Quadrature rules on manifolds: partitions

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July 3, 2023

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Numerical integration, a simple observation

Goal: Estimate the error in numerical integration: e.g.

$$\left|\int_0^1 f(x)dx - \sum_{j=1}^{N} \frac{1}{N} f(x_j)\right|.$$

Pick any point $x_j \in \left[\frac{j-1}{N}, \frac{j}{N}\right)$, for $j = 1, \ldots N$. Then, if f is Hölder continuous of degree $0 < \alpha \leq 1$

$$\left|\int_0^1 f(x)dx - \sum_{j=1}^{N} \frac{1}{N} f(x_j)\right| \leq \sum_{j=1}^{N} \int_{(j-1)/N}^{j/N} |f(x_j) - f(x)|\, dx$$

$$\leq \sup_{|y-x| \leq N^{-1}} |f(y) - f(x)| \leq \frac{1}{N^\alpha} |f|_{0,\alpha}$$

Numerical Approximation - the interval

We may also allow different weights.

Error for Lagrange interpolatory quadrature rules

$$\left| \int_a^b f(x)dx - \sum_{i=1}^{n} \omega_i f(x_i) \right| \leq \frac{(b-a)^{n+1}}{n!} \max_{x\in[a,b]} |f^{(n)}(x)|$$

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We need a priori estimates: for all (say) $f \in \mathcal{C}^\alpha$. Thus fix $n = \alpha \in \mathbb{N}$, and use composite rules: split $[a, b]$ into M subintervals and apply the rule to each subinterval

$$\left|\sum_{j=1}^M \left(\int_{a_j}^{a_{j+1}} f(x)dx - \sum_{i=1}^\alpha \omega_i f(x_i^j)\right)\right| \leq \sum_{j=1}^M \left(\frac{b-a}{M}\right)^{\alpha+1} \frac{1}{\alpha!} \max_{x\in[a,b]} |f^{(\alpha)}(x)|$$

$$\leq C_\alpha (\alpha M)^{-\alpha} \max_{x\in[a,b]} |f^{(\alpha)}(x)|$$

Koksma's inequality

In numerical integration, Koksma's inequality gives a bound for the error in the approximation of an integral by Riemann sums. Let $f \in C([0,1])$, $x_1, x_2, \ldots, x_N \in [0,1]$, then

$$\left| \int_0^1 f(x)\, dx - \frac{1}{N} \sum_{j=1}^{N} f(x_j) \right| \le \mathcal{D}^* \left(\{x_j\}_{j=1}^{N} \right) \mathcal{V}(f)$$

where

$$\begin{aligned} \mathcal{D}^* \left(\{x_j\}_{j=1}^{N} \right) &= \sup_{0 \le t \le 1} \left| t - \frac{1}{N} \sum_{j=1}^{N} \chi_{[0,t]}(x_j) \right| \\ &= \sup_{0 \le t \le 1} \left| \int_0^1 \chi_{[0,t]}(x)\, dx - \frac{1}{N} \sum_{j=1}^{N} \chi_{[0,t]}(x_j) \right| \end{aligned}$$

and

$$\mathcal{V}(f) = \sup_{0 = y_0 < y_1 < \cdots < y_k = 1} \left\{ \sum_{j=1}^{k} \left| f(y_k) - f(y_{k-1}) \right| \right\}$$

Discrepancy

- The quantity $\mathcal{D}^* \left(\{x_j\}_{j=1}^N \right)$ is called *discrepancy* of the distribution of points $x_1, x_2, \ldots, x_N$ and measures the error with respect to functions of the kind

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- In view of Koksma's inequality it is natural to ask if there are points with low discrepancy.
- Of course for any given N the points $x_j = \frac{j-1}{N-1}$ give

$$\mathcal{D}^* \left(\{x_j\}_{j=1}^N \right) = \frac{1}{N-1}$$

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is impossible.
- A remarkable theorem of Schmidt (1973) says that $D^*(N)$ cannot be $o\left(\frac{\log N}{N}\right)$.

