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Quasi-Monte Carlo integration on manifolds with mapped low-discrepancy points and greedy minimal Riesz *s*-energy points

Stefano De Marchi [a,*], Giacomo Elefante [b]

[a] *University of Padova, Department of Mathematics, Via Trieste, 63, I-35121 Padova, Italy*
[b] *University of Fribourg, Department of Mathematics, Chemin du Musée, 23, CH-1700 Fribourg, Switzerland*

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In this paper we consider two sets of points for Quasi-Monte Carlo integration on two-dimensional manifolds. The first is the set of mapped low-discrepancy sequence by a *measure preserving map*, from a rectangle $\mathcal{U} \subset \mathcal{R}^2$ to the manifold. The second is the *greedy minimal Riesz s-energy points* extracted from a suitable discretization of the manifold. Thanks to the *Poppy-seed Bagel Theorem* we know that the classes of points with minimal Riesz *s*-energy, under suitable assumptions, are asymptotically uniformly distributed with respect to the normalized Hausdorff measure. They can then be considered as quadrature points on manifolds via the Quasi-Monte Carlo (QMC) method. On the other hand, we do not know if the greedy minimal Riesz *s*-energy points are a good choice to integrate functions with the QMC method on manifolds. Through theoretical considerations, by showing some properties of these points and by numerical experiments, we attempt to answer to these questions.

1. Introduction

Monte Carlo (MC) and Quasi-Monte Carlo (QMC) methods are well-known techniques in numerical analysis, statistics, in economy, in financial engineering and in many fields where it is required to numerically compute fastly and accurately, the integral of a multivariate function f. Both MC and QMC methods approximate the integral $\int_X f(\boldsymbol{x})\mathrm{d}\mu(\boldsymbol{x})$, with $X \subset \mathbb{R}^d$, by the average of the function values at a set of N points of X uniformly distributed with respect to a given measure μ. Monte Carlo uses random points whereas the Quasi-Monte Carlo method considers deterministic point sets, in particular low-discrepancy sequences.

Let us consider the integral

$$\frac{1}{\mathcal{H}_d(\mathcal{M})}\int_{\mathcal{M}} f(\boldsymbol{x})\mathrm{d}\mathcal{H}_d(\boldsymbol{x}) \tag{1}$$

where $\mathcal{M}$ is a d-dimensional manifold and $\mathcal{H}_d$ is the *Hausdorff measure* (for the definition of this measure we refer to [8, §11.2]). In this case, the QMC method is preferable to other cubature techniques, since it requires only the knowledge

* Corresponding author.
E-mail addresses: demarchi@math.unipd.it (S. De Marchi), giacomo.elefante@unifr.ch (G. Elefante).

of f on a well-distributed points set of the manifold. It is worth mentioning, that other cubature techniques may require more information on the approximation space, like for example in the nonnegative least squares or those based on the Approximate Fekete Points (cf. [2]) where it is required the knowledge of a suitable polynomial basis of the manifold. There exist also Chebyshev-type quadrature formulas on multidimensional domains, as those studied for instance in [11].

Convergence results and error bounds for MC and QMC methods, are usually studied on $X = [0,1)^d$. In particular the error bound in $[0,1)^d$ for the QMC method is given by the well-known *Koksma–Hlawka inequality* (see Theorem 2 of Section 2). For other closed domains or manifolds there exist similar inequalities as recalled in Theorems 3 and 4 (cf. [1,4,18]).

In order to prove convergence to the integral on a manifold, we can choose a low-discrepancy sequence, which turns out to be uniformly distributed with respect to the Hausdorff measure of the manifold. Due to *Poppy-seed Bagel Theorem* (see the weighted version, Theorem 5 of Section 4) we know that minimal Riesz s-energy points, under some assumptions, are uniformly distributed with respect to the Hausdorff measure $\mathcal{H}_d$ (see [10,9]). Therefore these points represent potential candidates for integrating functions via the QMC method on manifolds. As observed in [3], it is also possible to use a continuous and positive on the diagonal (CPD) weight function, say w, to distribute these points uniformly with respect to a given density.

To compute the minimal Riesz s-energy points we make use of a *greedy* technique, obtaining the so-called *greedy k_s-energy points* (or *Léja–Gorski points*) and the greedy (w,s)-energy points in the weighted case (see Section 4, below). So far, we do not know if these approximate points of the minimal Riesz s-energy points are a good choice to integrate functions via the QMC method on general manifolds. As proved in [13], we only know that the greedy points are uniformly distributed on the d-dimensional unit sphere $\mathbb{S}^d$, $d \geq 1$.

In this work, we test these greedy points for the integration on different manifolds via QMC method, making a comparison with low-discrepancy sequences (like Halton points or Fibonacci lattices) mapped to the manifold by a measure preserving map aimed to maintain their uniform distribution with respect to the Hausdorff measure of the manifold (see Section 3), and also with the MC method by taking random points on the manifold itself.

The paper is organized as follows. After some necessary definitions, notations and results on MC and QMC integration, recalled in the next section, in Section 3 we present the mapping technique from the unit square $[0,1]^2$ to a general manifold $\mathcal{M} \subset \mathbb{R}^2$. In Section 4 we introduce other set of points, that is the minimal s-Riesz energy points, the weighted (w,s)-Riesz points and the greedy minimal (w,s)-energy points. In Section 5 we provide extensive numerical experiments for comparing these set of points for QMC integration on different functions on classical manifolds: cone, cylinder, sphere and torus. We conclude in Section 6 by summarizing the results and proposing some future works.

2. Preliminaries

Let X be a compact Hausdorff space and μ a regular unit Borel measure on X.

Definition 1. A sequence of points $\mathcal{S} = (\boldsymbol{x}_n)_{n\geq 1}$ in a compact Hausdorff space X is uniformly distributed with respect to the measure μ (or μ-*u.d.*) if for any real-valued bounded continuous function $f : X \to \mathbb{R}$ we have

$$\lim_{N\to\infty} \frac{\sum_{n=1}^{N} f(\boldsymbol{x}_n)}{N} = \int_X f(\boldsymbol{x}) \mathrm{d}\mu(\boldsymbol{x}).$$

This definition tells us that, if we have a sequence uniformly distributed with respect to a given measure μ, we can approximate $\int_X f \mathrm{d}\mu$ by using the QMC method.

Theorem 1 *(cf. [12]). A sequence $(\boldsymbol{x}_n)_{n\in\mathbb{N}}$ is μ-u.d. in X if and only if*

$$\lim_{N\to\infty} \frac{\#(J;N)}{N} = \mu(J)$$

holds for all μ-continuity sets $J \subseteq X$.

Here, by $\#(J;N)$ we mean the cardinality of the set $J \cap \{\boldsymbol{x}_n\}_{n=1}^N$.

An equivalent way to describe the uniform distribution of a sequence is in terms of the discrepancy $\left|\frac{\#(J;N)}{N} - \mu(J)\right|$.

For $[0,1)^d$ and $\mu = \lambda_d$ (the Lebesgue measure) it is commonly used the following definition of the discrepancy of a point set.

