A new quasi-Monte Carlo technique based on nonnegative least squares and approximate Fekete points[1]

Stefano De Marchi
Department of Mathematics - University of Padova

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[1] Joint work with Claudia Bittante and Alvise Sommariva

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- The use of as less (good) points as possible to approximate integrals on general domains;

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- The computation of integrals in high dimensions and on general domains, when no explicit cubature rules are known;
- The use of as less (good) points as possible to approximate integrals on general domains;
- Nonnegative least-square and approximate Fekete points for computing the cubature weights.

Outline

Cubature

Notation

- $\Omega = [0,1]^d$, i.e. the d-dimensional unit cube
- $X = \{x_1, \dots x_N\}$ of Ω, the set of samples
- Both MC and QMC compute

$$\int_\Omega f(x)dx \approx \frac{\lambda_d(\Omega)}{N} \sum_{i=1}^{N} f(x_i) \tag{1}$$

  where $\lambda_d(\Omega)$ is the Lebesgue measure of the domain Ω (in the case of the unit cube it is simply 1).

- In QMC the samples are taken as a low-discrepancy sequence (quasi-random points) (ex: Halton, Sobol);
- Using low-discrepancy sequences allow $\mathcal{O}(N^{-1})$ instead of $\mathcal{O}(N^{-1/2})$ convergence rate.

Definition

Given a sequence $X = \{x_1, ..., x_N\}$ its discrepancy is

$$D_N(X) := \sup_{B \in J} \left| \frac{\#(X,B)}{N} - \lambda_d(B) \right| \tag{2}$$

where

- $J := \prod_{i=1}^{d} [a_i, b_i) = \{x \in \mathbb{R}^d : \; a_i \leq x_i \leq b_i, \; 0 \leq a_i < b_i < 1\}$ (d-dimensional intervals),
- $\#(X, B)$ is the number of points of X in B.
- λ_d is Lebesgue measure

Note. When $D_N(X) \approx \mathtt{mis}(B)$ then D_N is called **low discrepancy**.

Why the discrepancy is important?

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Theorem (Koksma-Hlawka inequality)

Let $f : \Omega \to \mathbb{R}$ be BV with variation $V(f)$, and let $X \subset \Omega$ be a (low discrepancy) sequence of N points of Ω. Let $E_N(f)$ be the cubature error, then

$$E_N(f) \leq V(f) D_N \,. \tag{3}$$

Low-discrepancy examples

Halton and Sobol

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these sequences have discrepancy much lower than random points!

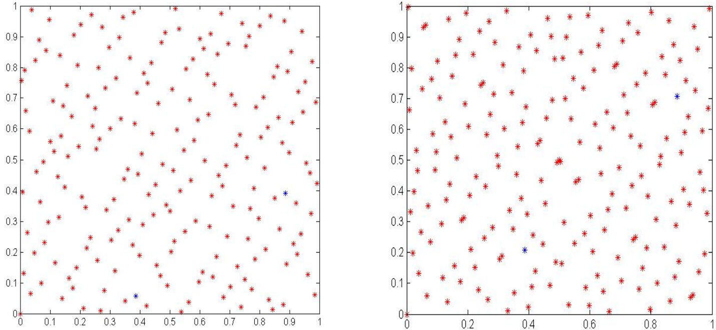

Figure : 200 Halton (Left) and Sobol points on the square. **Notice**: they form a nested sequence

For Halton points in dimension d, it is known $D_N(H_{N,d}) \leq \frac{C(\log N)^d}{N}$.

