$  in  $L^2(\Omega)$  where

$$G_k = 2 \sum_{n \geq k} 1(N(W) = n) \sum_{i=1}^n \nabla_{x_i} \Phi_n \cdot x_i.$$

From Lemma 4.1, we have the explicit expression of  $G$  depending only on  $\Psi$ :

$$G_k = 2 \sum_{n \geq k} 1(N(W) = n) \|x_{(k),n}\|^2 \Psi'(\|x_{(k),n}\|^2). \quad (\text{B.4})$$

The results (i)-(iii) combined with (B.4) precisely ensure that  $F \in \text{Dom}(\overline{D})$  and that  $\overline{\nabla} F = G_k$ .

## C Auxiliary density results

In this section, we state some density results used in the proof of Proposition 4.3. At first, we recall some basic properties of the trace operator, see Adams and Fournier (1975). Fix  $a \in \mathbb{R}$  and an integer  $m \geq (n+1)/2$ . The mapping  $\varphi \in \mathcal{D}(\mathbb{R}^{n+1}, \mathbb{R}) \subset H^m(\mathbb{R}^{n+1}, \mathbb{R}) \mapsto \varphi|_{r_{n+1}=0} \in H^{m-1/2}(\mathbb{R}^n, \mathbb{R})$  is continuous. The trace operator  $\gamma_{n,a}$  is defined as its continuous extension from  $H^m(\mathbb{R}^{n+1}, \mathbb{R})$  to  $H^{m-1/2}(\mathbb{R}^n, \mathbb{R})$ . In addition, we can give an explicit expression of the extension operator on the Schwartz class  $\mathcal{S}(\mathbb{R}^n)$ , see Zuily (2002, Lemma 1.17 of Chapter 11).

**Lemma C.1.** *Let  $a \in \mathbb{R}$ ,  $s > 0$ ,  $M > s/2$  and  $g \in \mathcal{S}(\mathbb{R}^n)$ . Then, the function  $f$  defined from  $g$  on  $\mathbb{R}^{n+1}$  in the Fourier domain by*

$$\widehat{f}(\xi', \xi_{n+1}) = K_M \frac{(1 + |\xi'|^2)^M \widehat{g}(\xi')}{(1 + |\xi'|^2 + \xi_{n+1}^2)^M}, \quad \forall \xi = (\xi', \xi_{n+1}) \in \mathbb{R}^{n+1} \quad (\text{C.1})$$

with  $K_M = \left(\int_{\mathbb{R}} (1 + \eta^2)^{-M-1/2} d\eta\right)^{-1}$  belongs to  $H^{s+1/2}(\mathbb{R}^{n+1})$ . In addition, for any  $\sigma \in (0, s]$  there exists  $C > 0$  only depending on  $n$  and  $s$ , such that for any  $f \in H^s(\mathbb{R}^n, \mathbb{R})$  we have

$$\|f\|_{H^{\sigma+1/2}(\mathbb{R}^{n+1})} \leq C \|g\|_{H^\sigma(\mathbb{R}^n)}, \quad (\text{C.2})$$

and  $\gamma_{n,a}f = g$ . Moreover, if  $g$  is symmetric, so is  $f$ .

**Remark C.2.** The function  $f$  is not unique since the trace operator is only a surjective operator.

*Proof.* All the conclusions of Lemma C.1 are stated and proved in Zuily (2002, Lemma 1.17 of Chapter 11), except (C.2) we now focus on. Fix  $\sigma \in (0, s]$ . In Zuily (2002, Lemma 1.17 of Chapter 11), it is proved that  $\|f\|_{H^{\sigma+1/2}} \leq C_\sigma \|g\|_{H^\sigma}$  with  $C_\sigma = K_M \left(\int_{\mathbb{R}} (1 + \eta^2)^{-2M-1/2+\sigma} d\eta\right)^{1/2}$ . Finally, since  $C_\sigma \leq K_M \left(\int_{\mathbb{R}} (1 + \eta^2)^{-2M-1} d\eta\right)^{1/2} < \infty$ ,  $C_\sigma$  can be replaced by a constant  $C$  (which is finite since  $M > 0$ ) depending only on  $s$  and  $n$ .  $\square$

As a consequence of the previous lemma, we can state.

