Integration on manifolds by mapped low-discrepancy points and greedy minimal k_s-energy points[1]

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[1] joint work with G. Elefante (Fribourg - CH)

Outline

Motivations and aims

Facts

- Integrate functions on manifolds by QMC method: low-discrepancy points (Sobol, Hammersley, Fibonacci lattices,...)

$$\int_X f(x)\mathrm{d}x \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i), \quad x_i \in X$$

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- Take

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

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- Poppy-seed Bagel Theorem (PsB) [Hardin, Saff 2004]: *"minimal Riesz s-energy points, under some assumptions, are uniformly distributed with respect to the Hausdorff measure $\mathcal{H}_d$"*

Aims

Observe that from the (PsB)-Theorem, the Riesz s-energy points can be useful for a QMC method when using the Hausdorff measure

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Ideas

- Find a measure preserving map so that we can map low discrepancy poins to points nearly uniformly distributed wrt the Hausdorff measure on the manifold
- Extract approximate minimal Riesz s-energy points from a suitable discretization of the manifold
- Compare results

Preserving measure maps (on 2-manifolds)

Error bound on bounded domains and discrepancy

Theorem (Zaremba 1970)

Let $B \subseteq [0,1)^d$ be a convex d-dimensional subset and f a function with bounded variation $V(f)$ on $[0,1)^d$ in the sense of Hardy and Krause. Then, for any points set $P = \{x_1, \ldots, x_N\} \subseteq [0,1)^d$, we have that

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

where $\mathbf{1} = \underbrace{(1, \ldots, 1)}_{d}$.

where $J_N(P)$ is the *isotropic discrepancy* of the points set P defined as $J_N(P) = D_N(C; P)$ with C a family of all convex subsets of $[0,1)^d$ and $D_N(C; P)$ the classical *discrepancy* of the set P.

Error bound on manifolds and discrepancy

Theorem (Brandolini et al. JoC 2013)

Let $\mathcal{M}$ be a smooth compact 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 $c > 0$ depending only on the local charts (not on the function f and the measure μ),

$$\left| \int_{\mathcal{M}} f(y)\overline{\mathrm{d}\mu(y)} \right| \le c\mathcal{D}(\mu)\|f\|_{W^{d,1}(\mathcal{M})}, \tag{2}$$

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

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

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Notice: if $\mathrm{d}\mu = \frac{1}{N} \sum_{x \in X_N} \delta_x - \mathrm{d}x$ in (2), we have the analogue of the Koksma-Hlawka inequality for manifolds

On $\mathcal{M} = \mathbb{S}^2$

- It is not easy to compute an estimate of the error using the previous inequality
- If $\mathcal{M} = \mathbb{S}^2$ [Marques et al. 2013] observed that minimizing the spherical cap discrepancy (s.c.d.) is equivalent to minimize the w.c.e. (worst case error)

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

with $\mathcal{H}$ a normed function space (C_0 are ok! polynomials $\rightarrow$ sperical design). By using the Stolarsky's invariance principle [Stolarsky '73, Brauchard&Dick 2013], the w.c.e is propotional to the distance-based energy metric

$$E_N(X_N) = \left(\frac{4}{3} - \frac{1}{N^2} \sum_{x_i, x_j \in X_N} |x_i - x_j| \right)^{1/2}.$$

Then we can maximize the term $\sum_{x_i, x_j \in X_N} |x_i - x_j|$ instead of the s.c.d.

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On different manifolds?

Preserving measure maps on 2-manifolds

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construct a sequence which is uniformly distributed w.r.t. Hausdorff measure on $\mathcal{M}$, by a preserving measure map.

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Letting $\mathcal{S} = (X_N)_{N\geq 1}$ uniformly distributed w.r.t. the Lebesgue measure λ on a rectangle $\mathcal{U} \subset \mathbb{R}^2$, $\mathcal{M}$ a regular manifold of dimension 2 and Φ an invertible map from $\mathcal{U}$ to $\mathcal{M}$.

Definition

Let us consider $A \subset \mathcal{M}$. We define the measure $\mu_\Phi(A)$ as

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↪ Hence the sequence of points $\Phi(\mathcal{S})$ is uniformly distributed with respect to the measure μ_Φ (by definition!).

Preserving measure maps on 2-manifolds (cont)

1. Take the measure $\mathcal{H}_2$ on the manifold $\mathcal{M}$ which, by means of the area formula [Folland, p. 353] is of the type

$$\int_{\mathcal{U}} g(x)\mathrm{d}x, \tag{4}$$

with g a density function (that depends on the parametrization Φ of $\mathcal{M}$).

