Spherical Discrepancy

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Abstract

Right now, one of my projects is focused on exploring the quality of measure on spheres. We'll look at the implementation of an algorithm for computing discrepancy, some of the analysis of a problem related to the quality of a set of points in the compact setting, and some of the open problems that go with them.

Discrepancy

You are probably familiar with discrepancy as a function

$$D : \mathbb{N} \times \mathbb{I}^{\mathbb{N}} \to \mathbb{I}$$

that measures the irregularity of the distribution of a sequence $\{x_i\}$ when truncated to length N

$$D_N(\{x_i\}) = \sup_{0 \leq a < b \leq 1} \left| \frac{\#(\{x_i\}_{i \leq N}) \cap [a, b]}{N} - (b - a) \right|.$$

This notion can be generalized in many ways to other spaces, for example, by identifying the end points of the interval and including all connected subsets containing the point $\{0 = 1\}$ gives a discrepancy for a sequence of points on $\mathbb{S}^1$, the spherical cap discrepancy.

Discrepancy

We like low discrepancy sequences (quasi-random) as replacements for uniformly distributed random points.
For example, one gets equidistribution... the approximate integral

$$\frac{1}{N}\sum_{i=1}^{N} f(x_i) \to \int_0^1 f(x)dx$$

converges like the discrepancy up to a factor of the total variation (Koksma-Hlawka).

Remark

Flavors of ergodic theory and number theory: Thue-Siegel-Roth sequences, Weyl equidistribution. Ratner's theorems step it up to homogeneous spaces, but getting a sphere as the closure of a unipotent flow?

Discrepancy

In general, given a sphere $\mathbb{S}^d$ in $\mathbb{R}^{d+1}$ with radius 1 and normalized uniform measure σ and an (open) spherical cap C in $\mathbb{S}^d$, the *local spherical cap discrepancy* of a set X_N of N distinct points in the d-sphere is given by

$$\mathrm{D}_C[X_N] := \left|\left[\mathrm{Vol}(C) - \frac{1}{N}\#|X_N \cap C|\right]\right|$$

which may be viewed as a normalized difference between the expected number of points in a cap of Vol(C) and the number of points found in cap C

$$\mathrm{D}_C[X_N] = \frac{1}{N}(\mathbb{E}[\#|X_N \cap C|] - \#|X_N \cap C|).$$

Integrating over the space of caps of fixed size (equivalently, integrated over the sphere), we define a variance

$$\mathrm{Var}_C[X_N] = \int_{\mathbb{S}^d} \mathrm{D}_C^2 \, \mathrm{d}\sigma.$$

Discrepancy

There are several measurements of the quality of the point set based on this method. One is the *spherical cap discrepancy*, given as

$$\mathrm{D}(X_N) := \sup_{C \in \mathbb{S}^d \times [-1,1]} \mathrm{D}_C[X_N].$$

Another is the $\mathbb{L}^2$-*discrepancy*, given by

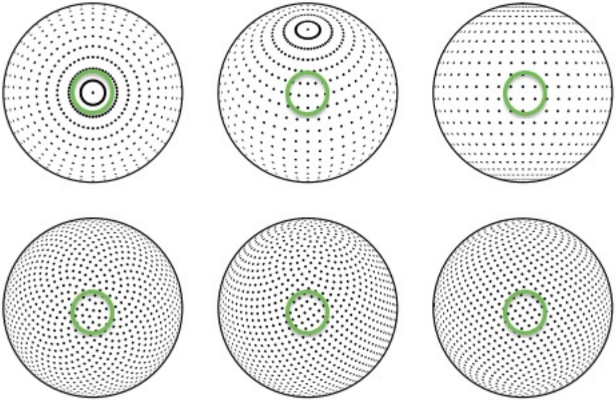
$$\mathrm{D}_{\mathbb{L}^2}[X_N] := \sqrt{\int_{-1}^{1} \mathrm{Var}_{C(t)}[X_N] \, \mathrm{d}t}$$

where $C(t)$ is a cap defined by the center z and all points with inner product greater than t.

Remark

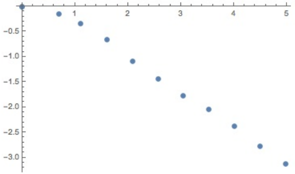
the local discrepancy is symmetric through the boundary of the cap, so these integrals double count in some sense.

Discrepancy



Spiral Points vs. Latitude/Longitude

```
ListPlot[Drop[RR, 0]]
DrRR[t_] := Drop[RR, t - 1]
Table[DrRR[i], {i, Length[Q] - 1}] // MatrixForm
Table[Fit[DrRR[i], {1, x}, x], {i, Length[Q] - 1}] //
 MatrixForm
```



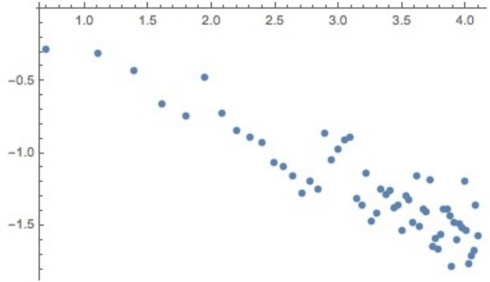
$$\begin{pmatrix} 0.194354 - 0.646505\,x \\ 0.260558 - 0.665517\,x \\ 0.395164 - 0.704171\,x \\ 0.43595 - 0.715185\,x \\ 0.429603 - 0.713532\,x \\ 0.360279 - 0.696243\,x \\ 0.371684 - 0.69898\,x \\ 0.434408 - 0.713471\,x \\ 0.62901 - 0.756827\,x \\ 0.726055 - 0.777701\,x \\ 0.474954 - 0.725491\,x \end{pmatrix}$$

