Quadrature rules on manifolds: designs

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- Orthonormal system of eigenfunctions $\{\varphi_k\}_{k=0}^{+\infty}$.
- Sobolev spaces: $-\infty < \alpha < +\infty$, $1 \leq p \leq +\infty$, $W^{\alpha,p}$ is the set of all distributions f on $\mathcal{M}$ with $(I + \Delta)^{\alpha/2} f \in L^p$

$$\|f\|_{\alpha,p} = \left\{ \int_{\mathcal{M}} \left| \sum_{k=0}^{+\infty} (1 + \lambda_k^2)^{\alpha/2} \, \widehat{f}(k) \varphi_k(x) \right|^p d\mu(x) \right\}^{1/p} < +\infty.$$

Numerical Approximation

- Want to approximate the integral of $f \in W^{\alpha,p}$, $\alpha > d/p$, with Riemann sums

$$\int_{\mathcal{M}} f(x) d\mu(x) \sim \sum_{j=1}^{N} \frac{1}{N} f(z_j).$$

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- The problem is therefore: $\forall N \in \mathbb{N}$, find N points $\{x_j\}_{j=1}^{N}$ in $\mathcal{M}$ such that for all $f \in W^{\alpha,p}$
$$\left| \frac{1}{N} \sum_{j=1}^{N} f(x_j) - \int_{\mathcal{M}} f(x)d\mu(x) \right| \leq CN^{-\beta} \|f\|_{\alpha,p}$$

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$$\left| \frac{1}{N} \sum_{j=1}^{N} f(x_j) - \int_{\mathcal{M}} f(x)d\mu(x) \right| \leq CN^{-\beta} \|f\|_{\alpha,p}$$
- $\beta \leq \alpha/d$ (Brandolini, Choirat, Colzani, G., Seri, Travaglini '14). $\forall 1 \leq p \leq +\infty$, $\forall \alpha > d/p$ $\exists C > 0$ s.t. $\forall \{x_j\}_{j=1}^N$ $\exists f^* \in W^{\alpha,p}$ s.t.
$$\left| \frac{1}{N} \sum_{j=1}^{N} f^*(x_j) - \int_{\mathcal{M}} f^*(x)d\mu(x) \right| \geq CN^{-\frac{\alpha}{d}} \|f^*\|_{\alpha,p}$$

The Bessel kernel

Let $\alpha > 0$. The Bessel kernel $B^\alpha(x,y) = \sum_{k=0}^{+\infty}(1+\lambda_k^2)^{-\alpha/2}\varphi_k(x)\overline{\varphi_k(y)}$

is positive, real, symmetric, and smooth in $\{x \neq y\}$.

- For $0 < \alpha < d$, $B^\alpha(x,y) \approx |x-y|^{\alpha-d}$
- For $\alpha = d$, $B^\alpha(x,y) \approx \log(1+|x-y|^{-1})$
- For $d < \alpha$, $B^\alpha(x,y) \approx 1$
- For $d < \alpha < d+1$, $|B^\alpha(x,y) - B^\alpha(x,z)| \leq c|y-z|^{\alpha-d}$
- For $d < \alpha < d+2$, $|B^\alpha(x,x) - B^\alpha(x,z)| \leq c|x-z|^{\alpha-d}$
- $\int_{\mathcal{M}} B^\alpha(x,y)d\mu(y) = 1$
- $$\int_{\mathcal{M}} B^\alpha(x,y)B^\beta(y,z)d\mu(y) = B^{\alpha+\beta}(x,z)$$
  $$= \sum_{k=0}^{+\infty}\sum_{m=0}^{+\infty}(1+\lambda_k^2)^{-\alpha/2}(1+\lambda_m^2)^{-\beta/2}\varphi_k(x)\overline{\varphi_m(z)}\int_{\mathcal{M}}\varphi_m(y)\overline{\varphi_k(y)}d\mu(y)$$

The Bessel kernel

- For $d < \alpha < d + 2$, $|B^\alpha(x, x) - B^\alpha(x, z)| \leq c|x - z|^{\alpha - d}$

When $\mathcal{M} = \mathbb{T}^d$, then

$$B^\alpha(x, y) = \sum_{k \in \mathbb{Z}^d} (1 + 4\pi^2 |k|^2)^{-\alpha/2} \cos(2\pi k(x - y))$$