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2. Consider the change of variables from another rectangle $\mathcal{U}' \subset \mathbb{R}^2$

$$\begin{array}{rccc} \Psi : & \mathcal{U}' & \longrightarrow & \mathcal{U} \\ & x' & \mapsto & \Psi(x') = x\,, \end{array} \tag{5}$$

so that

$$g(\Psi(x'))|J\Psi(x')| = g(x) = 1\,, \tag{6}$$

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3. Equating the "natural" measure $\mu_{\Phi\circ\Psi}$ (which comes from the parametrization) and the Hausdorff measure $\mathcal{H}_2$ on the manifold $\mathcal{M}$ we get

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

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Hence, by using (5), the sequence $\Phi(\Psi(\mathcal{S}'))$ ($\mathcal{S}'$ is a sequence uniformly distributed w.r.t. the Lebesgue meas on $\mathcal{U}' \subset \mathbb{R}^2$), will be uniformly distributed wrt the measure $\mathcal{H}_2$ on $\mathcal{M}$.

Practically

Examples: cylinder, cone, sphere

In order to determine the Lebesgue preserving measure's map we look for a nondecreasing function $\phi : I \to I'$, I, with $\phi(I) = I'$

$$\tilde{\Phi}(u, \theta) = (\phi(u)\cos(\theta), \phi(u)\sin(\theta), \phi(u))$$

will preserve the Lebesgue measure. The reparametrization (5) is

$$\Psi(u, \theta) = (\phi(u), \theta). \tag{7}$$

1. cylinder: $\mathcal{U} = [-1, 1] \times [0, 2\pi]$ and $(\phi(u) = u, v)$
2. cone: $\mathcal{U} = [0, 1] \times [0, 2\pi]$, $(\phi(u) = \sqrt{u}, v)$
3. sphere: $\mathcal{U} = [-1, 1] \times [0, 2\pi]$, $(\phi(u) = \arcsin(u), v)$

Minimal Riesz-energy points

s-Riesz energy and points [Hardin&Saff, 2004]

Definition (minimal s-Riesz energy points)

Let $X_N = \{x_1, \ldots, x_N\} \subset A \subseteq \mathbb{R}^d$ be a set of N distinct points. For each real $s > 0$, the s-Riesz energy of X_N is given by

$$E_s(X_N) := \sum_{y \in X_N} \sum_{\substack{x \in X_N \\ x \neq y}} \frac{1}{\|x - y\|_2^s}, \tag{8}$$

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Points that have

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

are minimal s-energy N-points over A.

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Definition

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 (Continuous and Positive on the Diagonal)-weight function on $A \times A$ if w is continuous at $\mathcal{H}_d$-almost every point of the diagonal $D(A) = \{(x, x) : x \in A\}$,

Weighted Riesz s-energy

Definition (weighted Riesz s-energy)

Let $s > 0$. Given N points $X_N = \{x_1, \ldots, x_N\} \subset A \subseteq \mathbb{R}^d$, the weighted Riesz s-energy of X_N is $E_s^w(X_N) := \sum_{1 \le i \ne j \le N} \frac{w(x_i, x_j)}{\|x_i - x_j\|_2^s}$, with $w : A \times A \to [0, \infty)$ a CPD-function while the N-point weighted Riesz s-energy of A is

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

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

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

Weighted Poppy-seed Bagel Theorem

The connection between the Riesz energy and a sequence uniformly distributed w.r.t. the Hausdorff measure is given by

Theorem (Hardin & Saff 2004, Borodachov et al. 2008)

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

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

with $\mathcal{B}^d$ the unit ball.

Greedy minimal Riesz-energy points

Greedy algorithm

General greedy algorithm

Let $k : X \times X \to \mathbb{R} \cup \{\infty\}$ be a symmetric 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) $a_{n+1},\ n \geq 1$

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

is called a greedy minimal k-energy sequence on A.

Greedy minimal k_s and (w, s)-energy points

The Riesz kernel in $X = \mathbb{R}^{d'}$, which depends on a parameter $s \in [0, +\infty)$
$K_s(\|x - y\|_2), \quad x, y \in \mathbb{R}^{d'}$, with

$$K_s(t) := \begin{cases} t^{-s} & \text{if } s > 0 \\ -\log(t) & \text{if } s = 0, \end{cases} \tag{11}$$

For $k = K_s$ we get the greedy minimal k_s-energy points.

Taking $k = w\,K_s$ we get the so-called greedy minimal (w, s)-energy points.

Remarks and questions

[Lopez-Garcia&Saff 2010] then proved

- Greedy k_d-energy points, say $X_{N,d}^w$, on $\mathbb{S}^d$ are asymptotically d-energy minimizing . This results does not hold for $s > d$.
- If $A \subset \mathbb{R}^d$ is a compact subset of a C^1 manifold and w is CPD on $A \times A$, then a (w, d)-energy sequence $X_{N,d}^w$, is dense in A.
- Taking $w = 1$, the same conclusion holds for greedy k_s-energy points.

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Questions

1. Can greedy (w, d)-energy points can be used for integration on manifolds wrt to $\mathcal{H}^w_d$?
2. Are they preferable to mapped low-discrepancy points on the manifold?

Numerical results

Integration

Compute the integral

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

by a QMC method with

(a) low discrepancy points mapped on the manifolds,

(b) greedy minimal k_s-energy points.