Note. Matlab has built-in functions `haltonset, sobolset`

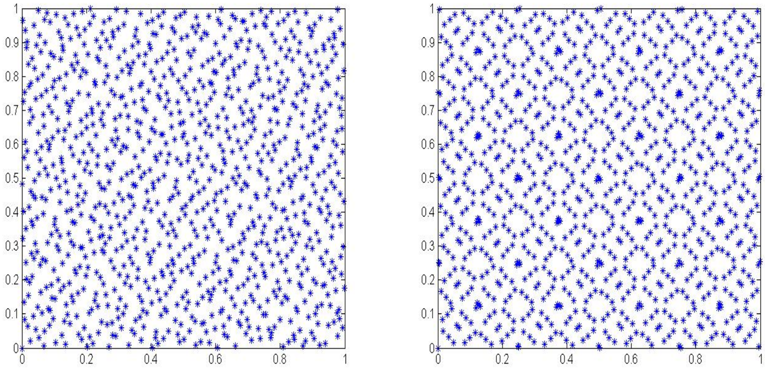

Figure : 1024 Halton points (Left) and Sobol points

Definition

Let A be a $m \times n$ matrix and $b \in \mathbb{R}^m$ a column vector, G a $r \times n$ matrix and $h \in \mathbb{R}^r$. A Linear System of Inequalities (LSI) problem is a least squares problem with linear constraints, that is the optimization problem

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2 \tag{4}$$
$$Gx \geq h\,.$$

Nonnegative Least Squares

How to use them for cubature

- $A = V^T$, with V the Vandermonde matrix at the sequence $X = \{x_i,\ i = 1, \ldots, n\}$ for the polynomial basis $\{p_j,\ j = 1, \ldots, m\}$;
- b being the column vector of size m of the moments, that is

$$b_j = \int_\Omega p_j(x) d\mu(x)$$

  for some measure μ on Ω
- $G = I$, $h = (0, \ldots, 0)^T$ both of order n
- then the problem $\arg\min_x \|V^T x - b\|_2$ subject to $x \geq 0$.

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- Algorithm : Lawson, Hanson *Solving Least Squares Problems, PH 1974, p. 161* gives the nonnegative weights x for the cubature at the point set X.
- Matlab has built-in function `lsqnonneg` in the optim toolbox.

Definition

Let $K \subset \mathbb{C}^d$ be a compact and $S_n = \mathrm{span}\{q_j,\, j = 1, \ldots, \nu_n\}$ a finite-dimensional space of linearly independent functions. The points $\{\xi_1, \ldots, \xi_{\nu_n}\}$ of K are Fekete points if they are unisolvent for the interpolation on S_n and maximize the absolute value of the Vandermonde determinant.

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- In polynomial interpolation $\nu_n = \dim(\mathbb{P}_n^d) = \binom{n+d}{d}$
- For Fekete points $|l_i| \le 1,\ \forall i$. As a consequence, $\Lambda_n = \max_{x\in\Omega} \sum_{i=1}^{\nu_n} |l_i(x)| \le \nu_n$. This bound is indeed an overestimate of the Lebegsue constant as it is known (see [Bos et al. NMTA11]), but gives the idea of the importance (and quasi-optimality) of Fekete points for interpolation/cubature.
- To compute Fekete points we have to solve a NP-hard (discrete) optimization problem (cf. [Civril&Magdon-Ismail TCS09]).
- Fekete points are known only on the interval, complex circle, square&cube for tensor product interpolation.

Given a *polynomial determining* compact set $K \subset \mathbb{R}^d$ or $K \subset \mathbb{C}^d$ (i.e., polynomials vanishing there are identically zero), [Calvi and Levenberg in JAT08] introduced the idea of Weakly Admissible Meshes (WAM) as sequence of discrete subsets $\mathcal{A}_n \subset K$ that satisfy the polynomial inequality

$$\boxed{\|p\|_K \leq C(\mathcal{A}_n)\|p\|_{\mathcal{A}_n}\,, \quad \forall p \in \mathbb{P}_n^d(K) \qquad (5)}$$

where both $\mathrm{card}(\mathcal{A}_n) \geq N := \dim(\mathbb{P}_n^d(K))$ and $C(\mathcal{A}_n)$ grow at most *polynomially* with n.

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- When $C(\mathcal{A}_n)$ is bounded we speak of an Admissible Mesh (AM).
- For our purposes it sufficies to consider WAMs.