Discrepancy

- This result is sharp since Van der Corput sequence

$$\begin{aligned}
&\frac{1}{2}, \\
&\frac{1}{4}, \quad \frac{1}{4}+\frac{1}{2}, \\
&\frac{1}{8}, \quad \frac{1}{8}+\frac{1}{2}, \quad \frac{1}{8}+\frac{1}{4}, \quad \frac{1}{8}+\frac{1}{4}+\frac{1}{2} \\
&\vdots
\end{aligned}$$

satisfies

$$\mathcal{D}^*(N) \leq c\frac{\log(N)}{N}.$$

A proof of "Koksma's inequality"

Let $g(x) = x - \lfloor x \rfloor - 1/2$ be the saw tooth function. Then

$$\left| \int_{\mathbb{T}} f(x)\, dx - \frac{1}{N} \sum_{j=1}^{N} f(x_j) \right| \leq \int_{\mathbb{T}} \left| f'(x) \right| \; dx \; \sup_{t \in \mathbb{T}} \left| \frac{1}{N} \sum_{j=1}^{N} g(t - x_j) \right|$$

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$$\frac{1}{N} \sum_{j=1}^{N} f(x_j) - \int_{\mathbb{T}} f(x)\, dx = \sum_{k \neq 0} \left(\frac{1}{N} \sum_{j=1}^{N} e^{2\pi i k x_j} \right) \widehat{f}(k)$$

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Since $g(x) = \sum_{k \neq 0} \frac{1}{-2\pi ik} e^{2\pi ikx}$ we have

$$\sum_{k \neq 0} \frac{1}{2\pi ik} \left(\frac{1}{N} \sum_{j=1}^{N} e^{2\pi ikx_j} \right) 2\pi ik \widehat{f}(k)$$

$$= \sum_{k \in \mathbb{Z}} \overline{\left(\frac{1}{N} \sum_{j=1}^{N} g(\cdot - x_j) \right)^{\wedge}(k)} \widehat{f'}(k)$$

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$$= \int_{\mathbb{T}} \overline{\frac{1}{N} \sum_{j=1}^{N} g(t + x_j)} f'(t) dt$$

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$$V(f) = \sup_{\substack{\text{partition } P \\ \text{of } [0,1]^d}} \left\{ \sum_{J \in P} |\Delta(f,J)| \right\}$$

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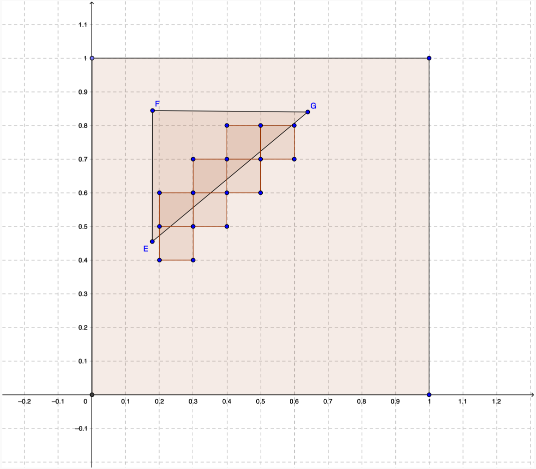
- The Hardy-Krause variation of f is

$$\mathcal{V}(f) = \sum_k V_k(f)$$

where the sum is over the Vitali variations $V_k(f)$ of the restrictions of f to all faces of all dimensions of $[0,1]^d$.

- Hardy-Krause variation works well for smooth functions, but it cannot be applied to most functions with simple discontinuities.
- The characteristic function of a convex polyhedron has bounded Hardy-Krause variation only if the polyhedron is a *d*-dimensional interval.



- The discrepancy of a finite point set $\{x_j\}_{j=1}^{N}$ in $[0,1]^d$ is defined by

$$\mathcal{D}\left(\{x_j\}\right) = \sup_I \left| \frac{1}{N} \sum_{j=1}^{N} \chi_I\left(x_j\right) - |I| \right|$$

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- The classical Koksma-Hlawka inequality states that if f has bounded Hardy-Krause variation, then

$$\left| N^{-1} \sum_{j=1}^{N} f\left(x_j\right) - \int_{[0,1]^d} f(x) dx \right| \leq \mathcal{D}\left(\{x_j\}\right) \mathcal{V}\left(f\right).$$

Higher dimension discrepancy

For $d > 1$ equally spaced points do not work very well. Let $N = K^d$ and consider the points (grid)

$$\left(\frac{k_1}{K}, \cdots, \frac{k_d}{K}\right), \; k_j = 0, 1, \ldots, K-1.$$