Definition 2. Let $P = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{N-1}\}$ denote a finite point set in $[0,1)^d$ and $\mathcal{B}$ a nonempty family of Jordan measurable subsets of $[0,1)^d$. Then

$$D_N(\mathcal{B};P) := \sup_{B\in\mathcal{B}} \left| \frac{\#(B;N;P)}{N} - \lambda_d(B) \right|.$$

Depending on the family $\mathcal{B}$ we can distinguish the discrepancies as follows.

- *Star discrepancy*: $D_N^*(P) = D_N(\mathcal{J}^*; P)$, where $\mathcal{J}^*$ is the family of all subintervals of $[0,1)^d$ of the form $\prod_{i=1}^d [0, a_i)$.
- *Extreme discrepancy*: $D_N(P) = D_N(\mathcal{J}; P)$, where $\mathcal{J}$ is the family of all subintervals of $[0,1)^d$ of the form $\prod_{i=1}^d [a_i, b_i)$.
- *Isotropic discrepancy*: $J_N(P) = D_N(\mathcal{C}; P)$, where $\mathcal{C}$ is the family of all convex subsets of $[0,1)^d$.

The star-discrepancy is important on $[0,1)^d$ in estimating the error of the QMC method by the Koksma–Hlawka inequality (see e.g. [12]).

Theorem 2 *(Koksma–Hlawka inequality). If f has multivariate bounded variation $V(f)$ on $[0,1)^d$ (in the sense of Hardy and Krause) then for every $P = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset [0,1)^d$*

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\boldsymbol{x}_n) - \int_{[0,1)^d} f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \right| \leq V(f) D_N^*(P), \tag{2}$$

where $D_N^*(P)$ is the star-discrepancy of P.

For the QMC method, thanks to this inequality it is natural to take low-discrepancy sequences. Low-discrepancy sequences are those whose star discrepancy has decay order $\log(N)^d/N$, which is the best known order of decay. Some examples of low-discrepancy sequences are: Halton, Hammersley, Sobol and the Fibonacci lattice (for details see e.g. [5]).

On the other hand, if we integrate a function using the QMC method on *convex* subsets of $[0,1)^d$ we have a similar inequality due to Zaremba (see [18]) where the isotropic discrepancy, J_N, is used.

Theorem 3. *Let $B \subseteq [0,1)^d$ be a convex subset and f a function with bounded variation $V(f)$ on $[0,1)^d$ in the sense of Hardy and Krause. Then, for any point set $P = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subseteq [0,1)^d$, we have that*

$$\left| \frac{1}{N} \sum_{\substack{i=1 \\ \boldsymbol{x}_i \in B}}^{N} f(\boldsymbol{x}_i) - \int_B f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \right| \leq (V(f) + |f(\mathbf{1})|) J_N(P), \tag{3}$$

where $\mathbf{1} = (1, \dots, 1)$.

On a smooth compact d-dimensional manifold there is a Koksma–Hlawka like inequality (see [4]).

Theorem 4. *Let $\mathcal{M}$ be a smooth compact d-dimensional manifold with a normalized measure $\mathrm{d}x$. Fix a family of local charts $\{\varphi_k\}_{k=1}^K$, $\varphi_k : [0,1)^d \to \mathcal{M}$, and a smooth partition of unity $\{\psi_k\}_{k=1}^K$ subordinate to these charts. Then, there exists a number $c > 0$, which depends on the local charts but not on the function f or the measure μ, such that*

$$\left| \int_{\mathcal{M}} f(y) \overline{\mathrm{d}\mu(\boldsymbol{y})} \right| \leq c \mathcal{D}(\mu) ||f||_{W^{d,1}(\mathcal{M})}, \tag{4}$$

where $\mathcal{D}(\mu) = \sup_{U \in \mathcal{A}} \left| \int_U \mathrm{d}\mu(\boldsymbol{y}) \right|$, $\mathcal{A}$ is the collection of all images of intervals in $\mathcal{M}$ and

$$||f||_{W^{n,p}(\mathcal{M})} = \sum_{1 \leq k \leq K} \sum_{|\alpha| \leq n} \left(\int_{[0,1)^d} \left| \frac{\partial^\alpha}{\partial x^\alpha} (\psi_k(\varphi_k(x)) f(\varphi_k(x))) \right|^p \mathrm{d}x \right)^{1/p},$$

with $W^{n,p}$ a Sobolev space.

Notice that, if $\mathrm{d}\mu = \frac{1}{N} \sum_{\boldsymbol{x} \in X_N} \delta_{\boldsymbol{x}} - \mathrm{d}\boldsymbol{x}$ in (4), we have the analogue of the Koksma–Hlawka inequality for manifolds. Therefore, in order to minimize the error, we have to minimize the discrepancy.

We also remark that in general is not easy to compute an estimate of the error using this inequality since we have to compute the supremum of the collection of all images of intervals in the manifold.

The case of the sphere has been solved by a different approach. Let $\mathbb{S}^2$ be the 2-sphere, then (see e.g. [14]) it is proved that, the worst case error

$$\sup_f \left| \frac{1}{N} \sum_{\boldsymbol{x} \in X_N} f(\boldsymbol{x}) - \frac{1}{4\pi} \int_{\mathbb{S}^2} f(\boldsymbol{x}) \mathrm{d}\sigma(\boldsymbol{x}) \right|$$

is proportional to the *distance-based energy metric*

$$E_N(X_N) = \left(\frac{4}{3} - \frac{1}{N^2} \sum_{\boldsymbol{x}_i \in X_N} \sum_{\boldsymbol{x}_j \in X_N} |\boldsymbol{x}_i - \boldsymbol{x}_j| \right)^{1/2}.$$

The proof is based on the *Stolarsky's invariance principle* (see e.g. [16,17,15]).

Thus, if we want to minimize the worst case error we have to maximize the sum of distance term $\sum_{\boldsymbol{x}_i \in X_N} \sum_{\boldsymbol{x}_j \in X_N} |\boldsymbol{x}_i - \boldsymbol{x}_j|$ which is easier to check computationally than the calculation of the spherical cap discrepancy.

This is the reason why in the next section we explore the use of sequences uniformly distributed with respect to the Hausdorff measure on a given manifold $\mathcal{M}$.

3. Measure preserving maps on 2-manifolds

Let $\mathcal{S} = (X_N)_{N \geq 1}$ be uniformly distributed with respect to the Lebesgue measure on a rectangle $\mathcal{U} \subset \mathbb{R}^2$, $\mathcal{M}$ a regular manifold of dimension 2 and Φ a map from $\mathcal{U}$ to $\mathcal{M}$.

Take $A \subset \mathcal{M}$. The measure μ_Φ of A in $\mathcal{M}$ is defined as

$$\mu_\Phi(A) := \lambda_2(\Phi^{-1}(A)) = \int_{\Phi^{-1}(A)} \mathrm{d}\lambda_2.$$

By construction, the sequence $\Phi(\mathcal{S})$ is then uniformly distributed with respect to the measure μ_Φ.