Discrete Extremal Sets

Idea: extracting a maximum determinant $N \times N$ submatrix from the $M \times N$ Vandermonde matrix $V = V(\mathbf{a}, \mathbf{p}) = [p_j(a_i)]$

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Key asymptotic result (cf. [Bos/De Marchi et al. NMTMA11]): Discrete Extremal Sets extracted from a WAM by the greedy algorithms below, have the same asymptotic behavior of the true Fekete points

$$\mu_n := \frac{1}{N}\sum_{j=1}^{N} \delta_{\xi_j} \xrightarrow{N\to\infty} d\mu_K$$

where μ_K is the pluripotential equilibrium measure of K

Approximate Fekete Points: algorithm

Idea: greedy maximization of submatrix volumes [Sommariva/Vianello ETNA10]

- core: select the largest norm row, $row_{i_k}(V)$, and remove from each row of V its orthogonal projection onto row_{i_k} onto the largest norm one (preserves volumes as with parallelograms)
- implementation: QR factorization with column pivoting [Businger/Golub 1965] applied to V^t
- Matlab script: $\boldsymbol{w} = V' \backslash \texttt{ones}(1:N)$; $ind = \texttt{find}(\boldsymbol{w} \neq \mathbf{0})$; $\xi = \boldsymbol{a}(ind)$

where $\boldsymbol{a}$ is the array of the WAM.

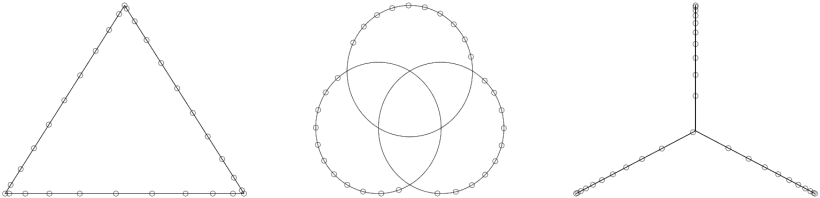

Figure : $N = 31$ AFP (deg $n = 30$) from Admissible Meshes on complex domains

Table 1. Numerically estimated Lebesgue constants of interpolation points in some 1-dimensional real and complex compacts

points	$n = 10$ $N = 11$	20 21	30 31	40 41	50 51	60 61
equisp intv	29.9	1e+4	6e+6	4e+8	7e+9	1e+10
Fekete intv	2.2	2.6	2.9	3.0	3.2	3.3
AFP intv	2.3	2.8	3.1	3.4	3.6	3.8
AFP 2intvs	3.1	6.3	7.1	7.6	7.5	7.2
AFP 3intvs	4.2	7.9	12.6	6.3	5.8	5.3
AFP disk	2.7	3.0	3.3	3.4	3.5	3.7
AFP triangle	3.2	6.2	5.2	4.8	9.6	6.1
AFP 3disks	5.1	3.0	7.6	10.6	3.8	8.3
AFP 3branches	4.7	3.5	3.8	8.3	5.0	4.8

- Unit disk: a symmetric polar WAM (invariant by rotations of $\pi/2$) is made by equally spaced angles and Chebyshev-Lobatto points along diameters [Bos at al. 2009]

$$\mathrm{card}(\mathcal{A}_n) = \mathcal{O}(n^2)\,, \quad C(\mathcal{A}_n) = \mathcal{O}(\log^2 n)$$

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- Unit simplex: starting from the WAM of the disk for polynomials of degree $2n$ containing only even powers, by the standard quadratic transformation

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- Square: Chebyshev-Lobatto grid, Padua points.

Notice: by affine transformation these WAMs can be mapped to any other triangle (**P1**) or polygon (**P4**).

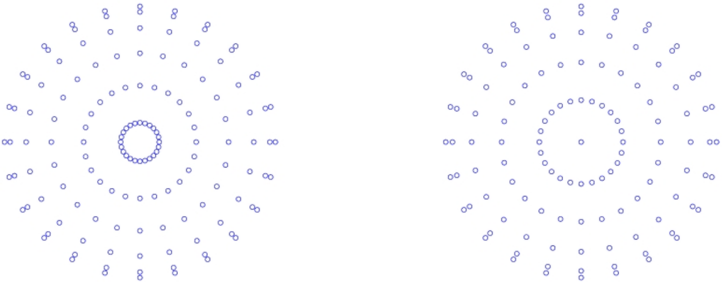


Figure : Left: for degree $n = 11$ with $144 = (n+1)^2$ points. Right: for $n = 10$ with $121 = (n+1)^2$ points.