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About (b): we start from a uniform mesh on a rectangle of $\mathbb{R}^2$ consisting of $N^2/2$ points and we map them to the manifold - if available by using the corresponding preserving measure map - and then we extract N greedy minimal k_s-energy points from this mapped mesh.

Functions and 2-manifolds

$$
\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\geq\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{12}
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Manifolds: cylinder, cone, sphere and torus.

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Manifolds: cylinder, cone, sphere and torus.

for the torus we do not know a preserving Lebesgue measure map, but we used simply

$$
[0,2\pi]\times[0,2\pi]\ \ni\ (u,v)\ \to\begin{cases}x=(2+\cos(u))\cos(v)\\ y=(2+\cos(u))\sin(v)\\ z=\sin(u)\end{cases}
\tag{13}
$$

Points and integral values

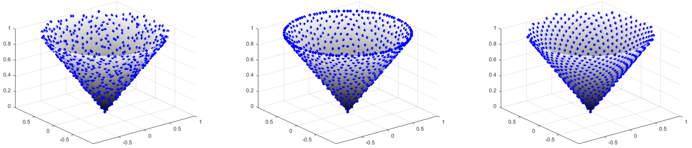
We compare the results with the greedy minimal k_2-energy points,

- QMC method using Halton points and Fibonacci lattice mapped on the manifolds.
- Fibonacci sequence from 144 (12-th Fibonacci number) up to 2584 (18-thFibonacci number)
- In the tables we present the results only for 144, 610 and 2584 points.

The exact value of the integrals taken by the built-in Matlab function `dblquad` with a tollerance of order 10^{-11}

The cone

function f_1



(a) Halton points (b) Greedy minimal k_2-energy points (c) Fibonacci points

Figure: 610 points on the cone

N	Halton	Fibonacci	GM k_2
144	1.215e-02	5.352e-03	2.097e-01
610	4.939e-03	1.270e-03	1.470e-01
2584	1.241e-03	3.029e-04	9.817e-02

Relative errors for f_1 on the cone

The cone

functions f_2, f_3 and f_4

N	Halton	Fibonacci	GM k_2
144	9.101e-03	6.250e-03	2.366e-01
610	5.277e-03	1.173e-03	1.764e-01
2584	6.766e-04	3.678e-04	1.212e-01

Relative errors for f_2 on the cone

N	Halton	Fibonacci	GM k_2
144	1.059e-02	1.416e-03	7.048e-02
610	3.763e-04	3.389e-04	7.172e-02
2584	1.289e-04	8.026e-05	3.790e-02

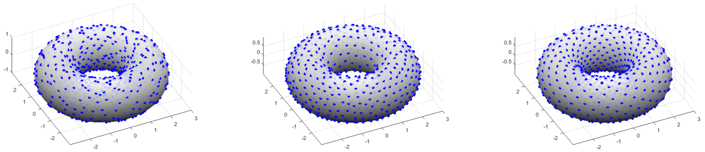
Relative errors for f_3 on the cone

N	Halton	Fibonacci	GM k_2
144	2.767e-02	1.384e-02	2.333e-01
610	9.623e-03	3.230e-03	1.782e-01
2584	3.068e-03	7.594e-04	1.313e-01

Relative errors for f_4 on the cone

The torus

function f_1



(a) Halton points

(b) Greedy minimal k_2-energy points

(c) Fibonacci points

Figure: 610 points on the torus

N	Halton	Fibonacci	GM k_2
144	2.152e-01	1.777e-01	6.894e-02
610	1.888e-01	1.780e-01	5.367e-02
2584	1.788e-01	1.780e-01	4.014e-02

Relative errors for f_1 on the torus

The torus

functions f_2, f_3 and f_4

N	Halton	Fibonacci	GM k_2
144	1.218e-01	1.690e-01	3.081e-02
610	1.453e-01	1.410e-01	4.728e-02
2584	1.414e-01	1.411e-01	2.297e-02

Relative errors for f_2 on the torus

N	Halton	Fibonacci	GM k_2
144	3.033e-02	3.426e-02	4.949e-03
610	2.716e-03	8.821e-03	1.349e-02
2584	8.763e-03	6.453e-03	1.673e-03

Relative errors for f_3 on the torus

N	Halton	Fibonacci	GM k_2
144	6.015e-01	5.339e-01	2.435e-01
610	5.109e-01	5.237e-01	1.874e-01
2584	5.252e-01	5.238e-01	1.319e-01

Relative errors for f_4 on the torus

Computational time for extracting greedy 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

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

Final remarks

- From numerical experiments we show the importance of knowing a measure preserving map (torus docet!)
- Adding more and more greedy points the error does not change significantly
- From experiments the time to extract the greedy minimal k_s-energy points grows: a good compromise, error vs computational time, is to use 610 points.
- By tuning the parameter s we have seen that, in the stationary case the bets choice is $s \leq 2$ (2=manifold dimension) ... except for the sphere.

Reference

S. De Marchi and G. Elefante: “Integration on manifolds by mapped low-discrepancy points and greedy minimal ks-energy points” (draft, Mar. 2016)

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Happy birthday Henryk!