Quadrature rules, Riesz energies, discrepancies and elliptic polynomials

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Point distributions webinar 2021

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Observe that

$$\dim \mathcal{P}_L = h_{L,d} \sim L^d$$

Fekete points

Let $\{x_j^L\}_{j=1}^{h_L} \subset \mathbb{S}^d$ be such that

$$|\det(Q_i^L(x_j^L))_{i,j}|$$

is maximal where $Q_1^L, \ldots, Q_{h_L}^L$ is an ON basis of $\mathcal{P}_L$.

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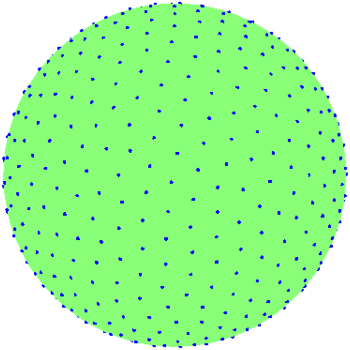
These sets of points are called Fekete (or extremal fundamental systems).



Rob Womersley web http://web.maths.unsw.edu.au/ rsw/Sphere/ 529 Fekete points

For $x_1^L, \dots, x_{h_L}^L \in \mathbb{S}^d$ Fekete points define

$$\ell_i^L(x) = \frac{\det \begin{pmatrix} Q_1(x_1^L) & \cdots & Q_1(x) & \cdots & Q_1(x_{h_L}^L) \\ \vdots & & \vdots & & \vdots \\ Q_{h_L}(x_1^L) & \cdots & Q_{h_L}(x) & \cdots & Q_{h_L}(x_{h_L}^L) \end{pmatrix}}{\det(Q_k(x_j^L))_{k,j}}$$

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Clearly

$$\ell_i^L(x_j^L) = \delta_{ij}, \;\; |\ell_i^L(x)| \leq 1.$$

For $Q \in \mathcal{P}_L$

$$Q = \sum_{j=1}^{h_L} Q(x_j^L)\ell_j^L$$

and

$$\int_{\mathbb{S}^d} Q \, d\sigma = \sum_{j=1}^{h_L} Q(x_j^L) \int_{\mathbb{S}^d} \ell_j^L \, d\sigma = \sum_{j=1}^{h_L} Q(x_j^L) w_j^L$$

where $w_j^L = \int_{\mathbb{S}^d} \ell_j^L \, d\sigma$ are the integration weights.

Theorem (M.-Ortega Cerdà 08) Fekete points are asymptotically uniformly distributed:

- for every $f \in \mathcal{C}(\mathbb{S}^d)$

$$\frac{1}{h_L}\sum_{j=1}^{h_L} f(x_j^L) \longrightarrow \int_{\mathbb{S}^d} f\, d\sigma \quad \text{as} \quad L \to +\infty.$$

or equivalently

- the (L^∞) spherical cap discrepancy

$$D_\infty(\{x_j^L\}_{j=1}^{h_L}) = \sup_{C\subset\mathbb{S}^d}\left|\frac{\#(\{x_j^L\}_{j=1}^{h_L}\cap C)}{h_L} - \sigma(C)\right|$$

satisfies

$$\lim_{L\to\infty} D_\infty(\{x_j^L\}_{j=1}^{h_L}) = 0.$$

$$\frac{1}{n_L}\sum_{j=1}^{n_L} Q(x_j^L) \xrightarrow[L]{} \int_{S^2} Q\,d\sigma = \sum_{j=1}^{n_L} Q(x_j^L)\, w_j^L \Rightarrow w_j^L \approx \frac{1}{n_L}$$

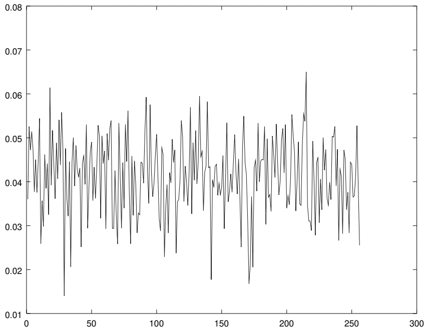
Reimer 93 $\boxed{w_j^L > 0}$ for P_2

$\boxed{L=2}$

numerically up to $L=191$

Sloan-Womersley

$\frac{4\pi}{256} \approx 0.049$



$16^2 = \Rightarrow L=15$

$2\pi\cdot$ weights corresponding to 256 Fekete points from Rob Womersley web http://web.maths.unsw.edu.au/ rsw/Sphere/