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$$B^\alpha(x,x) - B^\alpha(x,z) = 2\sum_{k\in\mathbb{Z}^d} (1+4\pi^2|k|^2)^{-\alpha/2} \sin^2(\pi k(x-z))$$

$$= 2\pi^2|x-z|^2 \sum_{|k|\leq|x-z|^{-1}} |k|^2(1+4\pi^2|k|^2)^{-\alpha/2} \quad \text{(div. for } \alpha < d+2\text{)}$$

$$+ 2\sum_{|k|>|x-z|^{-1}} (1+4\pi^2|k|^2)^{-\alpha/2} \leq C|x-z|^{\alpha-d}.$$

(conv for $\alpha > d$)

Probabilistic result

Theorem (Brandolini, Choirat, Colzani, G., Seri, Travaglini, 2014)
Let $d/2 < \alpha < d/2 + 1$. *Let* $\mathcal{M} = \cup_{j=1}^{N} U_j$ *(disjoint union),* $|U_j| = \omega_j$.
Then there is a constant $c > 0$ *independent of* N *such that*

$$\left(\int_{U_1} \dots \int_{U_N} \sup_{\|f\|_{\alpha,2} \leq 1} \left| \int_{\mathcal{M}} f(x)dx - \sum_{j=1}^{N} \omega_j f(x_j) \right|^2 \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N} \right)^{1/2}$$
$$\leq c \max_{1 \leq j \leq N} \mathrm{diam}(U_j)^{\alpha}.$$

In particular, if one manages to obtain $\mathrm{diam}(U_j) \leq cN^{-1/d}$ *(uniformly in* j *and* N*), then*

$$\dots \leq cN^{-\alpha/d}.$$

(here $dx_j = d\mu(x_j)$). Previous results: Brauchart-Saff-Sloan-Womersley (2014) for the sphere and with $\omega_j = 1/N$.

Proof - The norm of the functional

$$
\begin{aligned}
&\left| \int_{\mathcal{M}} f(x)dx - \sum_{j=1}^{N} \omega_j f(x_j) \right|^2 \\
&= \left| \int_{\mathcal{M}} \int_{\mathcal{M}} B^{\alpha}(x,y) g(y) dy dx - \sum_{j=1}^{N} \omega_j \int_{\mathcal{M}} B^{\alpha}(x_j,y) g(y) dy \right|^2 \\
&= \left| \int_{\mathcal{M}} \left(\int_{\mathcal{M}} B^{\alpha}(x,y) dx - \sum_{j=1}^{N} \omega_j B^{\alpha}(x_j,y) \right) g(y) dy \right|^2 \\
&\leq \int_{\mathcal{M}} \left| 1 - \sum_{j=1}^{N} \omega_j B^{\alpha}(x_j,y) \right|^2 dy \|f\|_{\alpha,2}^2
\end{aligned}
$$

Proof - The norm of the functional

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\begin{aligned}
&\int_{\mathcal{M}} \left| 1 - \sum_{j=1}^{N} \omega_j B^{\alpha}(x_j, y) \right|^2 dy \\
&= \int_{\mathcal{M}} (1 - \sum_{j=1}^{N} \omega_j B^{\alpha}(x_j, y))(1 - \sum_{i=1}^{N} \omega_i B^{\alpha}(x_i, y)) dy \\
&= 1 - 1 - 1 + \int_{\mathcal{M}} \sum_{j=1}^{N} \sum_{i=1}^{N} \omega_j \omega_i B^{\alpha}(x_j, y) B^{\alpha}(x_i, y) dy \\
&= -1 + \sum_{j=1}^{N} \sum_{i=1}^{N} \omega_j \omega_i B^{2\alpha}(x_j, x_i)
\end{aligned}
$$

Averaging the norm

$$\int_{U_1} \dots \int_{U_N} \left(-1 + \sum_{i,j=1}^{N} \omega_i \omega_j B^{2\alpha}(x_i, x_j) \right) \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N}$$

$$= -1 + \sum_{i,j=1}^{N} \int_{U_1} \dots \int_{U_N} \omega_i \omega_j B^{2\alpha}(x_i, x_j) \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N}$$

$$1 = \sum_{i,j=1}^{N} \int_{U_i} \int_{U_j} B^{2\alpha}(x, y) dx dy$$

$$= \sum_{i \neq j} \int_{U_i} \int_{U_j} B^{2\alpha}(x, y) dx dy + \sum_{j=1}^{N} \int_{U_j} \int_{U_j} B^{2\alpha}(x, y) dx dy$$

$$\sum_{i,j=1}^{N} \int_{U_1} \dots \int_{U_N} \omega_i \omega_j B^{2\alpha}(x_i, x_j) \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N}$$

$$= \sum_{i \neq j} \int_{U_i} \int_{U_j} \omega_i \omega_j B^{2\alpha}(x_i, x_j) \frac{dx_i}{\omega_i} \frac{dx_j}{\omega_j} + \sum_{j=1}^{N} \int_{U_j} \omega_j^2 B^{2\alpha}(x_j, x_j) \frac{dx_j}{\omega_j}$$

