## Workshop on Sphere Packing and Amorphous Materials

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# Geometric t-designs and t-cubature and their relations to sphere packings and coverings 

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## What is numerical cubature?

Given $X \subseteq \mathbb{R}^{d}$ and a (normalized) measure $\mu$ on $X$, we want to estimate:

$$
\int_{X} f(\vec{x}) d \mu \approx f(F) \stackrel{\text { def }}{=} \sum_{k} w_{k} f\left(\vec{p}_{k}\right)
$$

We want to choose $F$ so that the formula is exact for polynomials of degree $\leq t$.

## Example

Simpson's rule.

$$
\int_{0}^{1} f(x) d x \approx \frac{1}{6} f(0)+\frac{2}{3} f\left(\frac{1}{2}\right)+\frac{1}{6} f(1)
$$

Simpson's rule is exact if $f \in \mathbb{R}[x]_{\leq 3}$. One says quadrature in one dimension and cubature in higher dimensions.

## The cubature problem

Given $X, \mu$ and $t \in \mathbb{N}$, find $F$ so that

$$
\int_{X} P(\vec{x}) d \mu=P(F)
$$

for $P \in \mathbb{R}[\vec{x}]_{\leq t} . F$ is a $t$-cubature formula. We want positive and interior ( PI ) formulas: $w_{k}>0$ and $F \subseteq X$. These are also called weighted $t$-designs (Delsarte).

The basic $t$-cubature or $t$-design problem is to minimize the number of points.

Cubature in 1D (quadrature) was solved by Gauss and Christoffel. But in $\geq 2 \mathrm{D}$, cubature is an open-ended problem, just like the sphere packing problem.

## An exact duality

- Delsarte found that $t$-designs are dual to sphere packings. First, an exact duality.
- Suppose that the domain $X$ is a compact abelian group. Then an embedding $X \subseteq \mathbb{R}^{N}$ can be viewed as a "polynomial structure" on $X$. In math-speak, $X$ is an affine algebraic variety (or a subset of one).
- If the affine algebraic structure is compatible with the group action, the structure is equivalent to an integer-valued metric on its Pontryagin dual $\hat{X}$. (I.e., $\hat{X}$ is the Fourier space of $X$.)
- If $F \subseteq X$ is a subgroup (or "lattice"), then it has a dual $F^{*} \subseteq \hat{X}$. Fact: $F$ is a $t$-design if and only if $F^{*}$ has minimum distance $t+1$.
- Packings at radius $r \leftrightarrow$ sets with min distance $t+1=2 r+1$.


## An exact duality

## Example

$X=(\mathbb{R} / 2 \pi \mathbb{Z})^{d}=$ the $d$-torus with trigonometric polynomials

$$
P(\vec{\theta})=P\left(\cos \theta_{1}, \sin \theta_{1}, \ldots, \cos \theta_{d}, \sin \theta_{d}\right),
$$

using the usual degree. Then $\hat{X}=\mathbb{Z}^{d}$ with the $\ell^{1}$ or taxicab metric.

## Example

Let $X=(\mathbb{Z} / 2)^{d}$ be bit strings of length $d$, and define $t$-designs to be orthogonal arrays of strength $t$. Then $\hat{X}=(\mathbb{Z} / 2)^{d}$ with the Hamming metric.

## An exact duality

Example (Noskov)
Let $X=(\mathbb{R} / 2 \pi \mathbb{Z})^{2}$ and let $F$ be the five points drawn below. Then $F$ is a trigonometric 2-design. It is dual to a discrete sphere packing (in fact a tiling) of radius 1 .


The discrete $\ell^{1}$ spheres are "Aztec diamonds", or "plus signs" when $r=1$.

## Delsarte's duality

Delsarte found another duality. Suppose that $X$ is a 2 -point symmetric metric space. This means that $X$ has a symmetry group which is transitive on pairs of points $x$ and $y$ at fixed distance $\operatorname{dist}(x, y)$. Then symmetry induces a polynomial structure on $X$ using harmonic functions.

## Examples

The sphere $X=S^{d-1}$. Hamming space $X=(\mathbb{Z} / 2)^{d}$.
Delsarte's method: Given $F \subseteq X$ with minimum distance $r$, write down linear relations that the radial pair correlation function $\sigma$ must satisfy. Namely, $\sigma(s) \geq 0, \int \sigma(s) d s=1, \sigma(s)=0$ for $0<s<r$, and the transform $\hat{\sigma}(k) \geq 0$. By linear programming, these relations yield an upper bound on $|F|=1 / \sigma(0)$.

