A (Vague) Guiding Question

What is the most even distribution of $N$ points on the sphere $\mathbb{S}^d$?

Suppose we want to approximate

$$\frac{1}{|\mathbb{S}^d|} \int_{\mathbb{S}^d} f(x) dx \sim \frac{1}{N} \sum_{n=1}^{N} f(x_i).$$

How should we select the points? What if the domain is not $\mathbb{S}^d$?
Minimal Requirements

If we can pick 24 points on $\mathbb{S}^1$, this is how we should do it (admittedly: up to rotation but only up to rotation).
If we can pick 12 points on $S^2$, this is how we should do it (up to rotation but only up to rotation).
Sobolev-Lebedev Quadrature

Sergei Sobolev (1908–1989)

(Vyacheslav Lebedev, 1930–2010)
10. Cubature Formulas on the Sphere Invariant under Finite Groups of Rotations

S. L. Sobolev

A cubature formula on the surface of the sphere

\[ (l, f) = \int_S f(\vartheta, \varphi) \, dS - \sum_{k=1}^N c_k f(x^{(k)}) \equiv 0 \]  \hspace{1cm} (1)

is called *invariant* under transformations of a certain group \( G \) of sphere rotations if

\[ \left( l, f(\vartheta_1(\vartheta, \varphi), \varphi_1(\vartheta, \varphi)) \right) = \left( l, f(\vartheta, \varphi) \right), \]  \hspace{1cm} (2)

where

\[ \vartheta_1(\vartheta, \varphi), \quad \varphi_1(\vartheta, \varphi) \] \hspace{1cm} (3)

is a substitution in \( G \).

Integrate as many low-degree polynomials as possible exactly.
Suppose we want to approximate

\[ \frac{1}{|S^2|} \int_{S^2} f(x) \, dx \sim \frac{1}{N} \sum_{n=1}^{N} f(x_i). \]

How to select the points?

Idea (Sobolev 1962)

*Pick points such that as many spherical harmonics (polynomials in \( \mathbb{R}^3 \) restricted to \( S^2 \)) as possible are integrated exactly.*
Spherical Harmonics

- $m = 0, n = 1$
- $m = 1, n = 1$
- $m = 2, n = 2$
- $m = 4, n = 5$

- $m = 0, n = 2$
- $m = 1, n = 2$
- $m = 2, n = 3$
- $m = 5, n = 7$

- $m = 0, n = 3$
- $m = 1, n = 3$
- $m = 3, n = 6$
- $m = 6, n = 10$
Returning to our Minimal Requirements

Polynomials in $\mathbb{R}^2$ look like $x^m y^n$. On $\mathbb{S}^1$, they start looking like

$$(\cos \theta)^m (\sin \theta)^n$$

and trigonometric identities simplify this to classical Fourier series

$\sin \theta, \cos \theta, \sin 2\theta, \cos 2\theta, \ldots$. 

Basic Fact

$n$ equispaced points integrate

$$\sin (k\theta), \cos (k\theta) \quad \text{for all } 1 \leq k \leq n$$

exactly.

Proof.

$$\sum_{\ell=0}^{n-1} \cos \left(2\pi \frac{\ell}{n}\right) + i \sin \left(2\pi \frac{\ell}{n}\right) = \sum_{\ell=0}^{n-1} e^{2\pi i \frac{\ell}{n}}$$

= sum of roots of unity

= 0.
Returning to our Minimal Requirements

The Dodecahedron has a great degree of symmetry. It integrates all polynomials on $S^2$ up to degree 5 exactly ($\dim(V) = 36$). (Not quite as basic: this is optimal.)
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I want
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\frac{1}{|S^2|} \int_{S^2} f(x) \, dx \sim \frac{1}{N} \sum_{n=1}^{N} f(x_i)
\]
to be true for many polynomials. **What can we hope for?**
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to be true for many polynomials. **What can we hope for?**

2\(N\) parameters *should* solve 2\(N\) equations. If we additionally allow weights \(a_i \in \mathbb{R}\)

\[
\frac{1}{|S^2|} \int_{S^2} f(x) dx \sim \frac{1}{N} \sum_{n=1}^{N} a_i f(x_i)
\]

we *should* be able to do 3\(N\) equations. *(Open problem.)*
Figure: A set of 302 weighted points on $\mathbb{S}^2$ integrating all polynomials up to degree 29 exactly. Note that $30^2 = 900 \sim 3 \cdot 302$
The No-Miracles Theorem

