STOLARSKY'S INVARIANCE AND SPHERICAL DISCREPANCY IN THE HAMMING SPACE

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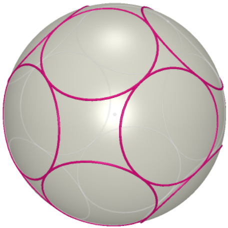
Point distributions webinar

Dec. 3, 2020

Quadratic discrepancy on the sphere



Quadratic discrepancy on the sphere $S^d(\mathbb{R})$

$$D^{L_2}_{\text{Cap}}(Z_N) = \int_{-1}^{1}\int_{S^d}\left(\frac{1}{N}|C(x,t)\cap Z_N| - \sigma(C(x,t))\right)^2 d\sigma(x)dt$$

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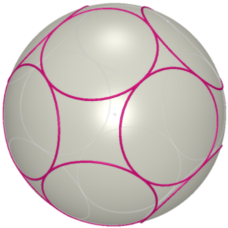

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A sequence of spherical point sets $(Z_N)_N$ is uniformly distributed if and only if

$$\lim_{N \to \infty} D^{L_2}_{\text{Cap}}(Z_N) = 0.$$

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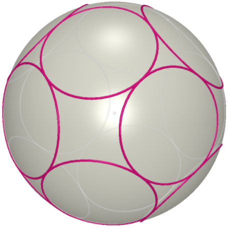

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Hyperuniform point sets: small number variance (Torquato-Stillinger, 2003). Applications in condensed matter physics, materials, chemical, engineering, and biological sciences.

Stolarsky's invariance principle for connected spaces

Stolarsky's invariance principle, 1973

$$c_d\left(D^{L_2}_{\mathrm{Cap}}(Z_N)\right)^2 = \iint\limits_{S^d \times S^d} \|x-y\| d\sigma(x) d\sigma(y) - \frac{1}{N^2}\sum_{i,j=1}^{N} \|z_i - z_j\|,$$

where $c_d = \frac{d\sqrt{\pi}\Gamma(d/2)}{\Gamma((d+1)/2)}$.

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General results regarding *universally optimal spherical codes* (Cohn-Kumar, 2007) imply that they minimize quadratic discrepancy

Bounds on D^{L_2} (the case of S^d)

- Classical results of BECK (1987) and ALEXANDER (1972) imply that for any Z_N of size N

$$D^{L_2}_{\text{Cap}} > cN^{-1/2(1+1/d)},$$

and that there exist point distributions such that

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- Optimal spherical designs of BONDARENKO-RADCHENKO-VIAZOVSKA (2013) meet the lower bound:

$$cN^{-1/2(1+1/d)} < D^{L_2}_{\text{Cap}} < CN^{-1/2(1+1/d)}$$

for sufficiently large N, absolute constants c and C (SKRIGANOV, 2019)

Finite spaces

Let $\mathcal{X}$ be a finite metric space; distances $d \in \{0, 1, \ldots, n\}$

$Z_N = \{z_1, \ldots, z_N\} \subset \mathcal{X}$

- Problem: Is Z_N "uniformly distributed" in $\mathcal{X}$?

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A subset Z_N is u.d. if for all $x \in \mathcal{X}, t \in \{0, 1, \ldots, n\}$

$$\frac{|B(x,t) \cap Z_N|}{N} = \text{vol}(B(x,t))$$

where $B(x,t) = \{z \in \mathcal{X} | d(z,x) \leqslant t\}$ is a metric ball in $\mathcal{X}$ centered at x

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Quadratic discrepancy of Z_N:

$$D^{L_2}(Z_N) = \sum_{t=0}^{n} (D_t(Z_N))^2$$

where

$$D_t(Z_N) := \left(\sum_{x \in \mathcal{X}} \left(\frac{|B(x,t) \cap Z_N|}{N} - \frac{1}{|\mathcal{X}|} |B(x,t)| \right)^2 \right)^{1/2}.$$

Finite metric spaces

Theorem (Stolarsky's invariance principle)

Let $Z_N = \{z_1, \dots, z_N\}$ be a subset of a finite metric space $\mathcal{X}$. Then

$$D^{L_2}(Z_N) = \frac{1}{2}\left(\frac{1}{|\mathcal{X}|^2}\sum_{x,y\in\mathcal{X}}\sum_{u\in\mathcal{X}}|d(x,u)-d(y,u)| - \frac{1}{N^2}\sum_{i,j=1}^{N}\sum_{u\in\mathcal{X}}|d(z_i,u)-d(z_j,u)|\right).$$