## Delsarte's duality

Delsarte, McEliece, Rodemich, Rumsey, Welch, Odlyzko, Sloane, Kabatiansky, Levenshtein, etc., found that the Delsarte method yields excellent bounds, sometimes optimal. Cohn and Elkies generalized the method to $X=\mathbb{R}^{d}$; it is thought to be optimal when $d \in\{2,8,24\}$.

The duality is that similar equations yield a lower bound on $|F|$, where $F$ is a $\mathrm{Pl} t$-design; sometimes $F$ is optimal for both.

| packings | designs |
| :---: | :---: |
| $\sigma(s) \geq 0$ | $\sigma(s) \geq 0$ |
| $\int \sigma(s) d s=1$ | $\int \sigma(s) d s=1$ |
| $\hat{\sigma}(k) \geq 0$ | $\hat{\sigma}(k) \geq 0$ |
| $\sigma(s)=0,0<s<r$ | $\hat{\sigma}(k)=0,0<k \leq t$ |
| $\min \sigma(0)$ | $\max \sigma(0)$ |

Trigonometric cubature and discrete sphere packings
Problem
Trigonometric $t$-cubature $F$ on $(\mathbb{R} / 2 \pi \mathbb{Z})^{d}$ for fixed $t$ and $d \rightarrow \infty$.
Or, packings $F^{*}$ in $\mathbb{Z}^{d}$ at radius $r$ with $t=2 r$.
For $r=1$, let $F^{*}$ be the set of $\vec{x}$ with

$$
x_{1}+2 x_{2}+3 x_{3}+\cdots+d x_{d} \equiv 0 \quad(\bmod 2 d+1) .
$$

Then this is a tiling of $d$-dimensional plus signs.


## Trigonometric cubature and discrete sphere packings

What about for higher $r$ ? Suppose that $p \geq 2 d+1$ is prime. Define a group homomorphism $\phi: \mathbb{Z}^{d} \rightarrow(\mathbb{Z} / p)^{r}$ by

$$
\phi(\vec{x})=\sum_{k=1}^{r} x_{k}\left(k, k^{3}, k^{5}, \ldots, k^{2 r-1}\right) \in(\mathbb{Z} / p)^{r}
$$

Then

$$
F^{*}=\Lambda \stackrel{\text { def }}{=} \operatorname{ker} \phi
$$

is a sphere packing with density $\rightarrow 1 / r$ ! as $d \rightarrow \infty$, i.e., within a constant factor of the volume bound.
Theorem (K.)
For each $t$, trigonometric $t$-designs exist with $O\left(d^{\lfloor t / 2\rfloor}\right)$ points.
It is easy to boost $t$ to $2 r+1$ by restricting to even points.

## Trigonometric cubature and discrete sphere packings

Theorem (Stroud)
A volume bound holds for any $t$-cubature formula.
We match Stroud's bound of $O\left(d^{\lfloor t / 2\rfloor}\right)$ points, for each fixed $t$.

- $\Lambda$ is a modified Craig lattice (Conway and Sloane). These lattices were described for Euclidean spheres, but they are even better for discrete $\ell^{1}$ spheres. ( $\ell^{1} \approx \ell^{2}$ for small $r$.)
- An analogy:

| $\mathbb{Z} / 2$ | $\mathbb{Z}$ |
| :---: | :---: |
| Hamming code | plus lattice |
| BCH code | Craig lattice |

- Is there a competitive statistical mechanics approach? Note: These constructions yield deeply overdetermined $t$-designs.


## A statistical mechanics result

Wandzura and Xiao (2001) used simulated annealing to find good $t$-cubature on the triangle $\Delta_{2}$ for large $t$ :


$$
\begin{aligned}
t & =30 \\
|F| & =175
\end{aligned}
$$

It looks like a sphere covering with anisotropy near the boundary.

## t-designs are coverings

## Theorem (K.)

A $t$-design on the simplex $\Delta_{d}$ has covering radius $O(1 / t)$ when pulled back to an orthant section of $S^{d}$ under the map

$$
\pi:\left(x_{0}, x_{1}, \ldots, x_{d}\right) \mapsto\left(x_{0}^{2}, x_{1}^{2}, \ldots, x_{d}^{2}\right)
$$

in barycentric coordinates.