Now, let us consider the Hausdorff measure $\mathcal{H}_2$ on the manifold $\mathcal{M}$ which, by means of the area formula [8, p. 353] is

$$\int_{\mathcal{U}} g(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}, \tag{5}$$

with g a density function that depends on the parametrization Φ of $\mathcal{M}$. We look for a change of variables from another rectangle $\mathcal{U}' \subset \mathbb{R}^2$ to $\mathcal{U}$ such that

$$\begin{array}{rccl} \Psi: & \mathcal{U}' & \longrightarrow & \mathcal{U} \\ & \boldsymbol{x}' & \longrightarrow & \Psi(\boldsymbol{x}') = \boldsymbol{x}. \end{array} \tag{6}$$

Then, we wish that

$$g(\Psi(\boldsymbol{x}'))|J\Psi(\boldsymbol{x}')| = g(\boldsymbol{x}) = 1. \tag{7}$$

This is equivalent to equalize the "natural" measure $\mu_{\Phi \circ \Psi}$ (which comes from the parametrization) and the Hausdorff measure $\mathcal{H}_2$ on the manifold $\mathcal{M}$:

$$\mathcal{H}_2(\mathcal{M}) = \int_{\mathcal{U}} g(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \int_{\mathcal{U}'} g(\Psi(\boldsymbol{x}'))|J\Psi(\boldsymbol{x}')| \mathrm{d}\boldsymbol{x}' = \int_{\mathcal{U}'} \mathrm{d}\boldsymbol{x}' = \mu_{\Phi \circ \Psi}(\mathcal{M}).$$

Summarizing, starting from a sequence $\mathcal{S}'$ uniformly distributed with respect to the Lebesgue measure on a rectangle $\mathcal{U}' \subset \mathbb{R}^2$, using the change of variables (6), we will get the sequence $\Phi(\Psi(\mathcal{S}'))$ that will be uniformly distributed with respect to the measure $\mathcal{H}_2$ on $\mathcal{M}$.

Proposition 1. *Let $\mathcal{U}$ be a reference rectangle in $\mathbb{R}^2$ and $\Phi : \mathcal{U} \to \mathcal{M}$ the corresponding measure preserving map. The measure preserving maps for the cone, cylinder and sphere are:*

$$\begin{array}{lll} \textit{cone:} & \mathcal{U} = [0,1] \times [0, 2\pi] & \Phi(u,\theta) = (\sqrt{u}\cos(\theta), \sqrt{u}\sin(\theta), \sqrt{u}) \\ \textit{cylinder:} & \mathcal{U} = [-1,1] \times [0, 2\pi] & \Phi(u,\theta) = (\cos(\theta), \sin(\theta), u) \\ \textit{sphere:} & \mathcal{U} = [-1,1] \times [0, 2\pi] & \Phi(u,\theta) = (\sqrt{1-u^2}\cos(\theta), \sqrt{1-u^2}\sin(\theta), u). \end{array}$$

Proof. It is an easy exercise. □

Notice that another possible way of computing the integral is by taking any coordinate chart for the parametrization $\varphi : \mathcal{U} \to \mathcal{M}$ of the manifold and then integrate with the QMC method directly in $\mathcal{U} \subset \mathbb{R}^2$ with a low-discrepancy sequence multiplying the integrating function by the determinant of the Jacobian of φ. Unfortunately, with this approach we will not have points which will lie on the manifold. In fact, mapping the points directly with the parametrization φ will not give a sequence of points uniformly distributed with respect to the Hausdorff measure of the manifold. This approach also depends on the determinant of the Jacobian since it will make the integrating function a different function.

4. Minimal Riesz-energy points

We start by introducing the s-Riesz energy of a set of points.

Definition 3 *(cf. [10]).* Let $X_N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \subset A \subseteq \mathbb{R}^d$ be a set of N distinct points. For each real $s > 0$, the s-Riesz energy of X_N is

$$E_s(X_N) := \sum_{\substack{\boldsymbol{x}, y \in X_N \\ \boldsymbol{x} \neq \boldsymbol{y}}} \frac{1}{|\boldsymbol{x} - \boldsymbol{y}|^s}, \tag{8}$$

where $|\cdot|$ denotes the Euclidean distance in $\mathbb{R}^d$. The N-point minimal s-energy over A is then

$$\mathcal{E}_s(A, N) := \inf_{X_N \subset A} E_s(X_N) \tag{9}$$

Note that in (9), by convention, the sum over an empty set of indices is taken to be zero and the infimum over an empty set is ∞. Notice also that $\mathcal{E}_s(A, N) = \mathcal{E}_s(\bar{A}, N)$ and $\mathcal{E}_s(A, N) = 0$ if A is unbounded. Hence, without loss of generality, we could restrict ourselves to the case when A is compact.

A Continuous and Positive on the Diagonal (CPD) weight function is defined as follows.

Definition 4. Let $A \subset \mathbb{R}^d$ be an infinite compact set whose d-dimensional Hausdorff measure $\mathcal{H}_d(A)$ is finite. A symmetric function $w : A \times A \to [0, +\infty)$ is called a CPD weight function on $A \times A$ if

(i) w is continuous as function on $A \times A$ at $\mathcal{H}_d$-almost every point of the diagonal $D(A) = \{(\boldsymbol{x}, \boldsymbol{x}) : \boldsymbol{x} \in A\}$,
(ii) there is some neighborhood G of $D(A)$ such that $\inf_G w > 0$,
(iii) w is bounded on any closed subset $B \subset A \times A$ such that $B \cap D(A) = \emptyset$.

This definition allows us to define the weighted Riesz s-energy of a point set X_N, of a subset $A \subset \mathbb{R}^d$ and the weighted Hausdorff measure of Borel sets $B \subset A$.

Definition 5. Let $s > 0$ and $X_N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \subset A$. The weighted Riesz s-energy of X_N is

$$E_s^w(X_N) := \sum_{1 \leq i \neq j \leq N} \frac{w(\boldsymbol{x}_i, \boldsymbol{x}_j)}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^s},$$

the N-point weighted Riesz s-energy of A is

$$\mathcal{E}_s^w(A, N) := \inf\{E_s^w(X_N) : X_N \subset A, \, \#X_N = N\},$$

and the weighted Hausdorff measure $\mathcal{H}_d^{s,w}$ on Borel sets $B \subset A$ is then

$$\mathcal{H}_d^{s,w}(B) := \int_B (w(\boldsymbol{x}, \boldsymbol{x}))^{-d/s} \mathrm{d}\mathcal{H}_d(\boldsymbol{x}).$$

We need another property for the set A. A set A is said to be d-rectifiable (see e.g. [7]) if and only if there exists a Lipschitz function ϕ mapping some bounded subset of $\mathbb{R}^d$ onto A, i.e. there exists a constant L and a compact set $B \subset \mathbb{R}^d$ such that

$$|\phi(\boldsymbol{x}) - \phi(\boldsymbol{y})| \leq L|\boldsymbol{x} - \boldsymbol{y}|, \ \forall \boldsymbol{x}, \boldsymbol{y} \in B$$

and $\phi(B) = A$.

The connection between the s-Riesz energy and a sequence uniformly distributed with respect to the Hausdorff measure is given by the **Weighted Poppy-seed Bagel Theorem** (cf. [3,10]).