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Rephrasing:

$$\lambda(x,y) := \frac{1}{2}\sum_{u\in\mathcal{X}}|d(x,u)-d(y,u)|$$

Then

$$D^{L_2}(Z_N) = \frac{1}{|\mathcal{X}|^2}\sum_{x,y\in\mathcal{X}}\lambda(x,y) - \frac{1}{N^2}\sum_{i,j=1}^{N}\lambda(z_i,z_j)$$

$$= \langle\lambda\rangle_{\mathcal{X}} - \langle\lambda\rangle_{Z_N}$$

Proof outline

$$D_t(Z_N)^2 = \sum_{x\in\mathcal{X}} \left(\frac{1}{N}\sum_{j=1}^{N} \mathbb{1}_{B(x,t)}(z_j) - \frac{1}{|\mathcal{X}|}|B(x,t)|\right)^2$$
$$= \frac{1}{N^2}\sum_{i,j=1}^{N} |B(z_i,t)\cap B(z_j,t)| - \frac{|B(u,t)|^2}{|\mathcal{X}|},$$

$$\sum_{t=0}^{n} |B(x,t)\cap B(y,t)| = |\mathcal{X}|(n+1) - \sum_{z\in\mathcal{X}} d(z,u) - \frac{1}{2}\sum_{z\in\mathcal{X}} |d(z,x)-d(z,y)| \quad \square$$

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Another form of the invariance principle: Define

$$\mu(x,y) = \sum_{t=0} \mu_t(x,y), \text{ where } \mu_t(x,y) := |B(x,t)\cap B(y,t)|$$

Then

$$D(Z_N)^2 = \langle\mu\rangle_{Z_N} - \langle\mu\rangle_{\mathcal{X}}$$

Kernel $\lambda(x, y)$ in the Hamming space

Lemma

Let $x, y \in \mathcal{X}_n$ be two points such that $d(x, y) = w$. Then

$$\lambda(x, y) = \lambda(w) := 2^{n-w} w \binom{w-1}{\lceil \frac{w}{2} \rceil - 1}, \quad w = 0, 1, \ldots, n.$$

We have

$$\frac{\lambda(2i+1)}{2i+1} = \frac{\lambda(2i)}{2i}, \quad i \geqslant 1,$$

and thus $\lambda(i)$ is a monotone non-decreasing function of i for all $i \geqslant 1$.

Generating function:

$$\sum_{i=0}^{\infty} \lambda(2i+1) x^i = 2^{n-1} (1-x)^{-3/2}$$

Average value $\langle\lambda\rangle_{\mathcal{X}_n}$

$$\begin{aligned}
\langle\lambda\rangle_{\mathcal{X}_n} &= 2^{-2n} \sum_{x,y\in\mathcal{X}_n} \lambda(d(x,y)) \\
&= 2^{-n} \sum_{w=0}^{n} \binom{n}{w} \lambda(w) \\
&= 2^{-n} \sum_{w=1}^{n} 2^{n-w} w \binom{n}{w} \binom{w-1}{\lceil \frac{w}{2} \rceil - 1} \\
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\end{aligned}
$$

Computed using

$$
\sum_{t=0}^{n} \left\{ \sum_{i=0}^{t} \binom{n}{i} \right\}^2 = 2^{2n-1}(n+2) - \frac{n}{2}\binom{2n}{n}
$$

(OEIS A002457)

Stolarsky's identity in the Hamming space

Distance distribution of the code $Z_N \subset \{0,1\}^n$:

$$A_w = \frac{1}{N}|\{(x,y) \in Z_N \mid d(x,y) = w\}|, \quad w = 0,1,\dots,n$$

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Theorem (Stolarsky's invariance for the Hamming space)

Let $Z_N \subset \{0,1\}^n$ be a subset of size N with distance distribution $A(Z_N) = (1, A_1, \ldots, A_n)$. Then

$$D^{L_2}(Z_N) = \Lambda_n - \frac{1}{N} \sum_{w=1}^{n} A_w \lambda(w),$$

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This result enables us to compute or estimate $D^{L_2}(Z_N)$ for various binary codes

