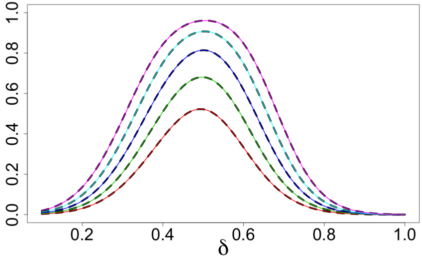
# Space filling; weak covering and quantization of high dimensional sets

Jack Noonan

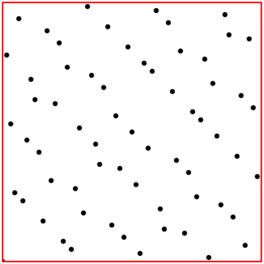



Workshop on kernel approximations and space-filling

July 1, 2022

# Space-filling designs

Space to be filled: $\mathcal{X} = [-1, 1]^d$
Design: $\mathbb{Z}_n = \{Z_1, \dots, Z_n\} \subset \mathcal{X}$
We want these points to be 'space-filling':

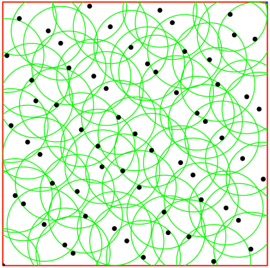


Designs $\mathbb{Z}_n$ which are well-spread within high-dimensional sets are required for efficient numerical integration, function approximation and global optimization.

# Covering radius = dispersion = fill radius = minimax crit.

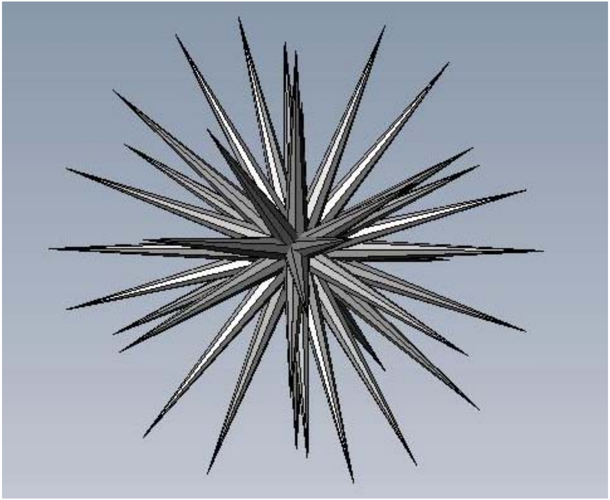
The main criteria for characterizing the spread of points are covering and packing radii, mean quantization error and various discrepancies.

$$CR(\mathbb{Z}_n) = \max_{x \in \mathcal{X}} \min_{i=1,\dots,n} \|x - Z_i\|$$



A.G.Sukharev: in the class of Lipschitz functions, $n$-point set with smallest covering radius provides the $n$-point min-max optimal:
(a) quadrature and (b) global optimization method.

If $d$ is not small (say, $d > 5$) then computation of $\mathrm{CR}(\mathbb{Z}_n)$ is very difficult to (a) compute given a point set, and (b) optimize with respect to the choice of the sets of points.

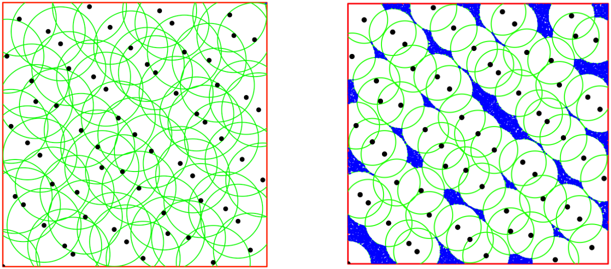


# Weak covering of high-dimensional sets

**Definition**

A design $\mathbb{Z}_n$ with radius $r$ makes a $(1-\gamma)$-covering of $\mathcal{X} = [-1,1]^d$ if

$$C_d(\mathbb{Z}_n, r) := \mathrm{vol}(\mathcal{X} \cap \mathcal{B}_d(\mathbb{Z}_n, r))/2^d = 1 - \gamma \, .$$



- We are only interested in a high covering of say 90%, 95% or 99%.