Definition (Delsarte-Goethals-Seidels, 1977)
A set of points \( \{x_1, \ldots, x_n\} \subset \mathbb{S}^d \) is called a spherical \( t \)–design if

\[
\frac{1}{|\mathbb{S}^d|} \int_{\mathbb{S}^d} f(x) dx = \frac{1}{N} \sum_{i=1}^{N} f(x_i)
\]

holds for all polynomials up to degree \( t \).
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\dim(\text{polynomials degree less than } t) \sim t^d
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Theorem (No Miracles, Delsarte-Goethals-Seidels, 1977)
If a spherical design integrates all polynomial of degree \( \leq t \), then

\[
N \gtrsim t^d
\]
Theorem (Delsarte-Goethals-Seidels, 1977)

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\[ N \gtrsim t^d \]

Theorem (Bondarenko-Radchenko-Viazovska, 2013)

\[ N \lesssim t^d \quad \text{is always possible.} \]

Summary: Linear Algebra is approximately correct.

\[ N \sim \dim(\text{polynomials degree less than } t). \]
‘Toroidal’ Designs

Same question is interesting for the two-dimensional torus $\mathbb{T}^2$

$$\frac{1}{4\pi^2} \int_{\mathbb{T}^2} f(x)dx \sim \frac{1}{N} \sum_{i=1}^{N} f(x_i).$$

Replace polynomials by trigonometric functions $e^{i\langle k, x \rangle}$ where $k \in \mathbb{Z}^2$. There is a natural ordering by $\|k\|$. Question: Is the Linear Algebra Heuristic still correct?
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**Question**

Is the Linear Algebra Heuristic still correct?
‘Toroidal’ Designs

Taking a regular grid of points shows that \( N \) points can integrate the first \( \sim N \) exponentials. Proof is actually exactly the same as before: the sum of roots of unity sum to 0, twice.
‘Toroidal’ Designs

Taking a regular grid of points shows that $N$ points can integrate the first $\sim N$ exponentials. Proof is actually exactly the same as before: the sum of roots of unity sum to 0, twice.

Lemma (Hugh Montgomery, 1980s)

$N$ points can integrate no more than $\sim N$ exponentials exactly.
Laplacian Eigenfunctions

What unites

- spherical harmonics (polynomials) on the sphere $S^d$ and
- exponential functions $\exp(i \langle k, x \rangle)$ on $\mathbb{T}^d$?
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They are both eigenfunctions of the Laplacian on the manifold

$$-\Delta_g \phi_k = \lambda_k \phi_k.$$
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- spherical harmonics (polynomials) on the sphere $\mathbb{S}^d$ and
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They are both eigenfunctions of the Laplacian on the manifold

$$-\Delta_g \phi_k = \lambda_k \phi_k.$$

If you feel you don’t have a good handle on what that means, *welcome to the club*: People have been trying to understand them for 200 years.
Theorem (General No Miracle Theorem, S 2019)

There exists a constant $c_d$ such that on any compact manifold $(M, g)$ any set of $N$ points cannot integrate more than the first $c_dN + o(N)$ Laplacian eigenfunctions exactly.
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$$c_d \leq \frac{(d/2 + 1)^{d/2+1}}{\Gamma(d/2 + 1)}.$$
Universal Limitations on Quadrature

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Conjecture. The optimal constant is $c_d = d$ (unweighted points) or $c_d = d + 1$ (weighted points).
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**Conjecture.** The optimal constant is $c_d = d$ (unweighted points) or $c_d = d + 1$ (weighted points). Rest of the talk: let’s go discrete.
‘Hey George, I proved a pretty useless result.’

George Linderman, MD. PhD. (Massachusetts General Hospital)
Sampling on Graphs

A basic problem: you are given a finite graph \( G = (V, E) \).
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You want to understand the average value of $f$ and are allowed to evaluate $f$ in 3 vertices. Which 3 vertices do you choose?
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A basic problem: you are given a finite graph $G = (V, E)$. You have an unknown function

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This was the actual question George had to deal with.
Sampling on Graphs
Sampling on Graphs


*Open Problem:* everything. Might be very important.
Some Vague Philosophy I
Sobolev Lebedev in Euclidean Space give Platonic Bodies.
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Some Vague Philosophy II
If we define the same thing on other abstract objects, we can find the 'Euclidean bodies' in that object.
Graphical Designs

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Sobolev Lebedev in Euclidean Space give Platonic Bodies.