Theorem 5. *Let $A \subset \mathbb{R}^{d'}$ be a compact subset of a d-dimensional $\mathcal{C}^1$-manifold in $\mathbb{R}^{d'}$, $d < d'$, and w is a CDP weight function on $A \times A$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_d^w(A,N)}{N^2 \log N} = \frac{\mathrm{Vol}(\mathcal{B}^d)}{\mathcal{H}_d^{d,w}(A)}. \tag{10}$$

Furthermore, if $\mathcal{H}_d(A) > 0$ and X_N^* is a sequence of configurations on A satisfying (10), with $\mathcal{E}_d^w(A,N)$ replaced by $E_d^w(X_N^*)$, then

$$\frac{1}{N}\sum_{\boldsymbol{x}\in X_N^*} \delta_{\boldsymbol{x}}(\cdot) \xrightarrow{*} \frac{\mathcal{H}_d^{d,w}(\cdot)_{|_A}}{\mathcal{H}_d^{d,w}(A)} \quad \text{as } N\to\infty. \tag{11}$$

Assume now that $A \subset \mathbb{R}^{d'}$ is a closed d-rectifiable set. Then for $s > d$,

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^w(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{(\mathcal{H}_d^{s,w}(A))^{s/d}}, \tag{12}$$

where $C_{s,d}$ is a finite positive number independent of A and d'. Moreover, if $\mathcal{H}_d(A) > 0$, any sequence X_N^* of configurations on A satisfying (12), with $E_s^w(X_N^*)$ instead of $\mathcal{E}_s^w(A,N)$, satisfies (11).

4.1. Greedy minimal Riesz-energy points

The computation of an approximation of these minimal Riesz s-energy points can be done by the following *greedy algorithm* which provides a good approximation of the minimal set and which attains the correct asymptotic main term for the energy for $s < d$.

Algorithm 1. Let $k : X \times X \to \mathbb{R}\cup\{\infty\}$ be a symmetric lower-semicontinuous kernel on a locally compact Hausdorff space X, and let $A \subset X$ be a compact set. A sequence $(a_n)_{n=1}^{\infty} \subset A$ such that

(i) a_1 is selected arbitrarily on A;
(ii) for $n \geq 1$, a_{n+1} is chosen so that

$$\sum_{i=1}^{n} k(a_{n+1}, a_i) = \inf_{\boldsymbol{x}\in A} \sum_{i=1}^{n} k(\boldsymbol{x}, a_i), \qquad \text{for every } n \geq 1.$$

The sequence $\{a_n\}_{n\geq 1}$ is called a `greedy minimal k-energy sequence on A` (or `Léja-Gorski points`). The Riesz kernel in $X = \mathbb{R}^{d'}$, which depends on the parameter $s \in [0, +\infty)$, is the radial kernel

$$k_s(\boldsymbol{x}, \boldsymbol{y}) := K_s(\|\boldsymbol{x} - \boldsymbol{y}\|), \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^{d'},$$

where $\|\cdot\|$ is the Euclidean norm, with

$$K_s(t) := \begin{cases} t^{-s} & \text{if } s > 0 \\ -\log(t) & \text{if } s = 0. \end{cases}$$

Hence, for $k = K_s$ we generate the **greedy minimal k_s-energy points**, while taking $k = w\, K_s$ we get the **greedy minimal (w,s)-energy points**.

As proved in [13] for the unit sphere $\mathbb{S}^d$, the greedy minimal (w,d)-energy points are asymptotically distributed as the real ones suggesting that they can be a good choice for integration on manifolds.

Theorem 6. *Assume that $w : \mathbb{S}^d \times \mathbb{S}^d \to [0, +\infty)$ is a continuous function such that $w(\boldsymbol{x}, \boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in \mathbb{S}^d$. Let $\{X_{N,d}^w\}$ be an arbitrary greedy (w,d)-energy sequence on $\mathbb{S}^d$, $d \geq 1$. Then*

$$\lim_{N\to\infty} \frac{E_d^w(X_{N,d}^w)}{N^2 \log N} = \frac{\mathrm{Vol}(\mathcal{B}^d)}{\mathcal{H}_d^{d,w}(\mathbb{S}^d)},$$

and furthermore

$$\frac{1}{N}\sum_{\boldsymbol{x}\in X_{N,d}^w} \delta_{\boldsymbol{x}}(\cdot) \to \frac{\mathcal{H}_d^{d,w}(\cdot)_{|_{\mathbb{S}^d}}}{\mathcal{H}_d^{d,w}(\mathbb{S}^d)}.$$

In particular, any greedy k_d-energy sequence $(X_{N,d})$ on $\mathbb{S}^d$ is asymptotically d-energy minimizing on $\mathbb{S}^d$.

Unfortunately this result is not valid for $s > d$. On the other hand, for any compact $A \subset \mathbb{R}^{d'}$ with $\mathcal{H}_\delta(A) > 0$ (where δ is arbitrary), the following order of growth for $E_s^w(X_{N,s}^w)$ holds (cf. [13]).

Theorem 7. *Let*

$$\mathcal{H}_\delta^\infty(A) := \inf\left\{\sum_i (\operatorname{diam} G_i)^\delta \,:\, A \subset \cup_i G_i\right\}, \quad 0 < \delta \le d'.$$

Assume $A \subset \mathbb{R}^{d'}$ be compact with $\mathcal{H}_\delta(A) > 0$. Let w be a bounded lower semicontinuous CDP weight function on $A \times A$ and consider an arbitrary greedy (w,s)-energy sequence $(X_{N,s}^w) \subset A$, for $s \ge \delta$. Then for $N \ge 2$

$$E_s^w(X_{N,s}^w) \le \begin{cases} M_{s,\delta,A}||w||\mathcal{H}_\delta^\infty(A)^{-s/\delta}N^{1+s/\delta}, & s > \delta \\ M_{\delta,A}||w||\mathcal{H}_\delta^\infty(A)^{-1}N^2\log N, & s = \delta, \end{cases} \tag{13}$$

where $M_{s,\delta,A}, M_{\delta,A} > 0$ are independent of w and N, and $||w|| = \sup\{w(\boldsymbol{x},\boldsymbol{y}) : \boldsymbol{x},\boldsymbol{y} \in A\}$.

The previous theorem leads us to the following Corollary which is helpful to understand the use of greedy (w,s)-sequences for integration on manifolds.

Corollary 1. *Let $A \subset \mathbb{R}^{d'}$ be a d-rectifiable set. Suppose $s > d$ and w is a bounded lower semicontinuous CDP weight function on $A \times A$. Consider an arbitrary greedy (w,s)-energy sequence $(X_{N,s}^w) \subset A$. Then $(X_{N,s}^w)$ is dense in A. If $s = d$ and A is assumed to be a compact subset of a d-dimensional $\mathcal{C}^1$-manifold, the same conclusion holds for any greedy (w,d)-energy sequence. Taking $w = 1$ the result is applicable to greedy k_s-energy sequences.*

Remark. We do not know yet if greedy minimal (w,d)-energy (or k_s) sequences are a good choice for integrating functions on a manifold with respect to the measure $\mathcal{H}_d^w$ as it is for the minimal energy points. Or whether we should prefer them to a low discrepancy sequences mapped on the manifold with measure preserving maps. This is what we try to understand by the numerical experiments in the next section.

5. Numerical experiments

In this section we present some numerical tests showing that the greedy minimal k_s-energy sequences are a good choice for integrating a function when a measure preserving map is available, whereas they have a similar behavior of low-discrepancy sequences if instead a generic map is used.