# Quantization error

## Definition

Let $X = (x_1, \ldots, x_d)$ be uniform random vector on $[-1,1]^d$. The mean squared quantization error for a design $\mathbb{Z}_n = \{Z_1, \ldots, Z_n\} \subset \mathbb{R}^d$ is defined by

$$\theta(\mathbb{Z}_n) = \mathbb{E}_X \varrho^2(X, \mathbb{Z}_n)\,, \quad \text{where} \;\; \varrho^2(X, \mathbb{Z}_n) = \min_{Z_i \in \mathbb{Z}_n} \|X - Z_i\|^2\,.$$

- $C_d(\mathbb{Z}_n, r)$, as a function of $r \geq 0$, is the c.d.f. of the r.v. $\varrho(X, \mathbb{Z}_n)$ while $\theta(\mathbb{Z}_n)$ is the second moment of the distribution with this c.d.f.:

$$\theta(\mathbb{Z}_n) = \int_{r \geq 0} r^2 dC_d(\mathbb{Z}_n, r)\,.$$

# Part 1
# Intersection of a ball and a cube

Based on:
*J. Noonan and A. Zhigljavsky (2020). Covering of high-dimensional cubes and quantization. SN Operations Research Forum*, 1(3) 1–32.
*J. Noonan and A. Zhigljavsky (2021). Non-lattice covering and quanitization of high dimensional sets. Black Box Optimization, Machine Learning, and No-Free Lunch Theorems.*

# Intersection of a ball and a cube

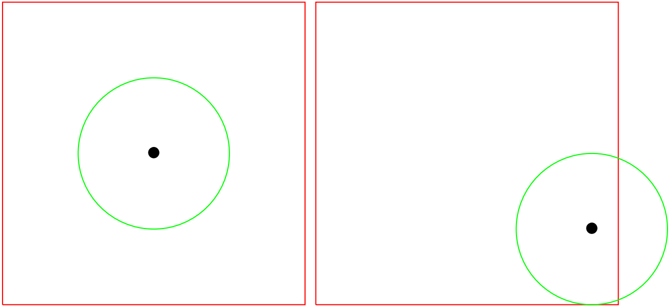
$\mathcal{X} = [-1, 1]^d$, $B_d(Z, r) = \{X \in \mathbb{R}^d : \|X - Z\| \le r\}$,

$$C_{d,Z,r} = \frac{\mathrm{vol}(\mathcal{X} \cap B_d(Z, r))}{\mathrm{vol}(\mathcal{X})} .$$

Let $U = (u_1, \ldots, u_d)$ have uniform distribution on $\mathcal{X}$. Then

$$C_{d,Z,r} = \Pr\left\{\|U - Z\|^2 \le r^2\right\} = \Pr\left\{\sum_{i=1}^{d}(u_i - z_i)^2 \le r^2\right\} .$$

# Intersection of a ball and a cube



There is no closed-form expression for $C_{d,Z,r}$, the c.d.f. of the r.v. $\sum_{i=1}^{d}(u_i - z_i)^2$ but we can approximate the c.d.f. in different ways; e.g., using characteristic functions of $(u_i - z_i)^2$.

## Intersection of a ball and a cube: Normal approximation I

$$C_{d,Z,r} = \Pr\left\{\|U - Z\|^2 \le r^2\right\} = \Pr\left\{\sum_{i=1}^{d}(u_i - z_i)^2 \le r^2\right\}$$

Consider the r.v. $\|U - Z\|^2$. Its mean and variance are:

$$\mu_{d,Z} = \mathbb{E}\|U - Z\|^2 = \|Z\|^2 + \frac{d}{3}$$

$$\sigma_{d,Z}^2 = \mathrm{var}(\|U - Z\|^2) = \frac{4}{3}\left(\|Z\|^2 + \frac{d}{15}\right)$$

The resulting normal approximation:

$$C_{d,Z,r} \cong \Phi\left(\frac{r^2 - \mu_{d,Z}}{\sigma_{d,Z}}\right),$$

where $\Phi(\cdot)$ is the c.d.f. of the standard normal distribution.