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If we define the same thing on other abstract objects, we can find the 'Euclidean bodies' in that object.

What’s the analogue of a platonic body on a Graph?
Some Graph Theory

We will work with finite, simple, connected Graphs $G = (V, E)$.

Functions are now simply maps $f : V \to \mathbb{R}$. The integral is

$$\int_G f := \frac{1}{|V|} \sum_{v \in V} f(v).$$
Some Graph Theory

We will work with finite, simple, connected Graphs \( G = (V, E) \).

**Question.** What is the analogue of a polynomial, a trigonometric polynomial or a Laplacian eigenfunctions?
Definition (Graphic Laplacian)

If \( f : V \rightarrow \mathbb{R} \), then the Graph Laplacian \((L_f) : V \rightarrow \mathbb{R}\) is given by

\[
(L_f)(u) = \sum_{v \sim E u} \left( \frac{f(v)}{\text{deg}(v)} - \frac{f(u)}{\text{deg}(u)} \right).
\]

where the sum runs over all vertices \( v \) adjacent to \( u \).

This is merely a linear operator, a \(|V| \times |V|\) matrix. It has eigenvalues and eigenvectors.
Definition (Graphical Design)

A graphical design on a Graph $G = (V, E)$ is a subset $W \subset V$
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A graphical design on a Graph \( G = (V, E) \) is a subset \( W \subset V \) such that, for as many eigenfunctions (eigenvectors) \( \phi_k \) of the Graph Laplacian (the matrix) as possible,
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A graphical design on a Graph $G = (V, E)$ is a subset $W \subset V$ such that, for as many eigenfunctions (eigenvectors) $\phi_k$ of the Graph Laplacian (the matrix) as possible,

$$\frac{1}{|W|} \sum_{w \in W} \phi_k(w) = \frac{1}{|V|} \sum_{v \in V} \phi_k(v).$$

Why should they even exist? Well, let’s have a look.
Graphical Design on Dyck Graph

8 vertices integrate the first 16 of 32 eigenfunctions.
6 vertices integrate 19 out of 24 eigenfunctions exactly.
Graphical Design on McGee Graph

8 vertices integrate the first 21 of 24 eigenfunctions.
8 vertices integrate the first 22 of 24 eigenfunctions.
Graphical Design on Sylvester Graph

6 vertices integrate the first 26 of 36 eigenfunctions.
Graphical Designs are non-Euclidean

Theorem (S, J. Graph Theory, 2019)
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A Graphical Design $W$ is either
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A Graphical Design $W$ is either
\begin{enumerate}
  \item not particularly good
  \item has $W$ large (for example $W = V$)
\end{enumerate}
Graphical Designs are non-Euclidean

Theorem (S, J. Graph Theory, 2019)
A Graphical Design $W$ is either
1. not particularly good
2. has $W$ large (for example $W = V$)
3. or has exponential growth of neighborhoods.
Zurich 2019: “Can you send me your slides?”

Konstantin Golubev
Figure: The Frucht Graph on 12 vertices: a subset $W$ of 4 vertices integrates the first 11 eigenfunctions exactly.

Definition (Extremal Graphical Design)
We call a graphical design extremal if it integrates all but 1 eigenvector exactly. (This is best possible.)
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$$\alpha(G) \leq \frac{\lambda_n}{\lambda_n - 1}.$$ 

This is sometimes sharp.
Konstantin’s Great Insight

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$$\alpha(G) \leq \frac{\lambda_n}{\lambda_n - 1}.$$  

This is sometimes sharp.