**Lemma C.3.** *Let  $a \in \mathbb{R}$ ,  $s > 0$  and  $g \in H^s(\mathbb{R}^n)$ . Then, there exists some function  $f$  belonging to  $H^{s+1/2}(\mathbb{R}^{n+1})$  such that  $\gamma_{n,a}f = g$ . In addition, there exists some  $C > 0$  depending only on  $n$  and  $s$  such that for any  $\sigma \in (0, s]$  we have  $\|f\|_{H^{\sigma+1/2}(\mathbb{R}^{n+1})} \leq C \|g\|_{H^\sigma(\mathbb{R}^n)}$ . Moreover, if  $g$  is symmetric  $f$  can also be chosen symmetric.*

*Proof.* We consider a sequence  $(g_\ell)$  of functions of  $\mathcal{S}(\mathbb{R}^n)$  converging to  $g$  in  $H^s$ . We fix some  $M > s/2$ . For any  $\ell$ , we define  $(f_\ell)$  from  $(g_\ell)$  using (C.1). Since  $(g_\ell)$  is a Cauchy sequence of  $H^s(\mathbb{R}^n)$ , we deduce by (C.2) applied with  $\sigma = s$  that

$$\|f_\ell - f_m\|_{H^{s+1/2}(\mathbb{R}^{n+1})} \leq C \|g_\ell - g_m\|_{H^s(\mathbb{R}^n)} \rightarrow 0$$

as  $\ell, m \rightarrow \infty$ . The sequence  $(f_\ell)$  is a Cauchy sequence in  $H^{s+1/2}(\mathbb{R}^{n+1})$  and converges to some function  $f$  in  $H^{s+1/2}(\mathbb{R}^{n+1})$ . This convergence also holds in  $H^{\sigma+1/2}(\mathbb{R}^{n+1})$  for any  $\sigma \in (0, s]$ . Hence, we can let  $\ell \rightarrow \infty$  in the inequality  $\|f_\ell\|_{H^{\sigma+1/2}(\mathbb{R}^{n+1})} \leq C \|g_\ell\|_{H^\sigma(\mathbb{R}^n)}$  (which is also valid in view of (C.2) applied to any  $\sigma \in (0, s]$ ) to get  $\|f\|_{H^{\sigma+1/2}(\mathbb{R}^{n+1})} \leq C \|g\|_{H^\sigma(\mathbb{R}^n)}$  for a constant  $C > 0$  which depends only on  $n$  and  $s$ . If  $g$  is symmetric, we can replace the sequence  $(g_\ell)$  by its symmetric part. Therefore, the functions  $(f_\ell)$  are symmetric and so is  $f$ .  $\square$

From this result, we can deduce the next proposition used in the proof of Lemma 4.4.

**Proposition C.4.** *Let  $a \in \mathbb{R}$  and  $k \in \mathbb{N} \setminus \{0\}$ . Let  $(\Phi_n)_{n \geq 0}$  be a sequence satisfying: (a)  $\Phi_n \equiv 0$  if  $n < k$ . (b) For any  $n \geq k$ ,  $\Phi_n$  is a symmetric function belonging to  $H^1(\mathbb{R}^n, \mathbb{R})$ . (c) For any  $n \geq 0$ ,  $\gamma_{n,a}\Phi_{n+1} \equiv \Phi_n$ . Then, there exists a sequence  $(g_{\ell,n})_{n \geq 0, \ell}$  such that*

- (A) For any  $\ell$  and any  $n < k$ ,  $g_{\ell,n} = 0$ .
- (B) For any  $n \geq k$  and  $\ell$ ,  $g_{\ell,n}$  are symmetric functions belonging to  $H^m(\mathbb{R}^n)$  with  $m > 1 + n/2$ . Since for  $m > 1 + n/2$   $H^m(\mathbb{R}^n) \hookrightarrow \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ , one deduces that for any  $n \geq 1$  and  $\ell$ ,  $g_{\ell,n} \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ .

(C) For any  $n$ ,  $g_{\ell,n} \rightarrow \Phi_n$  in  $H^1(\mathbb{R}^n, \mathbb{R})$  as  $\ell \rightarrow \infty$ .

(D) For any  $\ell$ , the sequence  $g_{\ell,n}$  also satisfies the relation  $\gamma_{n,a}g_{\ell,n+1} \equiv g_{\ell,n}$ .

*Proof.* Up to a translation, we can assume that  $a = 0$ . We can also assume that  $k = 1$ . We denote  $\gamma_n = \gamma_{n,0}$ .

*Step 1 : approximation of functions  $\Phi_n$  by smooth functions  $(h_{\ell,n})$ .* Set for any  $\ell$ ,  $g_{\ell,0} = h_{\ell,0} = 0$ . Hereafter, we apply classical density results and consider for any  $n \geq 1$ , a sequence  $(h_{\ell,n}) \in \mathcal{D}(\mathbb{R}^n, \mathbb{R})$  converging to  $\Phi_n$  in  $H^1(\mathbb{R}^n, \mathbb{R})$  as  $\ell \rightarrow \infty$ . We can replace the sequence  $(h_{\ell,n})$  by the symmetric part of each function and since each  $\Phi_n$  is symmetric, we can assume that all the functions  $(h_{\ell,n})$  are symmetric. We modify by induction the sequence  $(h_{\ell,n})$  in order to define a new sequence  $(g_{\ell,n})$  satisfying the compatibility relations (D).

*Step 2 : definition of the sequences  $(g_{\ell,n})$  for  $n \geq 0$ .* For  $n = 0$ , we set  $g_{\ell,0} = 0$  for any  $\ell$ . When  $n = 1$ , the continuity of the trace of functions of  $H^1(\mathbb{R}, \mathbb{R})$  yields  $\gamma_1 h_{\ell,1} = h_{\ell,1}(0) \rightarrow \Phi_1(0) = \Phi_0 = 0$  as  $\ell \rightarrow \infty$ . Let  $\varphi$  be a symmetric function belonging to  $\mathcal{D}(\mathbb{R}, \mathbb{R})$  such that  $\varphi(0) = 1$  and that  $g_{\ell,1} = h_{\ell,1} - h_{\ell,1}(0)\varphi$ . This sequence clearly belongs to  $H^m(\mathbb{R}, \mathbb{R})$  for any  $m > 1 + 1/2 = 3/2$ , and all functions  $g_{\ell,1}$  are symmetric. First, we can check that for any  $\ell$ ,  $g_{\ell,1}(1) = 0 = g_{\ell,0}$  and so (D) is satisfied for  $n = 0$ . Second, since  $h_{\ell,1}(0) \rightarrow 0$  and  $h_{\ell,1} \rightarrow \Phi_1$  in  $H^1(\mathbb{R}, \mathbb{R})$  as  $\ell \rightarrow \infty$ , we deduce that  $g_{\ell,1} \rightarrow \Phi_1$  in  $H^1(\mathbb{R}, \mathbb{R})$ .

Assume that we have defined for any  $\ell$  by induction some symmetric functions  $g_{\ell,1}, \dots, g_{\ell,N}$ , belonging respectively to  $H^{m_1}(\mathbb{R}, \mathbb{R}), \dots, H^{m_N}(\mathbb{R}^N, \mathbb{R})$  with  $m_1 > 1 + 1/2, \dots, m_N > 1 + N/2$ , satisfying (D) for  $n = 1, \dots, N$  and

$$\forall n \in \{0, \dots, N\}, g_{\ell,n} \rightarrow \Phi_n \text{ in } H^1(\mathbb{R}, \mathbb{R}) \text{ as } \ell \rightarrow \infty. \quad (\text{C.3})$$

Now, we define for any  $\ell$  the functions  $g_{\ell,N+1}$ . The function  $g_{\ell,N+1}$  will be of the form  $g_{\ell,N+1} = h_{\ell,N+1} + \tilde{h}_{\ell,N+1}^{(1)}$ , where  $\tilde{h}_{\ell,N+1}^{(1)}$  is a function depending on  $g_{\ell,N}$  and  $h_{\ell,N+1}$ .