# Improving the normal approximation

We use Edgeworth-type expansion in the CLT for sums of independent non-identically distributed r.v. by V.Petrov:

$$P\left(\frac{\|U-Z\|^2-\mu_{d,Z}}{\sigma_{d,Z}} \le x\right) = \Phi(x) + \sum_{\nu=1}^{\infty} \frac{Q_{\nu,d}(x)}{d^{\nu/2}}$$

where

$$Q_{\nu,d}(x) = -\phi(x) \sum H_{\nu+2s-1}(x) \prod_{m=1}^{\nu} \frac{1}{k_m!} \left(\frac{\lambda_{m+2,d}}{(m+2)!}\right)^{k_m}$$

where $H_m$ is the Chebyshev-Hermite polynomial of degree $m$ and the summation is carried out over all non-negative integer solutions of the equation

$$k_1 + 2k_2 + \cdots + \nu k_\nu = \nu$$
$$s = k_1 + k_2 + \cdots + k_\nu \,.$$

# Improving the normal approximation

The summation is carried out over all non-negative integer solutions of the equation

$$k_1 + 2k_2 + \cdots + \nu k_\nu = \nu\,.$$

In number theory, the partition function $p(\nu)$ represents the number of possible partitions of a non-negative integer $\nu$. The sequence has the generating function

$$\sum_{\nu=0}^{\infty} p(\nu)x^\nu = \prod_{k=1}^{\infty} \left(\frac{1}{1-x^k}\right)$$

The first few values are: 1, 1, 2, 3, 5, 7, 11, 15, 22, 30, 42, 56, 77, 101, 135, 176, 231, 297, 385, 490, 627, 792, 1002, 1255, 1575, 1958, 2436, 3010, 3718, 4565, 5604...

# Improving the normal approximation

Taking the first additional term in the Petrov expansion:

$$P\left(\frac{\|U-Z\|^2-\mu_{d,Z}}{\sigma_{d,Z}}\le x\right)\cong\Phi(x)+\frac{\mu_{d,Z}^{(3)}}{6(\sigma_{d,Z}^2)^{3/2}}(1-x^2)\phi(x),$$

where

$$\mu_{d,Z}^{(3)}=\mathbb{E}\left[\|U-Z\|^2-\mu_{d,Z}\right]^3=\frac{16}{15}\left(\|Z\|^2+\frac{d}{63}\right)$$

This leads to the following improved form of the normal approximation:

$$C_{d,Z,r}\cong\Phi(t)+\frac{\|Z\|^2+d/63}{5\sqrt{3}(\|Z\|^2+d/15)^{3/2}}(1-t^2)\phi(t)\,,$$

$$t=t_{d,\|Z\|,r}=\frac{r^2-\mu_{d,Z}}{\sigma_{d,Z}}=\frac{\sqrt{3}(r^2-\|Z\|^2-d/3)}{2\sqrt{\|Z\|^2+d/15}}\,.$$

# Intersection of a ball and a cube

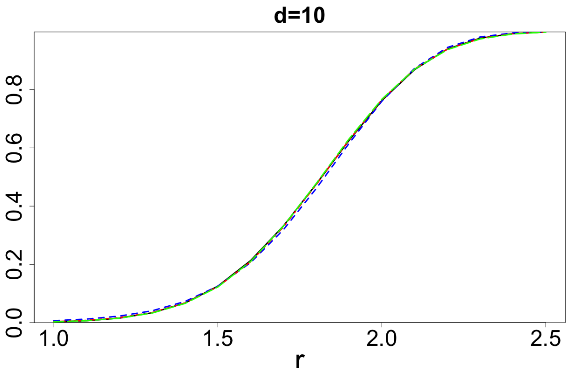



Figure 1: $d = 10,\ Z = 0,\ r \in [1, 2.5]$.

# Intersection of a ball and a cube

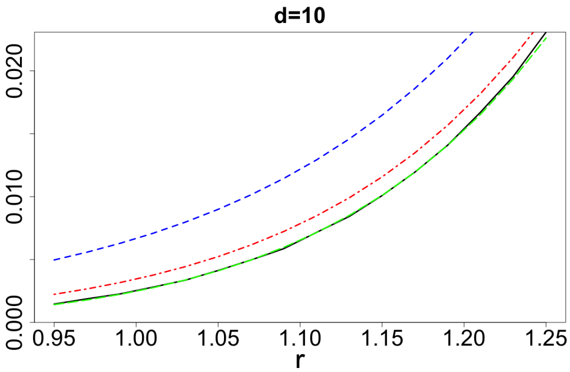



Figure 2: $d = 10,\ Z = 0,\ r \in [0.95, 1.25]$.