The functions we consider on the cone, cylinder, sphere and torus are

$$\begin{aligned} f_1(x,y,z) &:= \sqrt{(1+z)(1-z)}\cos\left(\frac{x}{2}+\frac{y}{3}+\frac{z}{5}\right), \\ f_2(x,y,z) &:= \begin{cases} \cos(30xyz) & \text{if } z < \frac{1}{2} \\ (x^2+y^2+z^2)^{3/2} & \text{if } z \ge \frac{1}{2}, \end{cases} \\ f_3(x,y,z) &:= e^{-\sin(2x^2+3y^2+5z^2)}, \\ f_4(x,y,z) &:= \frac{e^{-\sqrt{x^2+y^2+z^2}}}{1+x^2}\cos(1+x^2)\sin(1-y^2)e^{|z|}. \end{aligned} \tag{14}$$

To compute the integrals

$$\frac{1}{\mathcal{H}_d(\mathcal{M})}\int_{\mathcal{M}} f_i(\boldsymbol{x})\mathrm{d}\mathcal{H}_d(\boldsymbol{x}), \quad i = 1,\dots,4$$

we use the QMC method with

(a) low discrepancy points mapped on the manifolds,
(b) greedy minimal k_s-energy points.

To emphasize the significance of the QMC approach we did also a comparison with the MC method taking N points randomly distributed on the rectangle and then mapped on the manifolds. Because of the random nature of these points, we computed 10 times the integrals with MC and averaged them.

About (b), to compute N greedy minimal k_s-energy points we started from a uniform mesh on a rectangle consisting of $N^2/2$ points and mapped them, if available by using the corresponding measure preserving map, to the manifold. Then we

Table 1
Map for the torus (d).

$$[0,2\pi]\times[0,2\pi]\ni(u,v)\rightarrow\begin{cases}x=(2+\cos(u))\cos(v)\\ y=(2+\cos(u))\sin(v)\\ z=\sin(u)\end{cases}\tag{15}$$

Table 2
Exact values of the integrals.

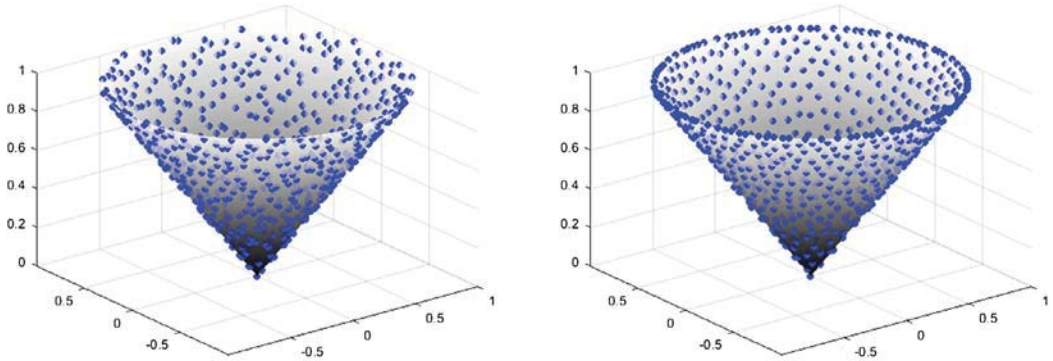
	Cone	Cylinder	Torus	Sphere
f_1	6.378e−01	7.125e−01	3.435e−01	7.295e−01
f_2	0.130e+01	5.784e−01	0.470e+01	2.809e−01
f_3	0.116e+01	0.132e+01	0.131e+01	0.1340e+01
f_4	1.458e−01	−1.160e−01	−1.269e−02	8.950e−02

extracted N greedy minimal k_s-energy points from this mapped mesh. Here $s=2$ because of the dimension of the manifold (a surface immersed in $\mathbb{R}^3$).

For the torus we used the map (Table 1) which does not preserve the Lebesgue measure.

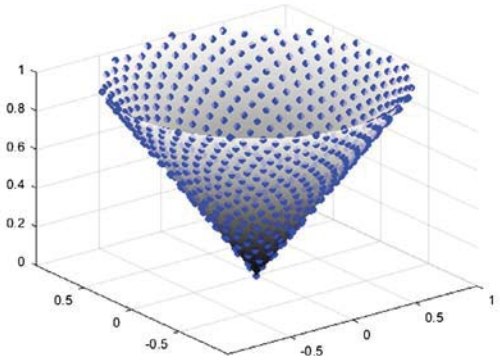
To compare the results with the greedy minimal k_2-energy points, we computed the integrals (Table 2) by QMC method using Halton points and Fibonacci lattices mapped on the manifolds. Because of the peculiarity of Fibonacci points, we generated for all sequences a number of points like the Fibonacci sequence, starting from 144 (i.e. the twelfth Fibonacci number) up to 2584, the eighteenth Fibonacci number (Figs. 1–4). But in the tables below (Tables 3–19) the results are only presented for 144, 610 and 2584 points. The exact value of the integral has been considered, after a variable change, using the built-in Matlab function *dblquad* with tolerance of 10^{-11}. The relative errors are then computed referring to this value. Here only some experiments on the cone, cylinder, sphere and the torus are presented. More experiments are available in the Master's thesis of the second author (see [6]). All the tests have been performed on a laptop with Intel Core i3-3120M @2.50 GHz, 4GB of RAM, Windows 10 and MATLAB 8.5.0.197613.

The Matlab package GMKs (*Greedy Minimal k_s points*) allows to reproduce all the experiments presented here and interested people can download it at http://www.math.unipd.it/~demarchi/software/GMKs.



(a) Halton points

(b) Greedy minimal k_2-energy points



(c) Fibonacci points

Fig. 1. 610 points on the cone.

Table 3
Relative errors for f_1 on the cone with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.215e−02	5.352e−03	2.097e−01	1.325e−02
610	4.939e−03	1.270e−03	1.470e−01	6.137e−03
2584	1.241e−03	3.029e−04	9.817e−02	4.850e−03

Table 4
Relative errors for f_2 on the cone with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

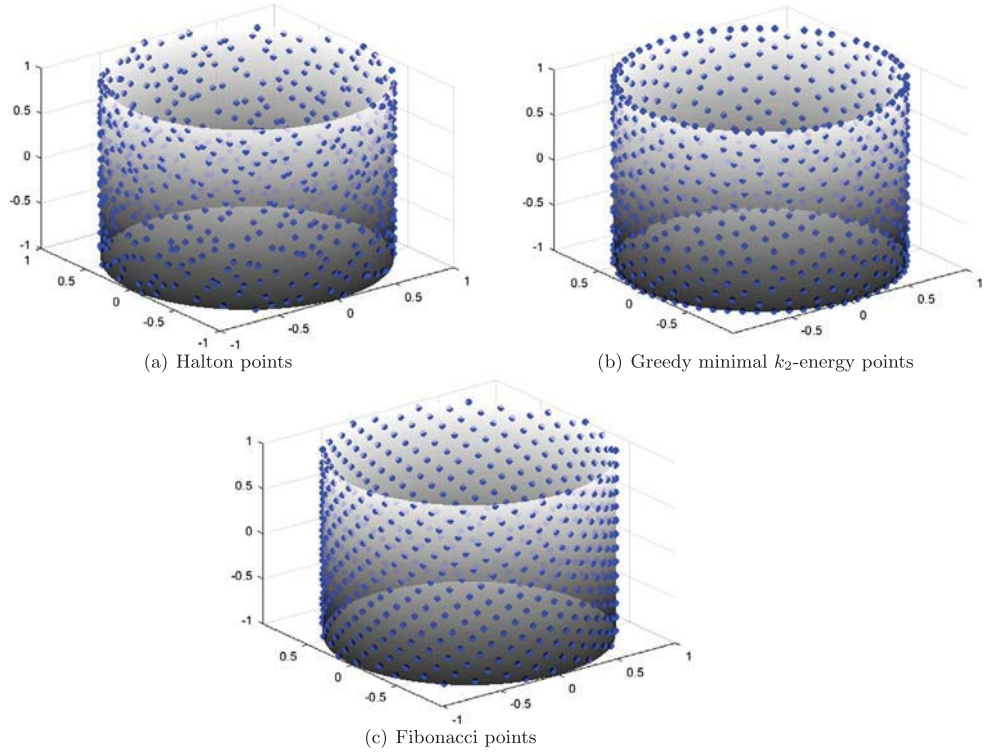
N	Halton	Fibonacci	GM k_2	MC
144	9.101e−03	6.250e−03	2.366e−01	3.498e−02
610	5.277e−03	1.173e−03	1.764e−01	2.294e−02
2584	6.766e−04	3.678e−04	1.212e−01	8.212e−03