Averaging the norm

Thus, for $d < 2\alpha < d + 2$,

$$\int_{U_1} \dots \int_{U_N} (-1 + \sum_{i,j=1}^{N} \omega_i \omega_j B^{2\alpha}(x_i, x_j)) \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N}$$

$$= \sum_{j=1}^{N} \int_{U_j} \int_{U_j} (B^{2\alpha}(x,x) - B^{2\alpha}(x,y)) dxdy$$

$$\leq \sum_{j=1}^{N} |U_j|^2 \sup_{x,y \in U_j} (B^{2\alpha}(x,x) - B^{2\alpha}(x,y))$$

$$\leq c \sum_{j=1}^{N} |U_j|^2 \mathrm{diam}(U_j)^{2\alpha - d} \leq c \sum_{j=1}^{N} |U_j| \mathrm{diam}(U_j)^{2\alpha} \leq \max_{1 \leq j \leq N} \mathrm{diam}(U_j)^{2\alpha}$$

General result

Theorem (Brandolini, Chen, Colzani, G, Travaglini, 2019)
Let $1 < p \leq +\infty$, $1/p + 1/q = 1$, $d/p < \alpha < d$. *Let* $\mathcal{M} = \cup_{j=1}^{N} U_j$ *(disjoint union),* $\omega_j = |U_j| \approx N^{-1}$ *and* $\mathrm{diam}(U_j) \approx N^{-1/d}$.

$$\left(\int_{U_1} \dots \int_{U_N} \sup_{\|f\|_{\alpha,p} \leq 1} \left| \int_{\mathcal{M}} f(x)dx - \sum_{j=1}^{N} \omega_j f(x_j) \right|^q \frac{dx_1}{\omega_1} \dots \frac{dx_N}{\omega_N} \right)^{1/q}$$

$$\approx \begin{cases} N^{-\alpha/d} & \alpha < d/2+1 \\ N^{-1/2-1/d}(\log N)^{1/2} & \alpha = d/2+1 \\ N^{-1/2-1/d} & \alpha > d/2+1 \end{cases}$$

Marcinkiewicz-Zygmund inequality

Theorem (1937)
Let $\mathcal{M} = \cup_{j=1}^{N} U_j$ (disjoint union), $\omega_j = |U_j|$. For every measurable g on $\mathcal{M}$,

$$\left(\int_{U_1} \cdots \int_{U_N} \left| \int_{\mathcal{M}} g(x)dx - \sum_{j=1}^{N} \omega_j g(x_j) \right|^q \frac{dx_1}{\omega_1} \cdots \frac{dx_N}{\omega_N} \right)^{1/q}$$

$$\approx \left(\int_{U_1} \cdots \int_{U_N} \left(\sum_{j=1}^{N} \left| \int_{U_j} g(y)dy - \omega_j g(x_j) \right|^2 \right)^{q/2} \frac{dx_1}{\omega_1} \cdots \frac{dx_N}{\omega_N} \right)^{1/q}$$

Area regular partitions

Theorem (G., Leopardi, '17)
$\forall N \in \mathbb{N}$ there exists an area regular partition $\mathcal{U} = \{U_1, \ldots, U_N\}$ of $\mathcal{M}$:

- $U_1 \cup \ldots \cup U_N = \mathcal{M}$.
- $\mu(U_i \cap U_j) = 0$ *if* $i \neq j$.
- $\mu(U_j) = N^{-1}$.
- $B(c_1 N^{-1/d}) \subset U_j \subset B(c_2 N^{-1/d})$ *for fixed* $0 < c_1 \leq c_2$, *where* $B(r)$ *is a ball of radius* r.

($\mathcal{M} = S^d$: Bourgain-Lindenstrauss ('88), Kuijlaars-Saff ('98) small constant c_2, Bondarenko-Radchenko-Viazovska ('15) convex sets).