# Intersection of a ball and a cube

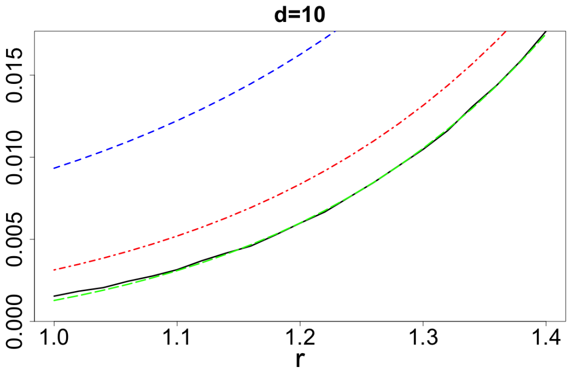



Figure 3: $Z$ is at half-diagonal with $\|Z\| = \frac{1}{2}\sqrt{10}$

# Part 2
# Random designs

Based on:

*J. Noonan and A. Zhigljavsky (2020). Covering of high-dimensional cubes and quantization. SN Operations Research Forum*, 1(3) 1–32.

*J. Noonan and A. Zhigljavsky (2021). Non-lattice covering and quanitization of high dimensional sets. Black Box Optimization, Machine Learning, and No-Free Lunch Theorems.*

# Intersection of a cube and $n$ random balls

Let $Z_1, \ldots, Z_n$ are i.i.d. random vectors uniformly distributed in the cube $[-\delta, \delta]^d$ with $0 < \delta \leq 1$. Then, for given $U = (u_1, \ldots, u_d)^\top \in \mathbb{R}^d$,

$$\begin{aligned}
\mathbb{P}\{U \in \mathcal{B}_d(\mathbb{Z}_n, r)\} &= 1 - \prod_{j=1}^{n} \mathbb{P}\{U \notin \mathcal{B}_d(Z_j, r)\} \\
&= 1 - \prod_{j=1}^{n} (1 - \mathbb{P}\{U \in \mathcal{B}_d(Z_j, r)\}) \\
&= 1 - \left(1 - \mathbb{P}_Z\{\|U - Z\| \leq r\}\right)^n
\end{aligned}$$

# Intersection of a cube and $n$ random balls

$$C_d(\mathbb{Z}_n, r) \simeq 1 - \int_{-\infty}^{\infty} \psi_2(s)\varphi(s)ds,$$

with

$$\psi_2(s) = \exp\left\{-n\left(\Phi(c_s) + \left(1+\frac{4}{d}\right)\frac{s' + d/21}{5[s'+d/5]^{3/2}}(1-c_s^2)\varphi(c_s)\right)\right\},$$

$$c_s = \frac{3(r/\delta)^2 - s' - d}{2\sqrt{s'+d/5}}, \quad s' = (d + 2s\sqrt{d/5})/\delta^2 .$$