Let us explain how the functions  $\tilde{h}_{\ell,N+1}^{(1)}$  are defined. Observe that, since we require that  $\gamma_N g_{\ell,N+1} = g_{\ell,N}$ , one necessarily has  $\gamma_N \tilde{h}_{\ell,N+1}^{(1)} = \gamma_N g_{\ell,N+1} - \gamma_N h_{\ell,N+1} = g_{\ell,N} - \gamma_N h_{\ell,N+1}$ . To define the function  $\tilde{h}_{\ell,N+1}^{(1)}$ , we have then to extend the function  $g_{\ell,N} - \gamma_N h_{\ell,N+1}$  to  $\mathbb{R}^{n+1}$ , which is possible in view of Lemma C.3. By the induction assumption  $g_{\ell,N} \in H^m(\mathbb{R}^n)$  for some  $m_N > 1 + n/2$  and then so does  $g_{\ell,N} - \gamma_N h_{\ell,N+1}$ . By applying Lemma C.3 to  $g = g_{\ell,N} - \gamma_N h_{\ell,N+1}$ ,  $s = m_N > 1 + N/2$  and  $\sigma = 1/2$ , we get the existence of a symmetric function  $\tilde{h}_{\ell,N+1}^{(1)} \in H^{m+1/2}(\mathbb{R}^{n+1})$  such that  $\gamma_N \tilde{h}_{\ell,N+1}^{(1)} = g_{\ell,N} - \gamma_N h_{\ell,N+1}$ .

*Step 3 : proof of Properties (A)–(D).* We now prove that  $g_{\ell,N+1} = h_{\ell,N+1} + \tilde{h}_{\ell,N+1}^{(1)}$  satisfies (A)–(D) stated in the lemma. Property (A) is obvious from the definition of the sequence  $(g_{\ell,0})$ . By construction, we have that, for any  $\ell$ ,  $\tilde{h}_{\ell,N+1}^{(1)}$  is a symmetric function belonging to  $H^{m_{N+1}}(\mathbb{R}^{n+1})$  with  $m_{N+1} = m_N + 1/2 > 1 + N/2 + 1/2 = 1 + (N + 1)/2$ , so does  $g_{\ell,N+1}$ . Hence, we deduce that (B) is satisfied. The relation  $\gamma_N g_{\ell,N+1} = g_{\ell,N}$  directly ensues from their definitions.

Now, we prove that (C) is satisfied. By the continuity of the trace mapping

$$\gamma_N \tilde{h}_{\ell,N+1}^{(1)} = g_{\ell,N} - \gamma_N h_{\ell,N+1} \rightarrow g_{\ell,N+1} - \gamma_N \Phi_{N+1} = g_{\ell,N} - \Phi_N \text{ in } H^{1/2}((0, 1)^N, \mathbb{R})$$

as  $\ell \rightarrow \infty$ . We deduce from the last display and (C.3) that  $\gamma_N \tilde{h}_{\ell, N+1} \rightarrow 0$  in  $H^{1/2}((0, 1)^N, \mathbb{R})$  as  $\ell \rightarrow \infty$ . By the continuity of the extension operator, we get

$$\|\tilde{h}_{\ell, N+1}^{(1)}\|_{H^1(\mathbb{R}^{N+1}, \mathbb{R})} \leq C \|\gamma_N \tilde{h}_{\ell, N+1}\|_{H^{1/2}(\mathbb{R}^N, \mathbb{R})} \rightarrow 0 \quad (\text{C.4})$$

as  $\ell \rightarrow \infty$ , where  $C > 0$  depends only on  $N$ . By the definition of  $g_{N+1, \ell}$  and from (C.4), we deduce that both sequences  $(g_{\ell, N+1})$  and  $(h_{\ell, N+1})$  have the same limit  $\Phi_{N+1}$  in  $H^1(\mathbb{R}^{N+1}, \mathbb{R})$  as  $\ell \rightarrow \infty$ , which ends the proof.  $\square$

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