Upper bound

Proposition

The expected discrepancy of a random code of size N in $\{0,1\}^n$ equals

$$\mathsf{E}[D^{L_2}(\mathcal{Z}_N)] = \frac{n}{N2^{n+1}}\binom{2n}{n} \approx \sqrt{\frac{n}{\pi}}\frac{2^{n-1}}{N}$$

As a result, there exist binary codes of length n and size N with discrepancy

$$D^{L_2}(\mathcal{Z}_N) \leqslant C\sqrt{n}\frac{2^n}{N}$$

Dual view of discrepancy

Define the dual distance distribution $A^{\perp}(Z_N) = (A_0^{\perp}, \ldots, A_n^{\perp})$ of the code Z_N:

$$A_w^{\perp} = \frac{1}{N} \sum_{i=0}^{n} K_w^{(n)}(i) A_i, \quad w = 0, 1, \ldots, n$$

where

$$K_k^{(n)}(x) = \binom{n}{k} {}_2F_1(-k, -x; -n; 2).$$

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We obtain

$$\begin{aligned} D^{L_2}(Z_N) &= \Lambda_n - \frac{1}{2^n} \sum_{i=0}^{n} A_i^{\perp} \sum_{w=0}^{n} K_w^{(n)}(i) \lambda(w) \\ &= -\frac{1}{2^n} \sum_{i=1}^{n} A_i^{\perp} \sum_{w=0}^{n} K_w^{(n)}(i) \lambda(w) \end{aligned}$$

Hamming codes

Theorem

The quadratic discrepancy of the Hamming code $Z_N = \mathcal{H}_m$ *of length* $n = 2^m - 1, m \geqslant 2$ *equals*

$$D^{L_2}(\mathcal{H}_m) = \frac{n}{2^n}\binom{n-1}{\frac{n-1}{2}}$$

For large n *the discrepancy* $D^{L_2}(\mathcal{H}_m) = \sqrt{n/4\pi}(1 - o(1))$.

Discrepancy of the Hamming codes and their duals

Hamming codes $\mathcal{H}_m, n = 2^m - 1, N = 2^{n-m}$							
m	4	5	6	7	8	9	10
$D^{L_2}(\mathcal{H}_m)$	1.571	2.239	3.179	4.50471	6.377	9.027	12.763
$\mathsf{E}D^{L_2}(N)$	17.336	50.058	143.016	406.518	1152.64	3264.14	9238.04
Hadamard codes $\mathcal{H}_m^{\perp}, n = 2^m - 1, N = 2^m$							
$2^{-n}D^{L_2}(\mathcal{H}_m^{\perp})$	0.058	0.042	0.030	0.021	0.015	0.011	0.008
$2^{-n}\mathsf{E}D^{L_2}(N)$	0.068	0.049	0.035	0.025	0.018	0.012	0.009

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First step: Compute a Krawtchouk expansion of $\lambda(x,y)=\lambda(w)$. Start with

$$\mu_t(x,y) := |B(x,t)\cap B(y,t)| = \sum_{z\in\mathcal{X}_n} \phi_t(d(x,z))\phi_t(d(z,y))$$

where $\phi_t = \mathbb{1}_{\{0,1,\dots,t\}}$

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where $\phi_t=\mathbb{1}_{\{0,1,\dots,t\}}$

For the indicator function f we compute

$$\phi_t(l)=2^{-n}\sum_{k=0}^{n}c_k(t)K_k^{(n)}(l),\quad l=0,1,\dots,n$$

where

$$c_0(t)=\sum_{i=0}^{t}\binom{n}{i};\;\; c_k(t)=\frac{1}{\binom{n}{k}}\sum_{i=0}^{t}\binom{n}{i}K_k^{(n)}(i)=K_t^{(n-1)}(k-1),\;\; k\geqslant 1$$

Fourier-Krawtchouk expansions, II

Lemma

Let $x, y \in \mathcal{X}_n$ *be such that* $d(x, y) = w$. *The Krawtchouk expansion of the kernel* $\mu_t(x, y), t = 0, \ldots, n$ *has the following form:*

$$\mu_t(x, y) = 2^{-n} \sum_{k=0}^{n} c_k(t)^2 K_k^{(n)}(w),$$

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Corollary

Let $x, y \in \mathcal{X}_n$ be such that $d(x,y) = w$. We have

$$\lambda(x,y) = \lambda(w) = \sum_{k=0}^{n} \hat{\lambda}_k K_k^{(n)}(w)$$

$$\hat{\lambda}_0 = \Lambda_n, \; \hat{\lambda}_k = -2^{-n} \frac{\binom{2n-2k}{n-k}\binom{2k-2}{k-1}}{\binom{n-1}{k-1}}, \; k = 1, 2, \dots, n,$$

and thus the kernel $(-\lambda(x,y))$ is positive definite up to an additive constant.

