Approximate Fekete points and discrete Leja points based on equal area partitions of the unit sphere

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Outline of talk

- The EQ spherical codes
- Approximately optimal interpolating sets
- Results for the EQ spherical codes
The partition $\text{EQ}(2,33)$ on $S^2 \subset \mathbb{R}^3$

EQ partitions: Recursive Zonal Equal Area partitions of the sphere, $\bigcup \text{EQ}(d, \mathcal{N}) = S^d$, with $|\text{EQ}(d, \mathcal{N})| = \mathcal{N}$. 
The spherical code EQP(2,33) on $S^2$

EQ codes: The Recursive Zonal Equal Area spherical codes, $\text{EQP}(d, \mathcal{N}) \subseteq S^d$, with $|\text{EQP}(d, \mathcal{N})| = \mathcal{N}$. 
Equal-area partitions of $\mathbb{S}^d \subset \mathbb{R}^d$

An equal area partition of $\mathbb{S}^d \subset \mathbb{R}^d$ is a finite set $\mathcal{P}$ of Lebesgue measurable subsets of $\mathbb{S}^d$, such that

$$\bigcup_{R \in \mathcal{P}} R = \mathbb{S}^d,$$

and for each $R \in \mathcal{P}$,

$$\lambda_d(R) = \frac{\lambda_d(\mathbb{S}^d)}{|\mathcal{P}|},$$

where $\lambda_d$ is the Lebesgue area measure on $\mathbb{S}^d$. 
Diameter bounded sets of partitions

The *diameter* of a region \( R \subset \mathbb{R}^{d+1} \) is defined by

\[
\text{diam } R := \sup \{ \| x - y \| \mid x, y \in R \}.
\]

A set \( \Xi \) of partitions of \( S^d \subset \mathbb{R}^{d+1} \) is *diameter-bounded* with *diameter bound* \( K \in \mathbb{R}_+ \) if for all \( \mathcal{P} \in \Xi \), for each \( R \in \mathcal{P} \),

\[
\text{diam } R \leq K |\mathcal{P}|^{-1/d}.
\]
Key properties of the **EQ** partition of $\mathbb{S}^d$

**EQ**($d, \mathcal{N}$) is the *recursive zonal equal area* partition of $\mathbb{S}^d$ into $\mathcal{N}$ regions.

The set of partitions $\mathbf{EQ}(d) := \{ \mathbf{EQ}(d, \mathcal{N}) \mid \mathcal{N} \in \mathbb{N}_+ \}$.

The **EQ** partition satisfies:

**Theorem 1**

For $d \geq 1$, $\mathcal{N} \geq 1$, $\mathbf{EQ}(d, \mathcal{N})$ is an equal-area partition.

**Theorem 2**

For $d \geq 1$, $\mathbf{EQ}(d)$ is diameter-bounded.
For \( \text{EIFP}(d, \mathcal{N}) \)

**Good:**
- Centre points of regions of diameter \( = \mathcal{O}(\mathcal{N}^{-1/d}) \),
- Mesh norm (covering radius) \( = \mathcal{O}(\mathcal{N}^{-1/d}) \),
- Minimum distance and packing radius \( = \Omega(\mathcal{N}^{-1/d}) \).

**Bad:**
- Mesh ratio \( = \Omega(\sqrt{d}) \),
- Packing density \( \leq \frac{\pi^{d/2}}{2^d \Gamma(d/2+1)} \) as \( \mathcal{N} \rightarrow \infty \).
Approximation properties

Not so bad?

- Normalized spherical cap discrepancy = $O(\mathcal{N}^{-1/d})$,
- Normalized $s$-energy

$$E_s = \begin{cases} I_s \pm O(\mathcal{N}^{-1/d}) & 0 < s < d - 1 \\ I_s \pm O(\mathcal{N}^{-1/d} \log \mathcal{N}) & s = d - 1 \\ I_s \pm O(\mathcal{N}^{s/d-1}) & d - 1 < s < d \\ O(\log \mathcal{N}) & s = d \\ O(\mathcal{N}^{s/d-1}) & s > d. \end{cases}$$

Ugly:

- Cannot be used for polynomial interpolation: proven for large enough $\mathcal{N}$, conjectured for small $\mathcal{N}$.
\[ V(\theta_c) = V_R = \sigma(S^3)/99 \]
\[ \Delta_1 = V_R^{1/3} \]

\[ \begin{align*}
\theta_{F,1} &= 14.8... \\
\theta_{F,2} &= 33.7... \\
\theta_{F,3} &= 33.7... \\
\theta_{F,4} &= 14.8... \\
\end{align*} \]

\[ \begin{align*}
m_1 &= 15 \\
m_2 &= 34 \\
m_3 &= 33 \\
m_4 &= 15 \\
\end{align*} \]
Admissible meshes

**Definition 3**

For compact $D \subset \mathbb{R}^d$, and $C(D)$ the space of continuous functions on $D$, given a sequence of finite dimensional subspaces $P_t(D) \subset C(D)$, a $P_t$-norming mesh is a sequence $(Z_t)$ of finite subsets of $D$ such that

$$\|p\|_\infty \leq c \sup_{z \in Z_t} |p(z)| \quad \text{for all } p \in P_t.$$

For a $P_t$-admissible mesh, $P_t(D)$ is the space of polynomials of maximum degree $t$ on $D$, and the cardinality $|Z_t| = O(t^s)$ for some $s \geq 1$.

(Calvi and Levenberg 2008, Vianello 2013)
Given a $\mathbb{P}_t$-admissible mesh with

$$n_t := |Z_t| \geq d_t := \dim(P_t(D)),$$

points $z_1, \ldots, z_{n_t} \in Z_t$, and a basis $\{p_1, \ldots, p_{d_t}\}$ of $P_t(D)$, the \textit{approximate Fekete points} of order $t$ are a subset of $Z_t$ with cardinality $d_t$, obtained from the Vandermonde matrix $A_t := [p_i(z_j)]$ via QR decomposition with column pivoting.