Sobolev spaces

For $\ell \geq 0$, $\mathcal{H}_\ell$ is the space of the spherical harmonics of degree ℓ

$$-\Delta Y = \ell(\ell + d - 1)Y, \quad Y \in \mathcal{H}_\ell.$$

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Then $L^2(\mathbb{S}^d) = \bigoplus_{\ell \geq 0} \mathcal{H}_\ell$ and for $f \in L^2(\mathbb{S}^d)$ the Fourier expansion is

$$f = \sum_{\ell,k} f_{\ell,k} Y_{\ell,k}, \qquad f_{\ell,k} = \langle f, Y_{\ell,k} \rangle = \int_{\mathbb{S}^d} f \, Y_{\ell,k} \, d\sigma,$$

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where $\{Y_{\ell,k}\}_{k=1}^{\dim \mathcal{H}_\ell}$ is an ON basis of $\mathcal{H}_\ell$. Given $s \geq 0$

$$\mathbb{H}^s(\mathbb{S}^d) = \left\{ f \in L^2(\mathbb{S}^d) \;:\; \sum_{\ell=0}^{+\infty} \sum_{k=1}^{\dim \mathcal{H}_\ell} (1 + \ell^2)^s |f_{\ell,k}|^2 < +\infty \right\}$$

with the norm

$$\|f\|_{\mathbb{H}^s(\mathbb{S}^d)} = \left(\sum_{\ell=0}^{+\infty} \sum_{k=1}^{\dim \mathcal{H}_\ell} (1 + \ell^2)^s |f_{\ell,k}|^2 \right)^{1/2}.$$

$\mathbb{H}^s(\mathbb{S}^d)$ is continuously embedded in $\mathcal{C}^k(\mathbb{S}^d)$ if $s > k + d/2$.

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For any $\epsilon > 0$, let $x_1, \ldots, x_N \in \mathbb{S}^d$ be a set of $N = h_{\lfloor (1+\epsilon)L \rfloor} \sim L^d$ Fekete points for $\mathcal{P}_{\lfloor (1+\epsilon)L \rfloor}$ and let $w_1, \ldots, w_N$ be the corresponding weights. Then for $s > d/2$

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By Brauchart-Hesse 07 this bound is optimal (see also Brandolini-Choirat-Colzani-Gigante-Seri-Travaglini 14).

Equal weights (Chebyshev quadrature)

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It can be shown that if $\mathrm{wce}(X_N, s) \sim N^{-s/d}$ for some $s > d/2$ and all N (i.e. (X_N) is a QMC design for H^s) then $\mathrm{wce}(X_N, s') \sim N^{-s'/d}$ for any $s \geq s' > d/2$.

Brauchart-Saff-Sloan-Womersley 14

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Brauchart-Saff-Sloan-Womersley 14

Then it is natural to ask for the larger s such that (X_N) is a QMC design for H^s (strength).

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asymptotic estimates of the maximal Riesz energy (Wagner 92) imply that energy maximizers form a sequence of QMC designs for H^s (By Stolarsky's formula $\mathrm{wce}(X_N, \frac{d+1}{2}) \equiv D_2(X_N) \leq D_\infty(X_N)$).

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• Numerical results for the strength in $\mathbb{S}^2$:

Fekete points 3/2

Coulomb energy minimizers 2

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  Fekete points 3/2
  Coulomb energy minimizers 2
  Logarithmic energy minimizers 3
- Random configurations (in expectation):
  Uniform and independent points are not QMC for any $s > d/2$
  Jittered sampling points are QMC if $\frac{d}{2} < s < \frac{d}{2} + 1$
  Spherical ensemble: Hirao 18, Berman 19 (concentration)

Extremal energies in $\mathbb{S}^2$

Define for $s < 2$ and $x_1, \dots, x_N \in \mathbb{S}^2$

$$E_s(x) = \sum_{i \neq j} \frac{1}{|x_i - x_j|^s} \quad \text{and} \quad E_{\log}(x) = \sum_{i \neq j} \log \frac{1}{|x_i - x_j|}.$$

Recall the conjecture about the extremal energy (Borodachov-Hardin-Saff 19)

$$\mathcal{E}_s(N) = \frac{2^{1-s}}{2-s} N^2 + \frac{(\sqrt{3}/2)^{s/2} \zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}} N^{1+s/2} + o(N^{1+s/2}), \quad N \to +\infty$$

Observe that

$$E_{-2}(x) = \sum_{i,j} |x_i - x_j|^2 = \sum_{i,j} (2 - 2x_i \cdot x_j) = 2N^2 - 2 \left| \sum_{i=1}^N x_i \right|^2 \leq 2N^2,$$

any configuration with 0 center of mass (vanishing dipole) attains the maximum $\mathcal{E}_{-2}(N) = 2N^2$.