Table 5
Relative errors for f_3 on the cone with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.059e−02	1.416e−03	7.048e−02	4.324e−02
610	3.763e−04	3.389e−04	7.172e−02	2.050e−02
2584	1.289e−04	8.026e−05	3.790e−02	1.613e−02

Table 6
Relative errors for f_4 on the cone with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	2.767e−02	1.384e−02	2.333e−01	8.209e−02
610	9.623e−03	3.230e−03	1.782e−01	1.708e−02
2584	3.068e−03	7.594e−04	1.313e−01	1.818e−02



(a) Halton points

(b) Greedy minimal k_2-energy points

(c) Fibonacci points

Fig. 2. 610 points on the cylinder.

Table 7
Relative errors for f_1 on the cylinder with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.092e−03	5.264e−04	2.240e−01	3.043e−02
610	3.131e−04	6.400e−05	1.603e−01	9.933e−03
2584	1.029e−04	6.929e−06	9.533e−02	5.645e−03

Table 8
Relative errors for f_2 on the cylinder with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

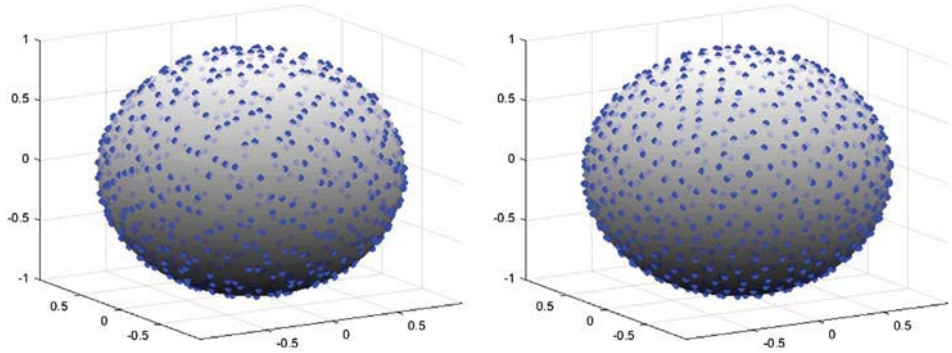
N	Halton	Fibonacci	GM k_2	MC
144	6.513e−02	8.764e−03	3.830e−01	1.597e−01
610	2.900e−02	2.964e−03	2.267e−01	4.026e−02
2584	1.436e−03	6.975e−04	1.502e−01	2.273e−02

Table 9
Relative errors for f_3 on the cylinder with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.792e−02	2.930e−04	1.150e−01	4.584e−02
610	2.359e−03	1.125e−05	8.751e−02	1.633e−02
2584	3.287e−04	6.267e−07	4.895e−02	7.310e−03

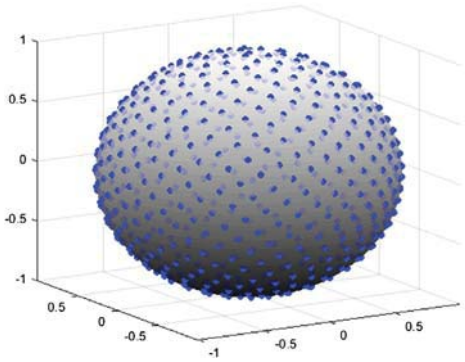
Table 10
Relative errors for f_4 on the cylinder with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	6.611e−03	1.506e−04	3.879e−02	2.047e−01
610	1.457e−02	8.382e−06	2.524e−02	8.602e−02
2584	4.730e−04	4.671e−07	2.339e−02	5.468e−02



(a) Halton points

(b) Greedy minimal k_2-energy points



(c) Fibonacci points

Fig. 3. 610 points on the sphere.

Table 11
Relative errors for f_1 on the sphere with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	2.833e−03	6.448e−04	1.595e−03	1.974e−02
610	1.001e−03	7.411e−05	1.202e−03	7.526e−03
2584	1.017e−04	8.504e−06	1.324e−03	4.495e−03

Table 12
Relative errors for f_2 on the sphere with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

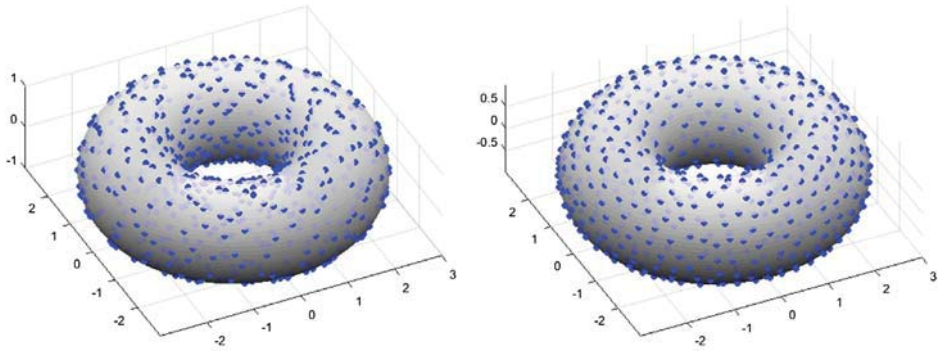
N	Halton	Fibonacci	GM k_2	MC
144	1.476e−01	1.089e−02	8.406e−02	1.281e−01
610	4.415e−02	8.045e−05	4.872e−03	1.080e−01
2584	6.847e−04	3.115e−06	5.177e−03	4.666e−02

Table 13
Relative errors for f_3 on the sphere with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	3.282e−03	1.025e−04	2.834e−03	4.531e−02
610	1.755e−03	5.727e−06	2.251e−03	1.244e−02
2584	7.294e−05	3.190e−07	1.325e−03	8.174e−03

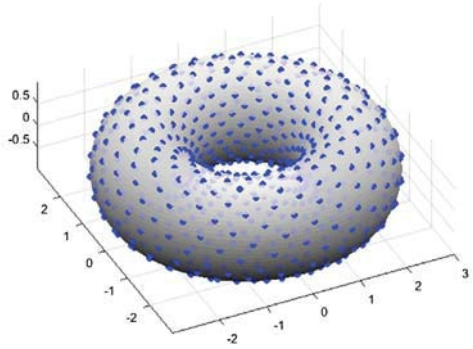
Table 14
Relative errors for f_4 on the sphere with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.549e−03	1.425e−03	1.912e−03	1.113e−01
610	6.631e−03	7.970e−05	3.702e−03	4.988e−02
2584	2.725e−04	4.442e−06	4.756e−03	1.955e−02



(a) Halton points

(b) Greedy minimal k_2-energy points



(c) Fibonacci points

Fig. 4. 610 points on the torus.