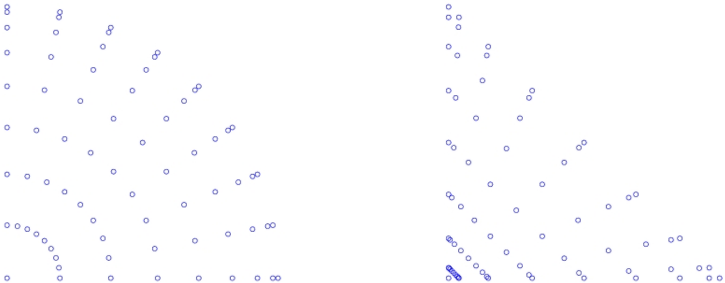


Figure : A WAM of the first quadrant for polynomial degree $n = 16$ (left) and the corresponding WAM of the simplex for $n = 8$ (right).

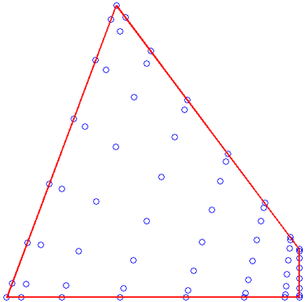


Figure : A WAM for a quadrangular domain for $n = 7$ obtained by the bilinear transformation of the Chebyshev–Lobatto grid of the square $[-1, 1]^2$

$$\frac{1}{4}[(1-u)(1-v)A+(1+u)(1-v)B+(1+u)(1+v)C+(1-u)(1+v)D]$$

Polygon WAMs: by triangulation/quadrangulation

$$\mathrm{card}(\mathcal{A}_n) = \mathcal{O}(n^2)\,, \quad C(\mathcal{A}_n) = \mathcal{O}(\log^2 n)$$

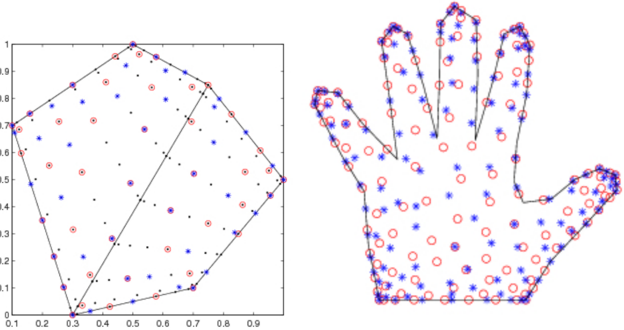
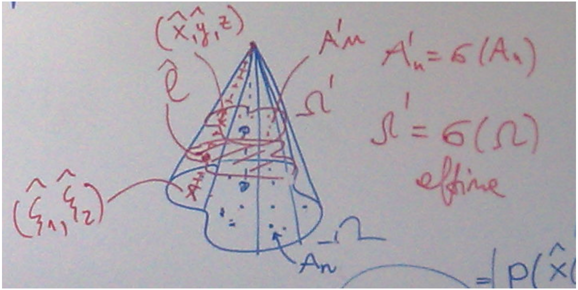


Figure : Left: $N = 45$ AFP ($\circ$) and DLP ($*$) of an hexagon for $n = 8$ from the WAM (dots) obtained by bilinear transformation of a 9×9 product Chebyshev grid on two quadrangle elements ($M = 153$ pts); Right: $N = 136$ AFP ($\circ$) and DLP ($*$) for degree $n = 15$ in a hand shaped polygon with 37 sides and a 23 element quadrangulation ($M \approx 5500$).

WAMs for (truncated) cones

Starting from a 2-dimensional domain WAM, we "repeat" the mesh along a Chebsyhev-Lobatto grid of the z-axis, as shown here in my handwritten notes (on my whiteboard).