# Probability of covering of a cube and $n$ random balls

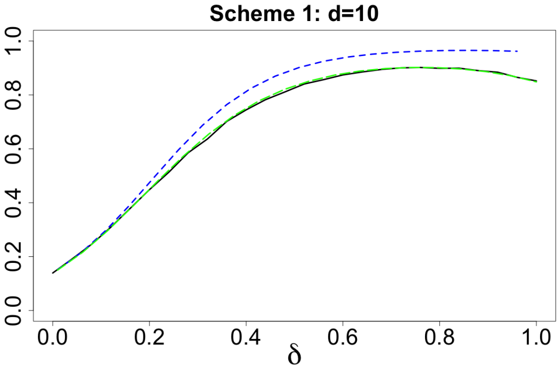



Figure 4: $n = 128$

# Probability of covering of a cube and $n$ random balls

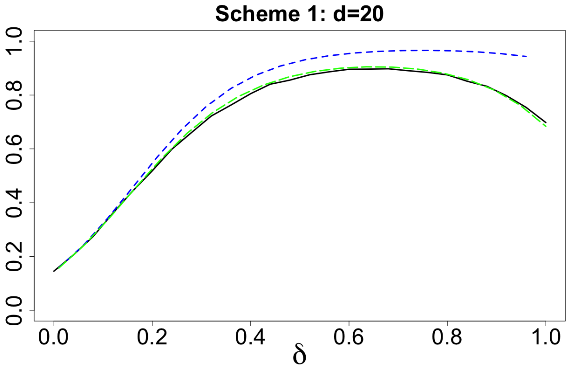



Figure 5: $n = 512$

# Probability of covering of a cube and $n$ random balls

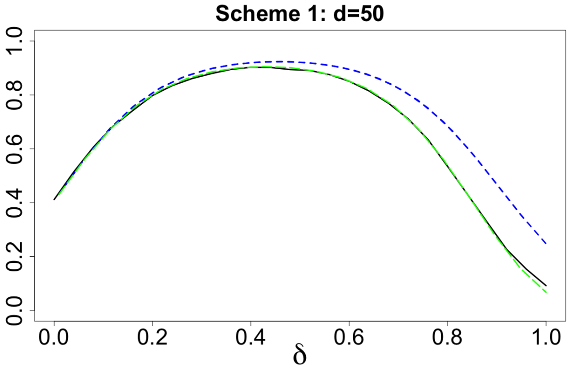



Figure 6: $n = 512$

# Approximations for quantization

$$\frac{d}{dr}(\mathbb{E}_{\mathbb{Z}_n} C_d(\mathbb{Z}_n, r)) \cong f_\delta(r) := \frac{n \cdot r}{\delta} \int_{-\infty}^{\infty} \frac{\varphi(s)\varphi(c_s)\psi_2(s)}{\sqrt{s' + k}}$$

$$\times \left[ \sqrt{3} + \left(1 + \frac{4}{d}\right) \frac{\left(s' + \frac{d\delta^2}{63}\right)}{5\,(s' + k)^{3/2}} \left\{ \delta(c_s^3 - c_s) - \frac{\sqrt{3}(r^2 - \frac{d\delta^2}{3} - s')}{\sqrt{s' + k}} \right\} \right] ds$$

Therefore the approximation for $\mathbb{E}_{\mathbb{Z}_n}\theta(\mathbb{Z}_n)$ is:

$$\mathbb{E}\theta_n = \mathbb{E}_{\mathbb{Z}_n}\theta(\mathbb{Z}_n) \cong \int_{r \geq 0} r^2 f_\delta(r) dr\,.$$

# Approximations for quantization

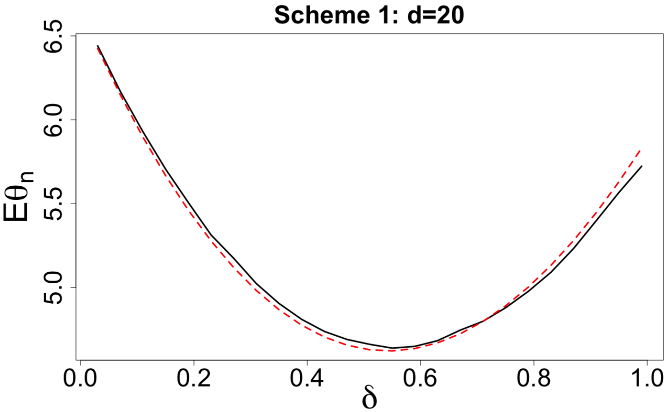



Figure 7: $\mathbb{E}\theta_n$ and approximation: $n = 128$.

# Approximations for quantization

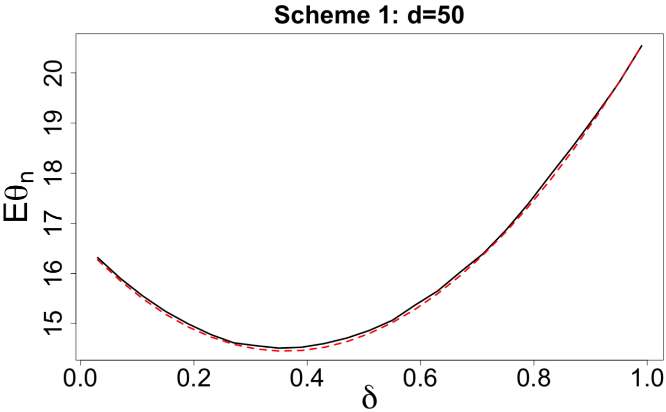



Figure 8: $\mathbb{E}\theta_n$ and approximation: $n = 128$.

# Part 3
# Deterministic designs

Based on: *J. Noonan and A. Zhigljavsky (2020). Efficient quantization and weak covering of high dimensional cubes. Discrete and Computational Geometry.*

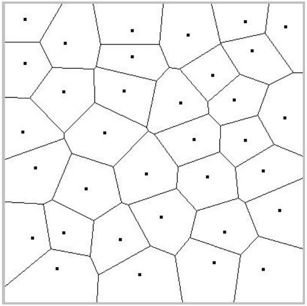
# Deterministic designs

**Design** $\mathbb{D}_{n,\delta}$**:** *a* $2^{d-1}$ *design defined on vertices of the cube* $[-\delta,\delta]^d$*,* $0 \le \delta \le 1$.
**Design** $\mathbb{D}_n^{(0)}$**:** *the collection of* $2^d$ *points* $(\pm\frac{1}{2},\dots,\pm\frac{1}{2})$*, all vertices of the cube* $[-\frac{1}{2},\frac{1}{2}]^d$*.*

The design $\mathbb{D}_{n,1/2}$ extends to the lattice $D_d$ (shifted by $\mathbf{\frac{1}{2}}$) containing points $X = (x_1,\dots,x_d)$ with integer components satisfying $x_1 + \ldots + x_d = 0 \pmod 2$, see [Conway and Sloane, Sect. 7.1, Ch. 4]; this lattice is sometimes called 'checkerboard lattice'.