Table 15
Relative errors for f_1 on the torus with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	2.152e−01	1.777e−01	6.894e−02	2.030e−01
610	1.888e−01	1.780e−01	5.367e−02	1.768e−01
2584	1.788e−01	1.780e−01	4.014e−02	1.687e−01

Table 16
Relative errors for f_2 on the torus with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	1.218e−01	1.690e−01	3.081e−02	1.778e−01
610	1.453e−01	1.410e−01	4.728e−02	1.272e−01
2584	1.414e−01	1.411e−01	2.297e−02	1.562e−01

Table 17
Relative errors for f_3 on the torus with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	3.033e−02	3.426e−02	4.949e−03	4.531e−01
610	2.716e−03	8.821e−03	1.349e−02	2.811e−01
2584	8.763e−03	6.453e−03	1.673e−03	1.049e−01

Table 18
Relative errors for f_4 on the torus with Fibonacci, Halton, Greedy Minimal k_2-energy points and MC method.

N	Halton	Fibonacci	GM k_2	MC
144	6.015e−01	5.339e−01	2.435e−01	5.692e−01
610	5.109e−01	5.237e−01	1.874e−01	4.779e−01
2584	5.252e−01	5.238e−01	1.319e−01	5.238e−01

Table 19
Time in seconds to compute the greedy minimal k_2-energy points.

N	Cone	Cylinder	Torus	Sphere
144	0.217	0.218	0.248	0.208
610	20.067	21.046	19.340	19.284
2584	1519.112	1513.211	1571.449	1511.768

5.1. Greedy minimal k_s-energy points: tuning the parameter s

In the previous section we set $s = 2$ because of the dimension, but we can consider a tuning of s and see how the errors change as a function of s. The script *demo2* of the Matlab package GMKs, previously mentioned, allows us to make the experiments that we are going to present.

In Figs. 5–8, we see the behavior of the relative errors of the integrals for $s \in [0, 10]$, with step 0.05, using 200 greedy minimal k_s-energy points.

6. Conclusion

In this paper we tested the QMC integration on manifolds by mapped low-discrepancy points and greedy minimal k_s-energy points.

Analyzing the relative errors we observed that if we have a measure preserving map it is better to use low-discrepancy sequences, especially the Fibonacci ones, than greedy minimal k_2-energy points. On the other hand, if we do not dispose of a measure preserving map, as in the case of the torus, or we use mapped points by another parametrization, the best approximation are with the greedy minimal k_2-energy points (as in the case of the functions f_1 and f_2). The time for extracting the greedy minimal k_s-energy points grows as the number of points. Therefore, in the case of greedy minimal energy points it is advisable to use less points especially in case of reduced computational resources. Moreover by using an increasing number of greedy minimal energy points the errors decay, but slower than mapped low-discrepancy points.

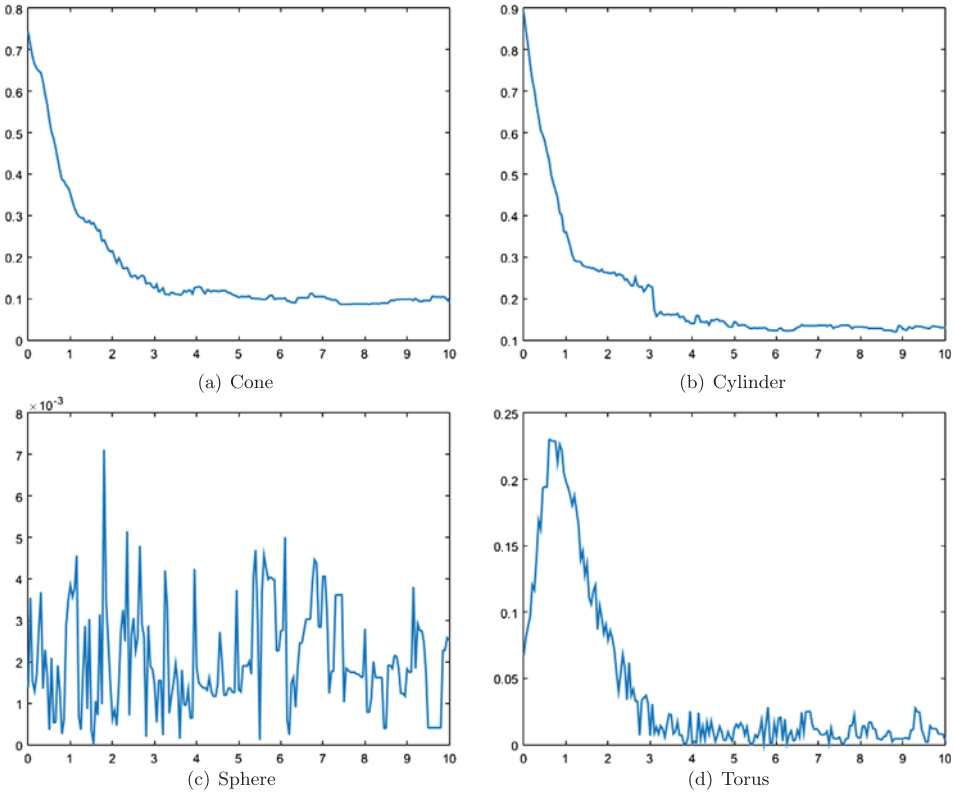


Fig. 5. Relative errors using 200 points for the function f_1.