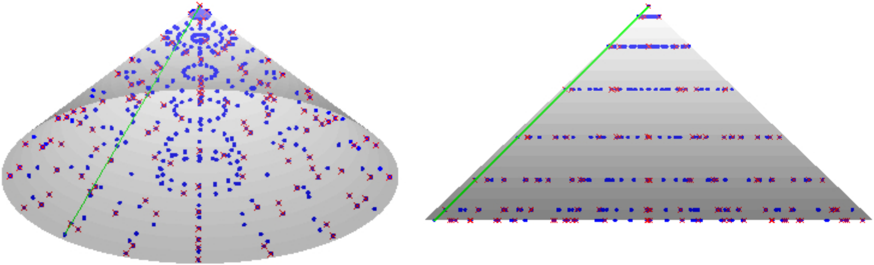
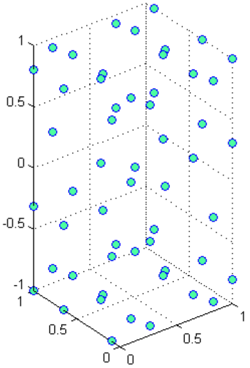


Figure : A WAM for the rectangular cone for $n = 7$

Here $C(A_n) = \mathcal{O}(\log^2 n)$ and the cardinality is $\mathcal{O}(n^3)$

The cube can be considered as a *cylinder with square basis*. WAMs for the cube with dimension $\mathcal{O}(n^3/4)$ were studied in [DeMarchi/Vianello/Xu 2009] in the framework of cubature and hyperinterpolation.
A WAM for the cube that for n even has $(n+2)^3/4$ points and for n odd $(n+1)(n+2)(n+3)/4$ points, is shown here for a parallelpiped with $n = 4$ (here $\#A_n = 54$)



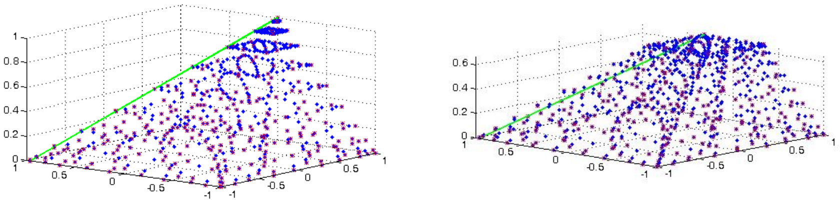


Figure : A WAM for a non-rectangular pyramid and a truncated one, made by using Padua points for $n = 10$. Notice the generating curve of Padua points that becomes a spiral

In this case $C(A_n) = \mathcal{O}(\log^2 n)$ and the cardinality is $\mathcal{O}(n^3/2)$

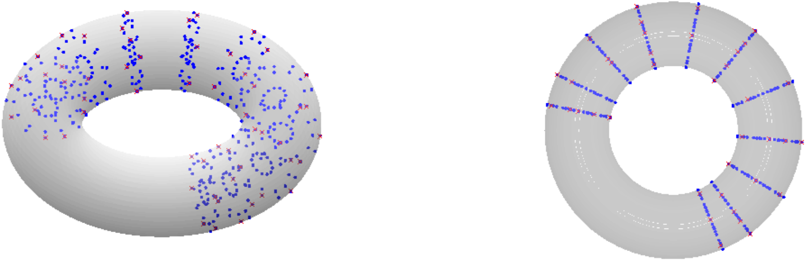


Figure : WAM for $n = 5$ on the torus centered in $z_0 = 0$ of radius $r_0 = 3$, with $-2/3\pi \leq \theta \leq 2/3\pi$.

In this case $C(A_n) = \mathcal{O}(\log^2 n)$ and the cardinality is $\mathcal{O}(2n^3)$

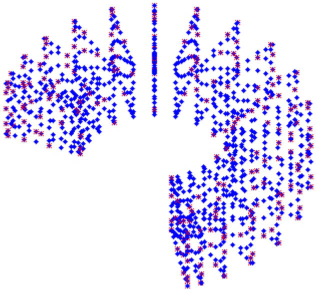


Figure : Padua points on the toroidal section with $z_0 = 0$, $r_0 = 3$ and opening $-2/3\pi \leq \theta \leq 2/3\pi$.

In this case $C(A_n) = \mathcal{O}(\log^2 n)$ and the cardinality is $\mathcal{O}(n^3)$.