Numerical Approximation, a different approach

- (Brandolini, Choirat, Colzani, G., Seri, Travaglini, '14) Let $1 \leq p \leq +\infty$ and $\alpha > d/p$. Assume that $\{x_j\}_{j=1}^N$ gives an exact quadrature rule for all eigenfunctions of the Laplace-Beltrami operator with eigenvalues $\lambda_k^2 \leq L^2$ (this is called L-design):

$$\int_{\mathcal{M}} \varphi_k(x) d\mu(x) - \sum_{j=1}^{N} \frac{1}{N} \varphi_k(x_j) = 0.$$

  then

$$\left| \int_{\mathcal{M}} f(x) d\mu(x) - \frac{1}{N} \sum_{j=1}^{N} f(x_j) \right| \leq C L^{-\alpha} \|f\|_{\alpha,p}$$

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- The problem now reduces to the following:

Korevaar-Meyers conjecture

$\forall N \in \mathbb{N}$, find a $CN^{1/d}$-design with N nodes.

Lemma
Let $f \in W^{\alpha,p}(\mathcal{M})$, $\alpha > d/p$ *and let* $1/p + 1/q = 1$, *then*

$$\left|\int_{\mathcal{M}} f(x)\,dx - \frac{1}{N}\sum_{j=1}^{N} f(x_j)\right| \leq \left\{\int_{\mathcal{M}} \left|1 - \sum_{j=1}^{N} B^{\alpha}(x_j, y)\right|^{q} dy\right\}^{1/q} \|f\|_{W^{\alpha,p}}$$

Lemma
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Proof.
Done, a few slides back. □

Lemma

Let ψ *be smooth and compactly supported in* $[1/2, 2]$, *and*

$$B_R^\alpha(x,y) = \sum_{k=0}^{+\infty} \psi(\lambda_k/R)\left(1+\lambda_k^2\right)^{-\alpha/2} \varphi_k(x)\,\overline{\varphi_k(y)}.$$

Then for every $n > 0$ *there exists* $c > 0$ *such that for* $R > 0$, $x, y \in \mathcal{M}$

$$|B_R^\alpha(x,y)| \leq cR^{d-\alpha}(1+R|x-y|)^{-n}.$$

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Proof.
By [Gariboldi, G., 2022] there exists a smooth positive function q such that if h is smooth and compactly supported, then for every n

$$\sum_{k=0}^{+\infty} h(\lambda_k/R)\varphi_k(x)\overline{\varphi_k(y)} = q(x, y)R^d \mathcal{F}_d h(R|x - y|) + O(R^{d-2}(1 + R|x - y|)^{-n}$$

$$B_R^{\alpha}(x, y) = \sum_{k} \psi(\lambda_k/R) \left(1 + \lambda_k^2\right)^{-\alpha/2} \varphi_k(x) \overline{\varphi_k(y)}$$

$$\sim R^{-\alpha} \sum_{k} \psi(\lambda_k/R)\varphi_k(x) \overline{\varphi_k(y)}$$

Lemma

Assume that for $\lambda_k^2 < L^2$

$$\frac{1}{N}\sum_{j=1}^{N}\varphi_k\left(x_j\right) = \int_M \varphi_k\left(x\right)dx = \begin{cases} 1 & k=0 \\ 0 & k>0 \end{cases} \qquad (1)$$

then for $1 \leq q \leq +\infty$, $\alpha > d\left(1-1/q\right)$, *then*

$$\left\{\int_{\mathcal{M}}\left|1-\sum_{j=1}^{N}B^{\alpha}(x_j,y)\right|^q dy\right\}^{1/q} \lesssim L^{-\alpha}$$

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Write $B^{\alpha}\left(x,y\right) = 1 + \sum_{j=-\infty}^{+\infty} B_{2^j}^{\alpha}\left(x,y\right)$. By (1) we have

$$\int_{\mathcal{M}} B^{\alpha}(x,y)d\nu(x) - 1 = \sum_{2^j \geq L}\int_{\mathcal{M}} B_{2^j}^{\alpha}\left(x,y\right)d\nu(x)$$

and the estimate follows from the estimates for $B_R^{\alpha}\left(x,y\right)$.

Designs on manifolds

The d-dimensional sphere S^d

- A. Bondarenko, D. Radchenko, M. Viazovska, Optimal asymptotic bounds for spherical designs, Annals of Mathematics **178** (2013), 443–452.

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- We would like to extend this result to the case of a compact connected Riemannian manifold without boundary.

First step of the proof

Theorem (Brouwer degree theory)
Let H be a finite dimensional Hilbert space. Let $f : H \to H$ continuous.
Let Ω be an open bounded subset of H containing 0.

If $\langle x, f(x) \rangle > 0$ for all $x \in \partial\Omega$, then there exists $x \in \Omega$ s.t. $f(x) = 0$.