Upper bounds for $0 < s < 2$

Rakhmanov-Saff-Zhou 94 (area regular partition)
For $\epsilon > 0$

$$\mathcal{E}_s(N) \leq \frac{2^{1-s}}{2-s} N^2 - \frac{1}{(2\sqrt{2\pi})^s}(1+\epsilon) N^{1+s/2},$$

for $N \geq N_0(\epsilon, s)$.
Alishahi-Zamani 15 (spherical ensemble)

$$\mathbb{E}_{X_N}[E_s(X_N)] \leq \frac{2^{1-s}}{2-s} N^2 - \frac{\Gamma\left(1-\frac{s}{2}\right)}{2^s} N^{1+s/2}$$

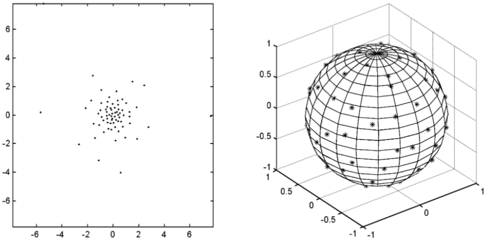
for $N \geq 2$.

Elliptic polynomials ($SU(2)$ or Kostlan-Shub-Smale)

We want to study the random points in the sphere associated with roots of random polynomials

$$\sum_{j=0}^{N} \sqrt{\binom{N}{j}} a_j z^j$$

via the stereographic projection, where a_j are normal (complex) random i.i.d.



From Armentano-Beltrán-Shub 11

The probability distribution corresponds to the classical unitarily invariant Hermitian structure in the space of homogeneous polynomials. Armentano-Beltrán-Shub (11)

$$\mathbb{E}_{X_N}[E_{\log}(X_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{N}{2}\log N - \left(\frac{1}{2} - \log 2\right) N.$$

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Considering a more general framework of holomorphic sections on Riemann surfaces. Zelditch-Zhong (08), Feng-Zelditch (13)

$$\mathbb{E}_{X_N}[E_s(X_N)] = \frac{2^{1-s}}{2-s} N^2 + C(s) N^{1+s/2} + O(N^{(1+s)/2} (\log N)^{1-s/2}),\ N \to +\infty$$

No explicit value for $C(s)$ and cannot recover the logarithmic case.

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Consider $f(z) = \sum_{j=0}^{N} \sqrt{\binom{N}{j}} a_j z^j$ as a Gaussian field. Computing the joint intensities of the zero sets by using Hammersley's formulas for GAFs

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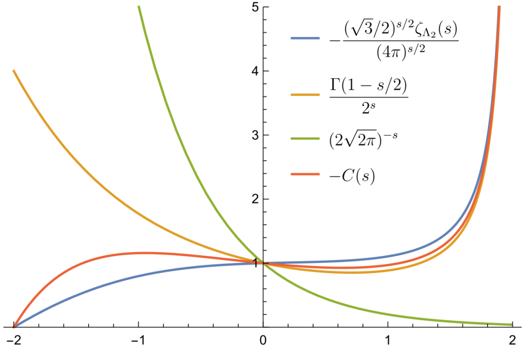
• If $x_1, \ldots, x_N \in \mathbb{S}^2$ are N points drawn as the zeros of elliptic polynomials $X_N = \{x_1, \ldots, x_N\}$

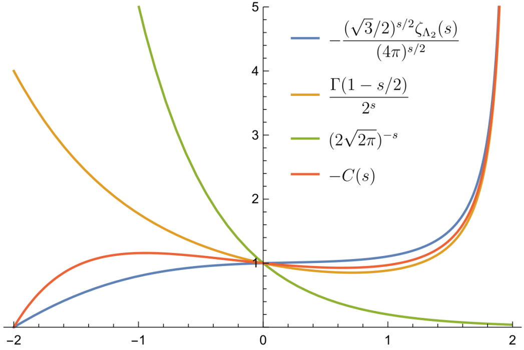
$$\mathbb{E}_{X_N}[E_s(X_N)] = \frac{2^{1-s}}{2-s} N^2 + C(s) N^{1+s/2} + \frac{sC(s-2)}{16} N^{s/2} + o(N^{s/2}), \ N \to +\infty$$

where

$$C(s) = \frac{2}{2^{s+1}} \left(1 + \frac{s}{2}\right) \Gamma\left(1 - \frac{s}{2}\right) \zeta\left(1 - \frac{s}{2}\right).$$



$-\frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}$
$\frac{\Gamma(1-s/2)}{2^s}$
$(2\sqrt{2\pi})^{-s}$
$-C(s)$
5
4
3
2
1
−2
−1
0
1
2



$$\mathbb{E}_{X_N}[E_{-2}(X_N)] = 2N^2 - 8\zeta(3)\frac{1}{N} + o(N^{-1}),\ N \to +\infty$$

• By using the expression of $\mathbb{E}_{X_N}[E_s(X_N)]$ for $-4 < s \leq -2$ we get that for the zeros of elliptic polynomials

$$\mathbb{E}_{X_N}[\mathrm{wce}(X_N, s)] = O(N^{-s/2}),$$

for $1 < s < 3$ and no they are not QMC in expectation for H^s if $s > 3$.

Thank you!