AFP and cubature

- If in the algorithm AFP we take as r.h.s.

$$\boldsymbol{b} = \boldsymbol{m} = \int_K \boldsymbol{p}(x)\, d\mu$$

  i.e. the moments of the polynomials basis with respect to a given measure μ,

- hence, the vector $\boldsymbol{w}(ind)$ gives directly the weights of an algebraic cubature formula at the corresponding AFP
- The Matlab function `approxfek` written by [Sommariva/Vianello CMA10], extracts approximate Fekete or Leja interpolation points from a 2d or 3d mesh/cloud and estimates their Lebesgue constant.

The lens is given by the intersection of two disks with centers and radii $C_1 = (0,0),\ r_1 = 5$ and $C_2 = (4,0),\ r_2 = 3$, respectively.

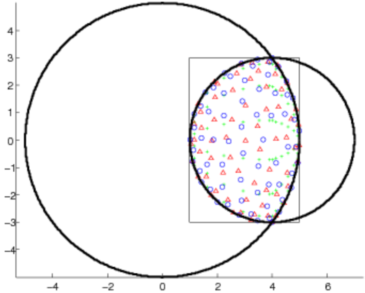


Figure : The lens approximated with $N = 200000$ Halton points. We extracted 66 points (corresponding to the dimension of $\mathbb{P}^2_{10}$).The points with `gqlens` are indicated with (+), the ones with `lsqnonneg` with exact moments with (△) and the AFP by `approxfek` (○) .

- The exact moments have been computed using nodes and weights provided by the Matlab function `gqlens`, which uses subperiodic trigonometric gaussian formulas [DaFies Vianello DRNA12].
- The QMC moments have been computed by starting from an initial grid of 600000 Halton points
- The nodes obtained with the `lsqnonneg` and the AFP accumulate along the boundary of the lens.
- A measure of stability

$$\rho = \frac{\sum_i w_i}{|\sum_i w_i|} \in [1, +\infty)\,, \tag{6}$$

says how many cubature weights of negative sign are present among all the weights

Tests on 2d domains

First test: the lens, continue...

	method	$N = 50000$	$N = 100000$	$N = 200000$
$n = 10$	gqlens	72 (1.00)	72 (1.00)	72 (1.00)
	QMC	37968	75925	151880
	lsqnonneg exact m.	66	66	66
	lsqnonneg QMC m.	66	66	66
	AFP exact m.	66 (1.02)	66 (1.00)	66 (1.04)
	AFP QMC m.	66 (1.02)	66 (1.00)	66 (1.04)
$n = 20$	gqlens	242 (1.00)	242 (1.00)	242 (1.00)
	QMC	37968	75925	151880
	lsqnonneg exact m.	210	209	207
	lsqnonneg QMC m.	231	231	231
	AFP exact m.	231 (1.03)	231 (1.04)	231 (1.04)
	AFP QMC m.	231 (1.03)	231 (1.04)	231 (1.04)
$n = 30$	gqlens	512 (1.00)	512 (1.00)	512 (1.00)
	QMC	37968	75925	151880
	lsqnonneg exact m.	416	413	409
	lsqnonneg QMC m.	496	495	495
	AFP exact m.	496 (1.01)	496 (1.03)	496 (1.01)
	AFP QMC m.	496 (1.02)	496 (1.04)	496 (1.02)

Table : Nodes on the lens extracted by `gqlens`, QMC, `lsqnonneg` with exact moments and approximated ones by QMC and the AFP by `approxfek`, again with exact moments or approximated by QMC. In parentheses the ratio (6).

First test

Test functions

used in many problems and applications

$$
\begin{aligned}
f_1(x,y) &= \frac{3}{4}e^{-\frac{1}{4}((9x-2)^2+(9y-2)^2)} + \frac{3}{4}e^{-\frac{1}{49}(9x+1)^2-\frac{1}{10}(9y+1)} \\
&\quad + \frac{1}{2}e^{-\frac{1}{4}((9x-7)^2+(9y-3)^2)} - \frac{1}{5}e^{-(9x-4)^2-(9y-7)^2} \qquad (7) \\
f_2(x,y) &= \sqrt{(x-0.5)^2+(y-0.5)^2} \qquad (8) \\
f_3(x,y) &= e^{-100((x-0.5)^2+(y-0.5)^2)} \qquad (9) \\
f_4(x,y) &= \cos(30(x+y)). \qquad (10)
\end{aligned}
$$

f_1 is the Franke function.