Then $\mathcal{D}\left(\{x_j\}\right) \approx N^{-1/d} = K^{-1}$

However it is possible to choose points $\{x_j\}_{j=1}^{N}$ such that

$$\mathcal{D}\left(\{x_j\}\right) \leq c \frac{\log^{d-1} N}{N}.$$

Higher dimension discrepancy

For example for $d = 2$ let

$$x_j = \left(\frac{j}{N}, r(j) \right)$$

where $r(j)$ is defined as follows. Let a_k be the binary digits of j, that is

$$j = a_0 + 2a_1 + 2^2 a_2 + 2^3 a_3 + \cdots$$

then

$$r(j) = \frac{a_0}{2} + \frac{a_1}{2^2} + \frac{a_2}{2^2} + \frac{a_3}{2^3} + \cdots$$

(the Van der Corput sequence !) It is not difficult to prove that for these points

$$D(x_j) \leq \frac{\log N}{N}.$$

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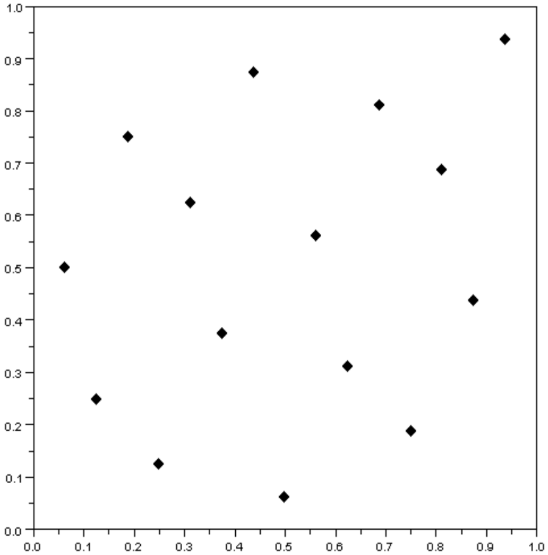

Higher dimension discrepancy

Theorem (Roth, 1954)
Let $\{x_j\}_{j=1}^{N} \subset \mathbb{T}^d$. *There exists a rectangle* $R \subset \mathbb{T}^d$ *having sides parallel to the axes such that*

$$\left| \frac{1}{N} \sum_{j=1}^{N} \chi_R\left(x_j\right) - |R| \right| \geq c_d \frac{(\log N)^{\frac{d-1}{2}}}{N}$$

with an absolute constant only depending on the dimension.

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- Schmidt (1973): True for $d \leq 2$.
- Bilyk, Lacey, Vagharshakyan (2008): $\exists\, \eta_d > 0$ s.t.
$$\ldots \geq c_d \frac{(\log N)^{\frac{d-1}{2}+\eta_d}}{N}$$

Monte Carlo Integration

- A second drawback with the grid

$$\left(\frac{k_1}{K}, \cdots, \frac{k_d}{K}\right),\ k_j = 0, 1, \ldots, K-1,$$

even if one repeats, a composite Lagrange interpolation rule in each dimension to evaluate the integral, is that the number of function evaluations increases exponentially with the dimension.

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- If $d = 200$, taking just $K = 2$, that is evaluating f at the vertices of $[0,1)^d$, gives $2^{200} > 10^{60}$ evaluations.
- One alternative is the Monte Carlo method. Let X be a probability space with measure dx. Then
$$\left\| \int_X f(x)dx - \sum_{j=1}^{N} \frac{1}{N} f(x_j) \right\|_{L^2(X^N, dx_1 \ldots dx_N)} = \frac{1}{\sqrt{N}} (\mathrm{Var}(f))^{1/2}$$

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- Works in high dimensions (the constant is 1 in all dimensions).
- It is hard to produce random points.

Monte Carlo integration

$$
\begin{aligned}
&\int_{X^N} \left| \int_X f(x)dx - \sum_{j=1}^{N} \frac{1}{N} f(x_j) \right|^2 dx_1 \dots dx_N \\
&= \int_{X^N} \left| \sum_{j=1}^{N} \frac{1}{N} \left(\int_X f(x)dx - f(x_j) \right) \right|^2 dx_1 \dots dx_N \\
&= \sum_{j=1}^{N} \sum_{i=1}^{N} \int_{X^N} \frac{1}{N} \left(\int_X f(x)dx - f(x_j) \right) \overline{\frac{1}{N} \left(\int_X f(x)dx - f(x_i) \right)} dx_1 \dots dx_N \\
&= \sum_{j=1}^{N} \int_X \frac{1}{N^2} \left| \int_X f(x)dx - f(x_j) \right|^2 dx_j \\
&= \frac{1}{N} \int_X \left| \int_X f(x)dx - f(y) \right|^2 dy
\end{aligned}
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- For example on $\mathbb{T}^d$, $\Delta = -\sum \partial^2/\partial x_j^2$, with eigenvalues $\left\{4\pi^2 |m|^2\right\}_{m\in\mathbb{Z}^d}$ and eigenfunctions $\{\exp(2\pi imx)\}_{k\in\mathbb{Z}^d}$.