They approximate the maximal determinant \textit{Fekete points} by having a large Vandermonde determinant and a small Lebesgue constant of interpolation.

(Sommariva and Vianello 2009)
Approximate Fekete points

The approximate Fekete points $z_{af}$ are obtained from the points $z$ and corresponding Vandermonde matrix $A$ as

$$\dim = \text{rows}(A);$$
$$y = \text{zeros}(\dim, 1);$$
$$y(1) = 1;$$

$$[Q, R, P] = \text{qr}(A);$$
$$w = P(:, 1:\dim) \times (R(:, 1:\dim) \backslash (Q' \times y));$$

$$z_{af} = z(:, \text{abs}(w) > \text{tol});$$

where $w$ is the optimal quadrature weight vector and $\text{tol}$ is a small tolerance. Here all elements of $w$ are non-zero, but $z_{af}$ may have dimension less than $\dim$.

(Sommariva and Vianello 2009)
Discrete Leja points

For the *Discrete Leja* points, LU decomposition with partial row pivoting is used instead.

```matlab
dim = rows(A);
y = zeros(dim, 1);
y(1) = 1;

[L, U, p] = lu(A’, ’vector’);
w = zeros(n, 1);
w(p(1:dim)) = L(1:dim, :)’ \ (U’ \ y);

z_dl = z(:, p(1:dim));
```

Here `z_dl` has dimension `dim`, but some elements of `w` may be zero.

(Bos, De Marchi, Sommariva and Vianello 2010)
We can also use *non-negative least squares* instead of either QR or LU decomposition.

```matlab
dim = rows(A);
y = zeros(dim, 1);
y(1) = 1;

w = lsqnonneg(A, y);

z_{nn} = z(:, abs(w) > tol);
```

Here all elements of $w$ are positive, but $z_{nn}$ may have dimension less than $dim$.

(Sommariva and Vianello 2014)
The EQ codes form an admissible mesh

**Theorem 4**

The EQ codes form a $\mathbb{P}_t$-admissible mesh.

**Proof.**

Any finite point set on the unit sphere $S^d$ with mesh norm at most $(1 - c)/t$ generates a norming set with constant $c$ for $\mathbb{P}_t$. The EQ spherical codes have mesh norm at most $C_d N^{1/d}$. Thus if $N \geq (C_d/(1 - c))^d t^d$, then EQP$(d, N)$ is a norming set with constant $c$ for $\mathbb{P}_t$.

(Jetter, Stöckler and Ward, 1998; L and Vianello 2014)
The Fekete points on the sphere $S^2$

The Fekete (maximal determinant) points on the sphere $S^2$ are the points that maximize the determinant of the Vandermonde-type matrix $A_t := [p_{t,i}(x_j)]$, where $i, j \in \{1, \ldots, (t + 1)^2\}$, the $p_{t,i}$ form an orthonormal basis of the spherical polynomials of degree at most $t$, and $x_j \in S^2$.

Rob Womersley has (approximately) computed these points up to degree $t = 165$, and their corresponding optimal quadrature weights, as well as the log of the determinant of the Gram matrix $G_t := A_t^T A_t$.

(Sloan and Womersley 2004; Womersley 2007)
The search algorithm

For each type of point set (approximate Fekete points, discrete Leja points, non-negative least squares points), for $t$ from 1 to 15, I used Octave with the EQ codes $\text{EQP}(2, \mathcal{N})$ for $\mathcal{N}$ from $(t + 1)^2$ to $(t + 1)^3$ to find:

- The smallest $\mathcal{N}$ such that the matrix $A$ has full rank, and the point set has all corresponding \textit{weights non-zero}.
- The smallest $\mathcal{N}$ such that the matrix $A$ has full rank, and the point set has all corresponding \textit{weights positive}.
- The value of $\mathcal{N}$ such that the matrix $A$ has full rank, the point set has all corresponding weights positive, and the Gram determinant is maximal.
Approximate Fekete points

The diagram shows the log of the Gram determinant as a function of the degree \( t \). The graphs are labeled as follows:

- Red dashed line: Non-zero weight
- Blue dotted line: Positive weight
- Green solid line: Maximum determinant
- Black solid line: Womersley

The log of the Gram determinant increases rapidly with increasing degree.
Discrete Leja points

The EQ spherical codes

Approximately optimal interpolating sets

Results for the EQ spherical codes

Log of Gram determinant

Degree \( t \)

Non-zero wt
Positive wt
Maximum det
Womersley
Non-negative least squares points

![Graph showing the log of the Gram determinant against degree t. The graph includes curves for Positive wt, Maximum det, and Womersley. The y-axis represents the log of the Gram determinant, and the x-axis represents degree t.]
Maximum determinant positive weight points

![Graph showing relative log of Gram determinant vs degree t for Approx Fekete, Discrete Leja, and NNLS methods.](image)

- **Approx Fekete**
- **Discrete Leja**
- **NNLS**

**Degree t**

**Relative log of Gram determinant**

0 0.2 0.4 0.6 0.8 1

0 2 4 6 8 10 12 14
Left to do

- Numerical examples for larger degree $t$.
  
  Searching can be done in parallel.

- Prove that for some $T > 0$, for all $t > T$, for sufficiently large $\mathcal{N}$, the EQ codes $\text{EQP}(2, \mathcal{N})$ yield positive weights for each of the 3 types of points. Estimate the $\mathcal{N}$ required.

- Investigate properties (mesh norm, discrepancy, energy) of the resulting point sets.