$\lambda(w)$

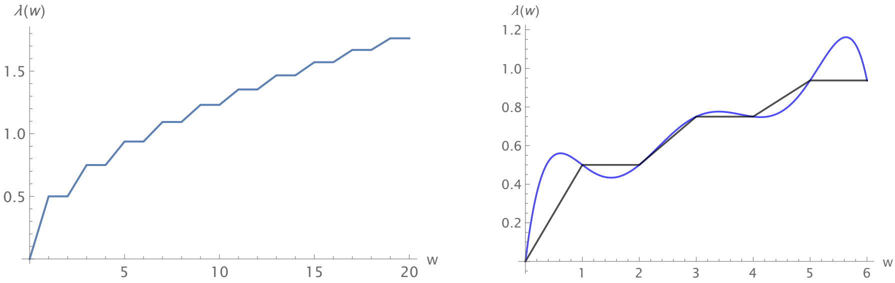

FIG.1: The plots show $\lambda(w)$ for $n = 20$ (left figure) and $n = 6$ (right figure). In the right plot we also show the Krawtchouk expansion, that is equal to $\lambda(w)$ at integer values of w. The plots are scaled by 2^{-n}.

Transform domain representation of $D^{L_2}(Z_N)$

We obtain an expansion of the discrepancy of the code Z_N

$$D^{L_2}(Z) = 2^{-n} \sum_{k=1}^{n} \frac{\binom{2n-2k}{n-k}\binom{2k-2}{k-1}}{\binom{n-1}{k-1}} A_k^{\perp}$$

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For instance, let $Z_N = \mathcal{H}_m$ be the Hamming code. We have $A^{\perp}_{\frac{n+1}{2}} = n$ and $A_k^{\perp} = 0$ o/w $(k \geqslant 1)$. Thus

$$D^{L_2}(\mathcal{H}_m) = -n\hat{\lambda}_{\frac{n+1}{2}}$$

$$\hat{\lambda}_{\frac{n+1}{2}} = -2^{-n}\binom{n-1}{\frac{n-1}{2}}$$

Discrepancy and energy minimization

Define the “potential energy” of the code $Z_N \subset \mathcal{X}_n$

$$E_\lambda(Z_N) = \frac{1}{N} \sum_{i,j=1}^{N} \lambda(d(z_i, z_j))$$

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Minimizing $D^{L_2}(Z_N)$ is equivalent to maximizing $E_\lambda(Z_N)$. This problem can be addressed by linear programming using the Delsarte conditions

$$\sum_{k=1}^{n} A_k K_i^{(n)}(k) \geqslant -\binom{n}{i}, i = 1, \ldots, n$$

and $\sum_{k=1}^{n} A_k = N - 1$.

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Dualizing, we obtain that any feasible solution of the linear program

$$\min \left\{ \sum_{i=0}^{n} \binom{n}{i} h_i - h_0 N \;\middle|\; \sum_{i=0}^{n} h_i K_i^{(n)}(k) \leqslant -\lambda(k), k = 1, \dots, n; h_i \geqslant 0, i = 1, \dots, n \right\}$$

gives an upper bound on $E_\lambda(Z_N)$

Linear programming bound

Proposition (LP)

Let $h(i) = \sum_{k=0}^{n} h_k K_k^{(n)}(i)$ *be a polynomial on* $\{0, 1, \ldots, n\}$ *such that*
(a), $h_k \geqslant 0$ *for all* $k \geqslant 1$ *such that* $A_k > 0$ *and*
(b)*,* $h(i) \leqslant -\lambda(i)$ *for all* $i \geqslant 1$ *such that* $A_i^{\perp} > 0$*. Then*

$$E_\lambda(Z_N) \leqslant h(0) - Nh_0$$

with equality if and only if all the inequalities in the assumptions (a),(b) are satisfied with equality.