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- Another example is the d-dimensional sphere $\mathbb{S}^d$, with Δ the angular component of the Laplacian in $\mathbb{R}^{d+1}$, eigenvalues $\{n(n+d-1)\}_{n=0}^{+\infty}$ and eigenfunctions the restriction to the sphere of homogeneous harmonic polynomials of degree n.

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- Set

$$\widehat{f}(k) = \int_{\mathcal{M}} f(x)\overline{\varphi_k(x)}d\mu(x)$$

Sobolev spaces - equivalent definitions

For $\alpha > 0$ and $1 \leq p \leq +\infty$ define the Sobolev space $W^{\alpha,p}(\mathcal{M})$:

- $f \in W^{\alpha,p}(\mathcal{M})$ if and only if $(1+\Delta)^{\alpha/2} f \in L^p(\mathcal{M})$, i.e.

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

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For $\alpha > 0$ and $1 \leq p \leq +\infty$ define the Sobolev space $W^{\alpha,p}(\mathcal{M})$:

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Quadrature rules on compact manifolds

- For given points $\{x_j\}$ and weights $\{\omega_j\}$, we want to give a priori estimates of the error

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- Choosing a point x_j in each U_j, one obtains the estimate

$$\left| N^{-1} \sum_{j=1}^{N} f(x_j) - \int_{\mathcal{M}} f(x) d\mu(x) \right| \leq \sum_{j=1}^{N} \int_{U_j} |f(x_j) - f(x)|\, d\mu(x)$$

$$\leq \sup_{|y-x| \leq cN^{-1/d}} \{|f(y) - f(x)|\} \leq cN^{-(\alpha - d/p)/d} \|f\|_{W^{\alpha,p}(\mathcal{M})}$$

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- This is the best possible

Lower bounds

Theorem (Brandolini, Choirat, Colzani, G, Seri, Travaglini, 2014)
For all $1 \leq p \leq +\infty$ *and* $\alpha > d/p$ *there exists* $c > 0$ *such that for all nodes* $\{x_j\}_{j=1}^{N}$ *and weights* $\{\omega_j\}_{j=1}^{N}$ *there exists* $f \in W^{\alpha,p}(\mathcal{M})$ *such that*

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

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Previous results:

- K. Hesse, I.H. Sloan (2005-2006): $\mathcal{M} = \mathcal{S}^d$, $p = 2$.
- A. Kushpel (2009): $\mathcal{M}$ compact two–point homogeneous, $p = +\infty$.

Proof.

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$$\|\psi_j\|_{\alpha,p} \leq cN^{\frac{\alpha}{d}-\frac{1}{p}} \qquad \int_{\mathcal{M}} \psi_j(x)\, d\mu(x) = N^{-1}.$$

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- Let $f(x) = \sum_{j=1}^{N} \psi_j(x)$:

$$\|f\|_{\alpha,p} \leq cN^{\frac{\alpha}{d}} \qquad \int_{\mathcal{M}} f(x)\, d\mu(x) = 1.$$

$$\left|\int_{\mathcal{M}} f(x)d\mu(x) - \sum_{j=0}^{N} \omega_j f(x_j)\right| = \left|\int_{\mathcal{M}} f(x)d\mu(x)\right| = 1 \geq \frac{1}{cN^{\frac{\alpha}{d}}}\|f\|_{\alpha,p}.$$

□

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 $\omega_j = 1/N$.

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 $\mathcal{M}$,

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

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

We have seen that

- For any choice of nodes $\{x_j\}$ and weights $\{\omega_j\}$,

$$\sup_{\|f\|_{\alpha,p}\leq 1} \left| \int_{\mathcal{M}} f(x)dx - \sum_{j=1}^{N} \omega_j f(x_j) \right| \geq cN^{-\alpha/d}$$

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- If one fixes $\{\omega_j\}$ (e.g. $\omega_j = 1/N$ for all j) beforehand, can we construct partitions as desired?