**Theorem (Golubev)**

*Assume the Hoffman bound is sharp. Then the independence set is an extremal graphical design.*
“Actually our first joint paper was done with Chao Ko, and was essentially finished in 1938, Curiously enough it was published only in 1961. One of the reasons for the delay was that at that time there was relatively little interest in combinatorics.” (Erdős)
Erdős-Ko-Rado Theorem

Let $A$ be a collection of $k$–element subsets of $\{1, 2, \ldots, n\}$ such that any two elements in $A$ have a non-empty intersection.
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This is sharp: take all subsets that contain the element 1.
Definition (Kneser Graph)

Let $V$ be the set of all $k$–element subsets of $\{1, \ldots, n\}$. Connect two vertices if the subsets are disjoint.
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Erdős-Ko-Rado determines the independence number of the graph.
Theorem (Golubev)

*Extremal Configurations for Erdos-Ko-Rado in the Kneser Graph are an extremal graphical design.*
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*Extremal Configurations for Erdos-Ko-Rado in the Kneser Graph are an extremal graphical design.*

Similar result for the Deza-Frankl Theorem (about fixed points of permutations on \( \{1, \ldots, n\} \)).
Things turn geometric!

General Equivalence Theorem (Babecki & Thomas, 2022)
Graphical Designs (with positive weight) are in bijection with the faces of a generalized eigenpolytope of the graph.
Things turn geometric!

General Existence Theorem (Babecki & Thomas, 2022)

There exists a graphical design on $k$ vertices integrating at least $k$ eigenvectors \textit{because} [...] on the corresponding polytope.
Random Walks

Random walks on graphs can be described by a sequence of probability measures

$$\mu_{k+1} = AD^{-1} \mu_k,$$

where $\mu_0$ is some probability distribution on the vertices, $D$ is the degree matrix and $A$ is the adjacency matrix.
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**Basic Fact**
This will generically converge to the uniform distribution at a rate given by $0 < |\lambda_2| < 1$, the second largest largest eigenvalue.
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**Basic Fact**
This will generically converge to the uniform distribution at a rate given by \( 0 < |\lambda_2| < 1 \), the second largest eigenvalue.

→ search for graphs with small \( |\lambda_2| \): **EXPANDER GRAPHS**.
Random Walks and Graphical Designs

Most probability measures on this graph converge to the uniform distribution at a rate given by $|\lambda^2| \sim 0.78$.

The uniform measure on the red vertices converges at a rate given by $|\lambda^9| \sim 0.47$. 
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Theorem (Rekha Thomas and S, 2022)

Let $G = (V, E)$ be a connected, regular graph on $n$ vertices and let $1 \leq \ell \leq n - 1$. 
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Let $G = (V, E)$ be a connected, regular graph on $n$ vertices and let $1 \leq \ell \leq n - 1$. There exists a probability measure $\mu_0$ supported on at most $\ell$ vertices in $V$. 
Theorem (Rekha Thomas and S, 2022)

Let $G = (V, E)$ be a connected, regular graph on $n$ vertices and let $1 \leq \ell \leq n - 1$. There exists a probability measure $\mu_0$ supported on at most $\ell$ vertices in $V$ such that the sequence of measures $\mu_{k+1} = AD^{-1}\mu_k$ satisfies

$$\sum_{v \in V} \left| \mu_k(v) - \frac{1}{n} \right|^2 \leq \lambda_{\ell+1}^{2k}.$$
Theorem 4.9. The Hamming code $H_r$ is a $(2^r - 1)$-design on $Q_{2^r-1}$, and

$$\text{efficacy}(H_r) = \frac{2^{2^r - r - 1}}{2^{2^r - 1} - \binom{2^r - 1}{2^{r-1}}} \sim \frac{1}{2^r}$$

asymptotically.
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Theorem 4.10. The Hamming code $H_r$ is the smallest linear code in cardinality which integrates all eigenspaces of $Q_{2^r-1}$ except for the eigenspace $\Lambda_{2^r-1}$.
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Conjecture 4.11. The Hamming code $H_r$ is an optimal design on $Q_{2^r - 1}$. 
Graphical Designs are hard to find

Theorem (Catherine Babecki and David Shiroma, 2022)
It is strongly NP-complete to determine if there is a graphical design smaller than the mentioned upper bound, and it is \#P-complete to count the number of minimal graphical designs.
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Theorem (Catherine Babecki and David Shiroma, 2022)
It is strongly NP-complete to determine if there is a graphical design smaller than the mentioned upper bound, and it is \#P-complete to count the number of minimal graphical designs. Many examples are here

https://sites.math.washington.edu/~GraphicalDesigns

(Often obtained via linear/semidefinite programming.)
Thank you!