Discrepancy of Spiral Points

Discrepancy

10000 Psudorandom Points

Discrepancy




```
Fit[Drop[Log[{Table[i, {i, 60}], ZZ}] // Transpose, 1], {1, x}, x]
0.0548572 - 0.402787 x
```

Discrepancy of Psudorandom Points

Discrepancy

- Computing the $\mathbb{L}^2$-discrepancy of a set of points is fairly easy, it follows from the *Stolarsky Invariance Principle*, which roughly states

$$\frac{1}{N^2}\sum_{i\neq j}|x_i - x_j| + \mathrm{D}_{\mathbb{L}^2}[X_N] = C_d.$$

- Based on results for star-discrepancy (where there is an analogous invariance principle, Warnock's formula), it is likely that computing the spherical cap discrepancy is NP-hard. However, there is still a nice algorithm for computing the cap discrepancy.

Computation

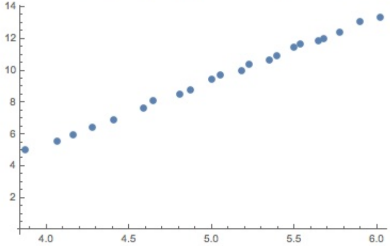
In the case of the star discrepancy an algorithm was described by Niederreiter that exactly computes the star discrepancy.

- Note that the discrepancy function achieves local extrema when the measuring sets are "captured."
- This is a finite set, so enumerate and take the maximum.

A similar approach works for spherical caps. It is a brute force approach but it is polynomial in the number of points (so is the original algorithm for star discrepancy)! Why? Because to "capture" a cap on $\mathbb{S}^d$ requires $d+1$ points or fewer, and $\binom{N}{d+1} = O(N^{d+1})$. Then comparing points gives an extra factor of N, so the runtime should be $O(N^{d+2})$, with possible improvements with clever sorting, etc.

Computation

```
ListPlot[Drop[Log[{Map[PottsTest3, Take[files, 32]], PrePots[[All, 3]]}] // Transpose, 10]]
```




```
Fit[Drop[Log[{Map[PottsTest3, Take[files, 32]], PrePots[[All, 3]]}] // Transpose, 10], {1, x}, x]
```

$-10.5834 + 3.99418\, x$

Runtime Estimate From Quadrature Points

Computation

This algorithm illustrates the issue of large constants in polynomial time algorithms. Using loops, this would probably take several hundred years for several thousand points. HOWEVER, it is a massively parallel problem. Just using matrix multiplication reduces the runtime by at least an order of 100 (mostly from better utilization of memory, since these are generally not sparse matrices and I don't think there is any good fast matrix multiplication implemented in my code.) Memory becomes a problem.

Remark

Implement and optimize this code in as a open parallel program, with good numerical error tracking. Build a database of discrepancies.

Computation

This algorithm also allows optimization to find minimal discrepancy point sets, but it is horrible since it depends on the labeled partitioning of N. So for a simplex, it is nice. Four points on $\mathbb{S}^2$ can be optimized by hand (almost). The minimum configuration and associated cap C allows one to pass support points across the boundary by symmetry and there happens to be a strong duality with four points. Then at the minimum discrepancy configuration

$$|\operatorname{Vol}(C) - 1/4| = |1 - \operatorname{Vol}(C)| \implies \operatorname{Vol}(C) = 5/8, \mathrm{D}(X_N) \geq 3/8.$$

This is not true for the regular simplex. We are also ignoring the 2-point discrepancy at the moment.

Computation

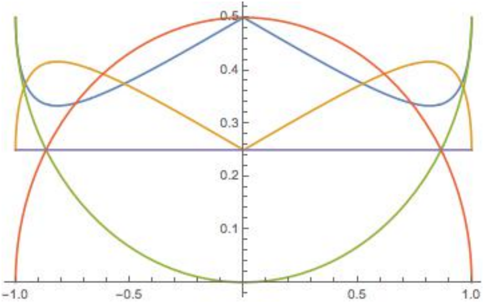
Numerical minimization hinted at $.375 = 3/8$ and one can symbolically solve to give discrepancies of

$$\frac{512 + 19\sqrt{466 - 38\sqrt{105}} + \sqrt{210\left(233 - 19\sqrt{105}\right)}}{2048}$$

$$\frac{1024 - 19\sqrt{466 - 38\sqrt{105}} - \sqrt{210\left(233 - 19\sqrt{105}\right)}}{2048}$$

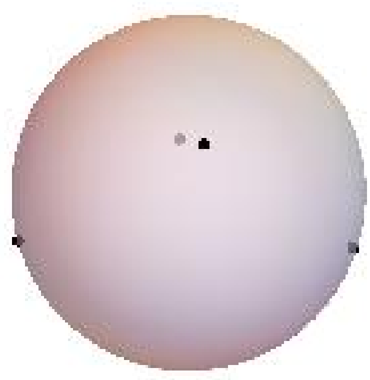
(which happen to be $3/8$!)

Computation



Simplex Discrepancy

Computation



Minimal Discrepancy Points

Variance

One last remark is that the variance

$$\mathsf{Var}_C[X_N] = \int_{\mathbb{S}^d} \mathsf{D}_C^2 \, \mathrm{d}\sigma.$$

is interesting on its own. There are some nice ways to look at it as a quality of measures parametrized by the radius of the cap size and the function spaces that the intersection volume serves as an evaluation kernel for. It also seems to fit well with a statistical mechanical property of point processes (hyperuniformity) and their behavior in the thermodynamic limit.

Remark

Understand these quantities from multiple perspectives (integral geometry, measure theory, optimal transport, statistical mechanics, discrete/combinatorial geometry).