First test

Errors for f_1

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	method	$N = 50000$	$N = 100000$	$N = 200000$
	QMC	2.0e-02	2.2e-02	2.7e-02
	lsqnonneg exact m.	2.9e-02	1.7e-02	4.4e-02
$n = 10$	lsqnonneg QMC m.	3.9e-02	2.9e-02	2.6e-02
	AFP m. esatti	1.8e-02	2.4e-02	5.7e-02
	AFP QMC m.	1.8e-02	2.4e-02	5.7e-02
	QMC	1.4e-02	1.2e-02	7.2e-03
	lsqnonneg exact m.	8.5e-04	1.8e-02	2.3e-02
$n = 20$	lsqnonneg QMC m.	1.1e-02	1.4e-04	1.3e-02
	AFP exact m.	6.0e-02	2.4e-02	1.7e-02
	AFP QMC m.	6.0e-02	2.4e-02	1.7e-02
	QMC	7.6e-03	5.7e-03	6.5e-04
	lsqnonneg exact m.	3.3e-03	1.5e-03	9.3e-04
$n = 30$	lsqnonneg QMC m.	1.9e-02	7.6e-03	9.1e-04
	AFP exact m.	1.6e-03	2.1e-03	5.5e-03
	AFP QMC m.	1.4e-03	4.0e-03	4.5e-04

Table : Relative errors for f_1 on the lens, using QMC on Halton points. The values of the integral were computed with `gqlens`.

Similarly for f_2, f_3 and f_4.

The non-convex domain given by overlapping i) the disk with center $C = (0,0)$ and radius $r = 3$; ii) the square $[0,4] \times [0,4]$ iii) the closed polygon with vertices $V_1 = (1,1)$, $V_2 = (6,2)$, $V_3 = (7,4)$, $V_4 = (10,3)$, $V_5 = (9,6)$, $V_6 = (6,7)$, $V_7 = (4,5)$, $V_8 = (1,6)$, $V_9 = V_1$.

For this domain does not exist a cubature formula exact on the polynomials neither a way to compute the exact moments.

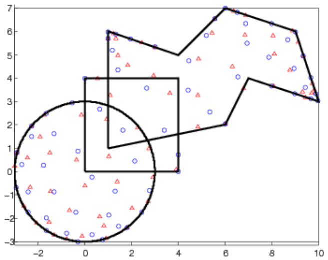


Figure : The composed domain approximated with $N = 200000$ Halton points and $n = 10$ (i.e. 66 points). The points selected with `lsqnonneg` are: with exact moments QMC with (Δ) and the AFP ($\circ$) .

Second test

A composite domain, continue ...

	method	$N = 50000$	$N = 100000$	$N = 200000$
$n = 10$	QMC	23323	46619	93269
	lsqnonneg	66	66	66
	AFP	66 (1.03)	66 (1.08)	66 (1.03)
$n = 20$	QMC	23323	46619	93269
	lsqnonneg	231	231	231
	AFP	231 (1.35)	231 (1.28)	231 (1.29)
$n = 30$	QMC	23323	46619	93269
	lsqnonneg	496	496	496
	AFP	496 (8544.15)	496 (5092.41)	496 (20346.70)

Table : For the composite domain, varying the number N of Halton points, we show the points extracted by `lsqnonneg` and the the AFP via `approxfek` at different n. We also show the ratio ρ (in brackets).

Second test

Errors for f_1

	method	$N = 50000$	$N = 100000$	$N = 200000$
$n = 10$	lsqnonneg	4.1e-02	3.4e-02	5.3e-02
	AFP	5.7e-02	1.1e-01	3.0e-02
$n = 20$	lsqnonneg	1.3e-02	4.1e-03	6.9e-03
	AFP	3.0e-02	4.3e-03	1.1e-02
$n = 30$	lsqnonneg	3.6e-03	2.8e-03	3.8e-03
	AFP	9.4e+00	3.3e+03	3.8e+00

Table : Relative errors for f_1 on the composite domain.