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- Set $H = \Pi_L^0 = \mathrm{span}\{\varphi_k : 0 < \lambda_k^2 \leq L^2\}$ (diffusion polynomials).

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- Set $\Omega = \{P \in \Pi_L^0 : \int_{\mathcal{M}} \|\nabla P(x)\| d\mu(x) < 1\}$.

This allows to reduce the problem to the following

Lemma
$\exists F : \Pi_L^0 \to \mathcal{M}^N$ continuous, $F(P) = (x_1(P), \ldots, x_N(P))$ s.t. $\forall P \in \partial\Omega$

$$\sum_{j=1}^{N} P(x_j(P)) > 0.$$

($f : P \mapsto G_{x_1(P)} + \ldots + G_{x_N(P)}$, where $G_x \in \Pi_L^0$ is s.t. $\langle P, G_x\rangle = P(x)$.
Thus
$\langle Q, f(P)\rangle = \langle Q, G_{x_1(P)} + \ldots + G_{x_N(P)}\rangle = Q(x_1(P)) + \ldots + Q(x_N(P))$.)

Strategy

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- Bondarenko, Radchenko and Viazovska begin with a "well distributed" collection of points $\{x_j\}_{j=1}^N$.
- Precisely, they take $x_j \in U_j$, where $\mathcal{U} = \{U_j\}_{j=1}^N$ is an *area regular partition* of $\mathcal{M}$.
- For all $P \in \Pi_L^0$ s.t. $\int_{\mathcal{M}} \|\nabla P(x)\| d\mu(x) = 1$, move each point x_j along the gradient vector field of P, increasing each value $P(x_j(P))$ until

$$\sum_{j=1}^{N} P(x_j(P)) > 0.$$

Final Ingredient

To prove the Lemma they need the following version of the Marcinkiewicz-Zygmund inequality for gradients of diffusion polynomials.

Theorem (Mhaskar-Narcowich-Ward, 2001)
Let $\mathcal{M} = S^d$. For any $0 < c_1 \le c_2$ there exists a constant C_3 such that for all $N \in \mathbb{N}$, for all area regular partitions $\mathcal{U} = \{U_j\}_{j=1}^N$ with constants c_1 and c_2, for all $x_j \in U_j$, for all $L \le N^{1/d}$, for all $P \in \Pi_L^0$,

$$\left| \sum_{j=1}^N \frac{1}{N} \|\nabla P(x_j)\| - \int_{\mathcal{M}} \|\nabla P(x)\| d\mu(x) \right| \le C_3 L N^{-1/d} \int_{\mathcal{M}} \|\nabla P(x)\| d\mu(x).$$

- In fact, they prove this result with ∇P replaced with P, but when $\mathcal{M} = S^d$, P is a polynomial in $d+1$ variables of degree at most L, and so is ∇P (degree at most $L+1$).

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- Filbir-Mhaskar (2010) prove this result when $\mathcal{M}$ is a Riemannian manifold (and in other cases), but again with ∇P replaced with P.

Back to manifolds

Theorem (Gariboldi, G. 2018)
Let $\mathcal{M}$ be a compact connected orientable d-dimensional Riemannian manifold without boundary. For any $0 < c_1 \leq c_2$ there exists a constant C_3 such that for all $N \in \mathbb{N}$, for all area regular partitions $\mathcal{U} = \{U_j\}_{j=1}^N$ with constants c_1 and c_2, for all $x_j \in U_j$, for all $L \leq N^{1/d}$, for all $P \in \Pi_L^0$,

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Back to manifolds

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Corollary (Korevaar-Meyers for manifolds)
For all (N, L) with $L \leq cN^{1/d}$ there exists an L-design in $\mathcal{M}$ with N nodes.

Corollary (Optimal numerical approximation)
Let $1 \leq p \leq +\infty$ and $\alpha > d/p$. There exists a constant $C > 0$ s.t. for all $N \in \mathbb{N}$ there is a point distribution $\{x_j\}_{j=1}^N$ such that

$$\left| \frac{1}{N} \sum_{j=1}^{N} f(x_j) - \int_{\mathcal{M}} f(x) d\mu(x) \right| \leq CN^{-\alpha/d} \|f\|_{\alpha,p}$$

Variations and extensions

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- M. Ehler, U. Etayo, B. Gariboldi, G, T. Peter (2021). Prefixed non-constant weights $\{w_j\}_{j=1}^N$ with $w_j \leq cN^{-1}$, both for compact Riemannian manifolds and for compact algebraic manifolds in $\mathbb{R}^n$, Π_L polynomials in $\mathbb{R}^n$ of degree L.