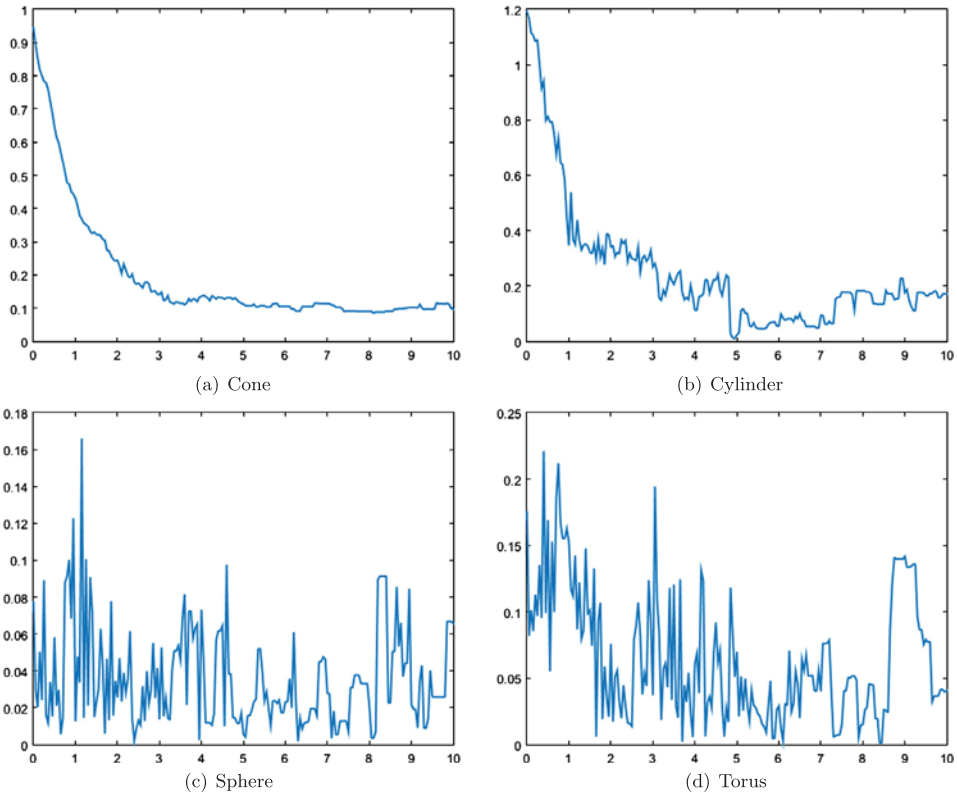


Fig. 6. Relative errors using 200 points for the function f_2.

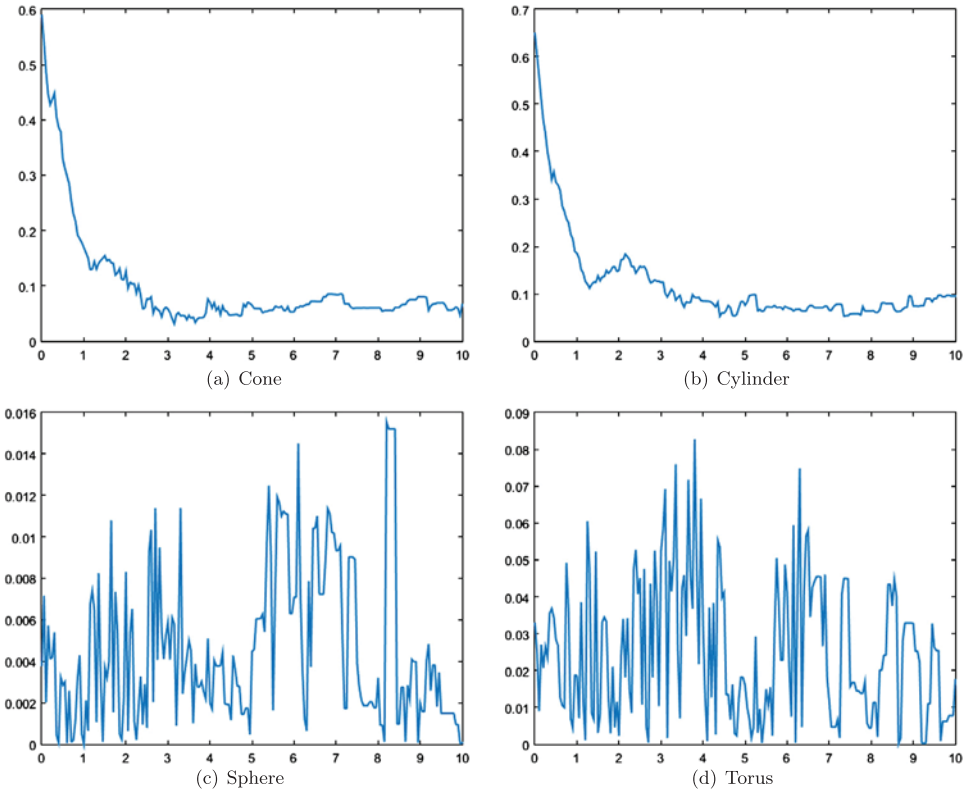


Fig. 7. Relative errors using 200 points for the function f_3.

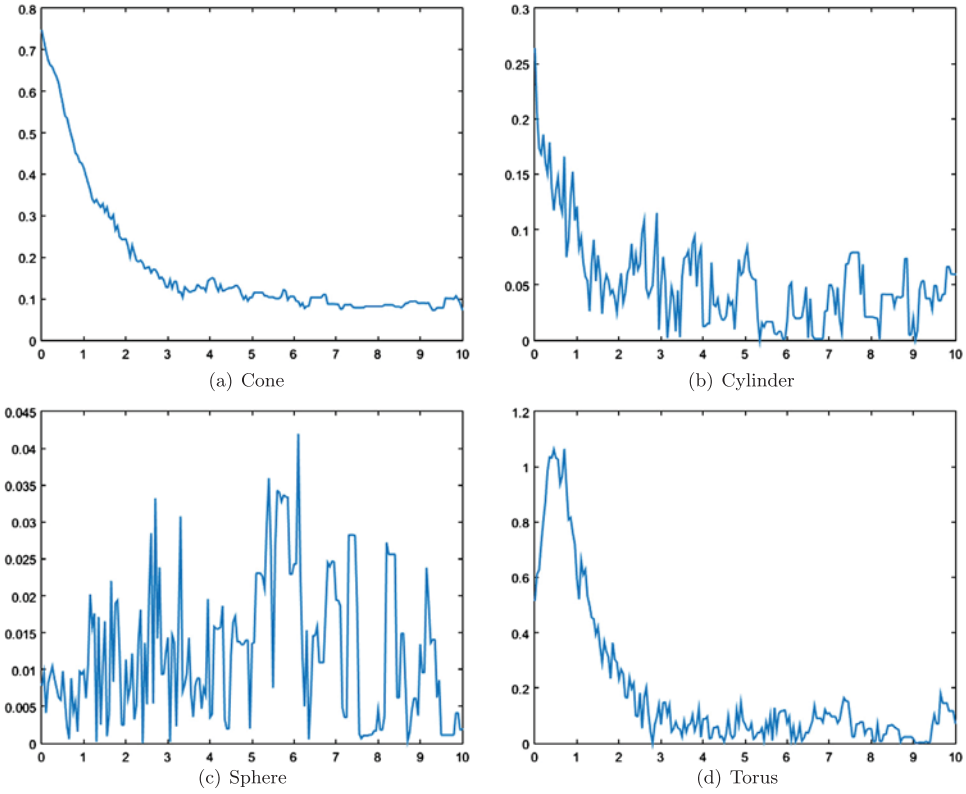


Fig. 8. Relative errors using 200 points for the function f_4.

We have also noticed that keeping the same number of points but tuning the parameter s, values below the manifold dimension (in our case $s = 2$) should be avoidable since the relative errors are worse than those for $s > 2$. Indeed for $s > 2$ the relative errors showed to be almost of the same order and, as suggested by the theory, the "optimal" s is around the manifold dimension. The only exception is the sphere, where we obtained relative errors of the same order for all values of the parameter.

We wish also to underline that the QMC approach for integration on manifolds is preferable to the MC method as confirmed by all tests. Producing points well distributed on a manifold could be useful not only for QMC integration on manifolds but also for other approximation methods involving sequences of points on manifolds such as radial basis functions (RBF) approximation or meshless approximation of PDEs. These are future works that we wish to investigate more deeply.

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