Similarly for f_2, f_3 and f_4

Third example

Three dimensional domain

The union of the cube $[0, 0.75] \times [0, 0.75] \times [0, 0.75]$ with the sphere centered in $C = (0.5, 0.5, 0.5)$ and radius $r = 0.5$

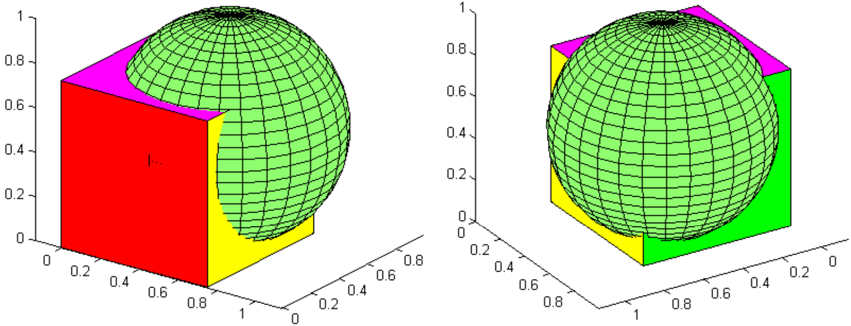
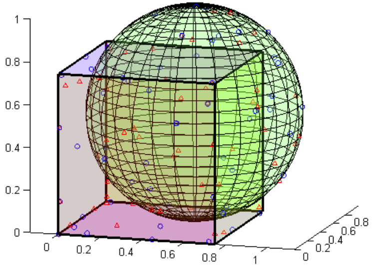


Figure : Composite domain: union of a cube and a sphere

Third example

Points extracted: plots



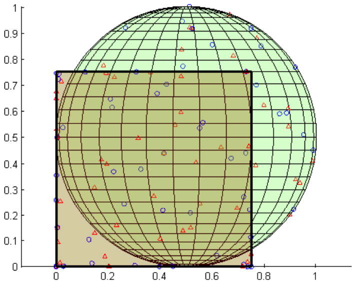


Figure : From $N = 100000$ Halton points the points extracted `lsqnonneg` (Δ) and the the AFP via `approxfek`($\circ$) for $n = 5$ (i.e. 56 points).

Third example

Points extracted: table

	method	$N = 50000$	$N = 100000$	$N = 200000$
	QMC	32212	64431	128793
$n = 5$	lsqnonneg QMC m.	56	56	56
	AFP QMC m.	56 (1.47)	56 (1.62)	56 (1.28)
	QMC	32212	64431	128793
$n = 7$	lsqnonneg QMC m.	120	120	120
	AFP QMC m.	120 (1.48)	120 (1.15)	120 (1.18)
	QMC	32212	64431	128793
$n = 9$	lsqnonneg QMC m.	220	220	216
	AFP QMC m.	220 (1.27)	220 (1.24)	220 (1.26)

Table : For the 3d domain, varying the number N of Halton points, we show the number of points extracted with different n. We also show the ratio ρ (in brackets).

First test

Errors

	method	$N = 50000$	$N = 100000$	$N = 200000$
$n = 5$	lsqnonneg QMC m.	1.97e-02	3.70e-02	4.58e-03
	AFP QMC m.	1.99e-02	5.11e-02	1.33e-02
$n = 7$	lsqnonneg QMC m.	5.49e-04	4.62e-03	3.43e-03
	AFP QMC m.	2.64e-02	3.92e-03	1.07e-02
$n = 9$	lsqnonneg QMC m.	8.34e-05	3.01e-03	7.80e-03
	AFP QMC m.	2.19e-03	2.25e-04	2.82e-05

Table : Relative errors for the 3d Franke function on the composite domain of Fig. 14. Errors are computed with respect to the QMC method.

Similar behaviour for other functions

Conclusions

Done and to do

Done

- We have provided a general compression technique.
- The method applies to every space dimension
- Nonnegative least-squares and AFP have shown a better behaviour than QMC, except for functions with high variation. But this is also the case for the classical QMC

To do

- A faster way of finding AFP
- Error analysis

Essential bibliography

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#thankyou!