Delsarte 1972-73, Yudin 1992, Ashikhmin-B-Litsyn 1999-2001, Cohn-Kumar 2007, Cohn-Zhao 2014, many others.

Bounds on discrepancy

Theorem

For any $N \geqslant 1$

$$D^{L_2}(n,N) \geqslant \Lambda_n - \frac{N-1}{N}\lambda(n). \tag{1}$$

For $n = 2t-1, N \geqslant 1$

$$D^{L_2}(n,N) \geqslant \begin{cases} \Lambda_n - \frac{2N-1}{2N}\lambda(t) & t \text{ even} \\ \Lambda_n - \frac{Nn-(n-1)/2}{N(n+1)}\lambda(t) & t \text{ odd.} \end{cases} \tag{2}$$

For any $N \geqslant 1$

$$D^{L_2}(n,N) \geqslant \begin{cases} -(\frac{2^n}{N} - 1)\hat{\lambda}_{\frac{n}{2}}, & n \text{ even} \\ -(\frac{2^n}{N} - 1)\hat{\lambda}_{\frac{n+1}{2}}, & n \text{ odd.} \end{cases} \tag{3}$$

Bounds on discrepancy

Theorem

For any $N \geqslant 1$

$$D^{L_2}(n,N) \geqslant \Lambda_n - \frac{N-1}{N}\lambda(n). \tag{1}$$

For $n = 2t-1, N \geqslant 1$

$$D^{L_2}(n,N) \geqslant \begin{cases} \Lambda_n - \frac{2N-1}{2N}\lambda(t) & t \text{ even} \\ \Lambda_n - \frac{Nn-(n-1)/2}{N(n+1)}\lambda(t) & t \text{ odd.} \end{cases} \tag{2}$$

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- Proof by fitting a polynomial to satisfy the conditions in Proposition (LP).
- Computations are aided by knowing the Fourier coefficients $\hat{\lambda}_k$
- The bounds are obtained by using $h(x)$ of degree 0 and n

Discrepancy minimizers

Theorem: *Binary perfect codes are discrepancy minimizers*

The following codes were found to be discrepancy minimizers by computer:

1. the Golay code with $n = 23, N = 4096$
2. the shortened Golay code
3. the twice shortened Golay code
4. the quadratic residue code with $n = 17, N = 512$
5. the 2-error-correcting BCH codes with $n = 31, N = 2^{21}$ and $n = 127, N = 2^{113}$ and their shortened codes.

Bounds on discrepancy

In summary, we proved the following bounds on the quadratic discrepancy of binary codes in the Hamming space:

Theorem

For large n and $N = o(2^n)$ we have the asymptotic bounds

$$c\frac{1}{\sqrt{n}}\frac{2^n}{N} \leqslant D^{L_2}(n,N) \leqslant C\sqrt{n}\frac{2^n}{N}$$

for some constants c, C. The discrepancy $D^{L_2}(n,N)$ is bounded away from zero unless $\frac{2^n}{\sqrt{n}} = o(N)$.
If $N = 2^{rn}, 0 < r < 1$, then

$$(\log N)^{-1/2}N^{\alpha} \lesssim D^{L_2}(n,N) \lesssim (\log N)^{1/2}N^{\alpha},$$

where $\alpha = \frac{1}{r} - 1$.

Generalization: Weighted L_p discrepancies

(This part is based on a joint work with Maxim Skriganov, arXiV:2007)

(Weighted) L_p discrepancy:

$$D_p(G, Z_n) = \Big(\sum_{t=0}^{n} g_t \sum_{x \in \mathcal{X}_n} |D(Z_n, y, t)|^p \Big)^{1/p}, \quad 0 < p < \infty$$

where

$$D(Z_n, x, t) = \frac{|B(x,t) \cap Z_N|}{N} - 2^{-n}|B(x,t)|$$

is the local discrepancy, and $G = (g_0, g_1, \dots, g_n), g_t \geqslant 0, \sum_{t=0}^{n} g_t = 1$ is a vector of weights.

REMARK: L_p discrepancies have been earlier considered for the case of spherical sets (M.M. Skriganov, *J. Complexity*, 2020)

Bounds on L_p discrepancy

Idea: Choose N points randomly in $\mathcal{X}_n$, then

$$D(Z_n, x, t) = \sum_{i=1}^{N} \frac{1}{N} \zeta_i$$

where $\zeta_i(x, t) = \mathbb{1}_{B(x,t)}(z_i) - 2^{-n}|B(x, t)|, i = 1, \ldots, N$ are zero-mean random variables. Khinchine-type inequalities for the pth moment of the sum of independent RVs enable one to derive estimates of D^{L_p}.