This is for weighted $t$-designs. For unweighted $t$-designs, the result is even stronger, because crowding at the edges forces more points in the middle just to make the weights equal.

## Positive islands

The proof uses a polynomial $P(\vec{x})$ of degree $t$ with

$$
\int_{\Delta_{d}} P(\vec{x}) d \vec{x}>0
$$

but which is only positive on a small positive island:


Any PI formula has a point in the island, so it is an sphere covering in a metric in which the islands are approximately round.

## Archimedes' theorem and $t$-designs

Theorem (Archimedes)
An axis projection of $S^{2}$ preserves normalized volume.


This explains Simpson's rule: It is the projection of a set in $S^{2}$ which is a 3 -design by symmetry. But that is another story.

## Archimedes' theorem and $t$-designs

- Archimedes' map generalizes to the moment map

$$
\pi: \mathbb{C} P^{d} \rightarrow \Delta_{d} \quad \mathbb{C} P^{1}=S^{2}
$$

- Here $\mathbb{C} P^{d}$ is an affine real algebraic variety in coordinates $\operatorname{Re} z_{j} \overline{z_{k}}$ and $\operatorname{Im} z_{j} \overline{z_{k}}$, and

$$
\pi(\vec{z})=\left(\left|z_{0}\right|^{2},\left|z_{1}\right|^{2}, \ldots,\left|z_{d}\right|^{2}\right)
$$

in barycentric coordinates on $\Delta_{d}$. Because $\mathbb{C} P^{d}$ is a projective toric variety, its moment map $\pi$ preserves volume and is linear.

- In physics-speak, $\mathbb{C} P^{d}$ is the space of quantum states in the Hilbert space $\mathbb{C}^{d+1}$. It is also a classical phase space, and $\pi$ is a vector of conservation laws from $d$ commuting symmetries.


## Archimedes' theorem and $t$-designs

## Example

The 240 kissing points of $E_{8} \subseteq S^{7}$ (the sphere kissing problem solution in 8 dimensions) project to 60 or 40 points on $\mathbb{C} P^{3}$.
Those project to 3-designs on $\Delta_{3}$ with 8 and 11 points.


They are described in Abramowitz and Stegun (1964)! Again, another story.

## The positive island

We actually define $P$ on $\mathbb{C} P^{d}$, rotate it to the desired position, and project to $\Delta_{d}$ by averaging over fibers. Before rotation, $P(\vec{z})=P\left(\left|z_{0}\right|\right)$. It is made using numerical quadrature on $[0,1]$ with $\mu(x)=x^{d-1}$. I.e., $P\left(\left|z_{0}\right|\right)$ comes from a Jacobi polynomial.


## Tao's question

Terry Tao posed this "congestion" (conjecture or question) in MathOverflow.

Question (Tao)
Suppose that $K$ is a symmetric convex body in $\mathbb{R}^{d}$ which and $\Lambda$ is a lattice packing of $K$. Then is the reciprocal lattice a covering of $r K^{*}$, where $K^{*}$ is the reciprocal convex body, with $r=d / 2$ or at least $r=O(d)$ ?
The constant $d / 2$ is from the putative worst case of a $d$-cube.

## Tao's question

I can prove $r=O\left(d^{3 / 2}\right)$ using the positive island method.

- First, replace $K$ with an ellipsoid $E$. By John's theorem, this sacrifices a factor of $O\left(d^{1 / 2}\right)$. Apply a linear map to make $E$ a standard sphere.
- Let $f: \mathbb{R}^{d} \rightarrow \mathbb{R}$ be a band-limited function, i.e., $\hat{f}(\vec{k})=0$ when $\|\vec{k}\|>t$. We can view $f$ as a "polynomial" of degree $t$. Then we can define Fourier $t$-designs on $\mathbb{R}^{d}$ with $t \in \mathbb{R}_{\geq 0}$ (cf., Cohn and Elkies).
- $\Lambda^{*}$ is a $t$-design with $t=2$ by duality. Does that force it to have a good covering radius? We can let $f$ be a band-limited positive island function using a Bessel function, with radius $O(d)$ QED.


## Open problems

- In the discrete $\ell^{1}$-ball or $\ell^{2}$-ball packing problem, what if $d, r \rightarrow \infty$ together at some rate?
- A $t$-design on a simplex $\Delta_{d}$ has covering radius $O(1 / t)$ on the orthant. Is this an optimal local density estimate?
- What is the answer to Tao's question?

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