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Theorem

For all $N \leqslant 2^{n-1}$, we have

$$D_p(G, n, N) \leqslant 2^{-(n/p)+1} N^{-1/2} (p+1)^{1/2}$$

for $1 \leqslant p < \infty$, and $D_p(G, n, N) \leqslant 2^{-(n/p)+3/2} N^{-1/2}$ for $0 < p < 1$.

Discrepancy for hemispheres

Let $n = 2m + 1$ and consider only balls of radius $t = m$

For a subset $Z_N \subset \mathcal{X}_n$ define

$$D_p^{(m)}(Z_N) = \left(\sum\nolimits_{x \in \mathcal{X}_n} |D(Z_N, x, m)|^p \right)^{1/p}, \quad 0 < p < \infty\,,$$

where

$$D(Z_N, x, m) = \frac{|B(x, m) \cap Z_N|}{N} - \frac{1}{2}$$

Let

$$D_\infty^{(m)}(Z_N) = \max_{x \in \mathcal{X}_n} |D(Z_n, x)|$$

Main results for $D_p^{(m)}$

- Let $N = 2K$ be even, then

$$D_p^{(m)}(Z_N) \geqslant 0 \quad \forall Z_N \subseteq \mathcal{X}_n, p \in (0, \infty],$$

with equality for subsets Z_N consisting of K pairs of antipodal points. For $p = 2$ the condition for equality is also necessary.

- Let $N = 2K + 1$ be odd, then

$$D_p^{(m)}(Z_N) \geqslant 2^{n/p-1}/N \quad \forall Z_N \subseteq \mathcal{X}_n, p \in (0, \infty],$$

with equality for subsets Z_N consisting of K pairs of antipodal points supplemented with a single point.

Weighted invariance principle

Given a vector of weights $G = (g_0, g_1, \ldots, g_n)$, define the *weighted discrepancy* as

$$D_G^{L_2}(Z_N) = \sum_{t=0}^{n} g_t \cdot \left(D_t(Z_N)\right)^2$$

Proposition (Weighted invariance)

$$D_G^{L_2}(Z_N) = \langle \lambda_G \rangle_{Z_N} - \langle \lambda_G \rangle_{\mathcal{X}},$$

where for $x, y \in \mathcal{X}_n$

$$\lambda_G(x,y) := \frac{1}{2} \sum_{z \in \mathcal{X}_n} |\gamma(d(x,z)) - \gamma(d(y,z))|$$

and $\gamma(t) := \sum_{i=t}^{n} g_t$.

"Probabilistic potential" in the Hamming space

(joint work with Madhura Pathegama)

Let $v(x,y) = v(d(x,y))$ be a radial potential function on $\{0,1\}^n$; let $V = (v(x,y))_{x,y}$
Let p be a probability vector on $\{0,1\}^n$
Consier the energy $E_v = p^T V p$

Proposition

The uniform distribution $p = (2^{-n})$ is a minimizer of E_v if and only if the potential v is negative definite up to an additive constant.

$$v(d) = \sum_{i=0}^{n} \hat{v}_i K_i(d), \quad v_i \leqslant 0, i \geqslant 1$$

E.g.,

$$v(d) = d = \frac{n}{2} K_0^{(n)}(d) - \frac{1}{2} K_1^{(n)}(d)$$

$$\hat{\lambda}_k = -2^{-n} \frac{\binom{2n-2k}{n-k}\binom{2k-2}{k-1}}{\binom{n-1}{k-1}}, \ k = 1, 2, \ldots, n$$

Summary and open problems

- Previously the invariance principle was studied only for connected spaces such as S^d and related projective spaces (Riemannian symmetric spaces of rank one). Concrete results relied on analytic methods specific to such spaces.
- Finite metric spaces require different methods (combinatorial, etc.). Some of the results for the Hamming space have no direct analogs in the continuous case.

A multitude of open questions:

- Find necessary and sufficient conditions for minimizing discrepancy
- Classify discrepancy minimizers
- Structural results for other distance transitive finite (or disconnected infinite) metric spaces
- Explore applications of sets with small discrepancy