# Voronoi cells; Quantization

Voronoi cells $V_i = \{x \in \mathcal{X} : \|x - x_i\| \leq \|x - x_j\|, j \neq i\}$:



$$\theta(\mathbb{Z}_n) = \mathbb{E}_X \min_{i=1,\ldots,n} \|X - Z_i\|^2 = \frac{1}{\mathrm{vol}([-1,1]^{\mathrm{d}})} \sum_{i=1}^{n} \int_{V(Z_i)} \|X - Z_i\|^2 dX \, ,$$

where $X = (x_1, \ldots, x_d)$ and $dX = dx_1 dx_2 \cdots dx_d$.

If all of the Voronoi cells $V(Z_i), i = 1, \ldots, n$, are congruent, then

$$\theta(\mathbb{Z}_n) = \frac{1}{\mathrm{vol}(V(Z_1))} \int_{V(Z_1)} \|X - Z_1\|^2 dX \,.$$

### Theorem

*Consider the design* $\mathbb{D}_n^{(0)}$*, the collection of* $n = 2^d$ *points* $(\pm 1/2, \ldots, \pm 1/2)$*. The Voronoi cells for this design are all congruent. The Voronoi cell for the point* $\mathbf{1/2} = (1/2, 1/2, \ldots, 1/2)$ *is the cube*

$$C_0 = \left\{ X = (x_1, \ldots, x_d) \in \mathbb{R}^d : \ 0 \leq x_i \leq 1, \ i = 1, 2, \ldots, d \right\} \,.$$

## Theorem

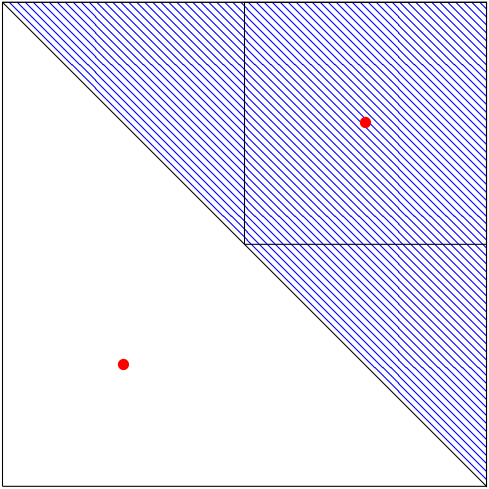
*The Voronoi cells of the design* $\mathbb{D}_{n,\delta} = \{Z_1, \ldots, Z_n\}$ *are all congruent.* *The Voronoi cell for the point* $Z_1 = \boldsymbol{\delta} = (\delta, \delta, \ldots, \delta) \in \mathbb{R}^d$ *is*

$$V(Z_1) = C_0 \bigcup \left[ \bigcup_{j=1}^{d} U_j \right]$$

*where*

$$U_j = \left\{ X = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d : -1 \leq x_j \leq 0, |x_j| \leq x_k \leq 1 \text{ for all } k \neq j \right\}$$

*The volume of* $V(Z_1)$ *is* $\mathrm{vol}(V(Z_1)) = 2$.



## Theorem

*For the design* $\mathbb{D}_n^{(0)}$, *we obtain:*

$$\theta(\mathbb{D}_n^{(0)}) \quad = \quad d/12,$$

*For the design* $\mathbb{D}_{n,\delta}$ *with* $0 \leq \delta \leq 1$, *we obtain:*

$$\theta(\mathbb{D}_{n,\delta}) \quad = \quad d\left(\delta^2 - \delta + \frac{1}{3}\right) + \frac{2\delta}{d+1},$$

## Corollary

*The optimal value of* $\delta$ *minimising* $\theta(\mathbb{D}_{n,\delta})$ *is*

$$\delta^* = \frac{1}{2} - \frac{1}{d(d+1)}.$$

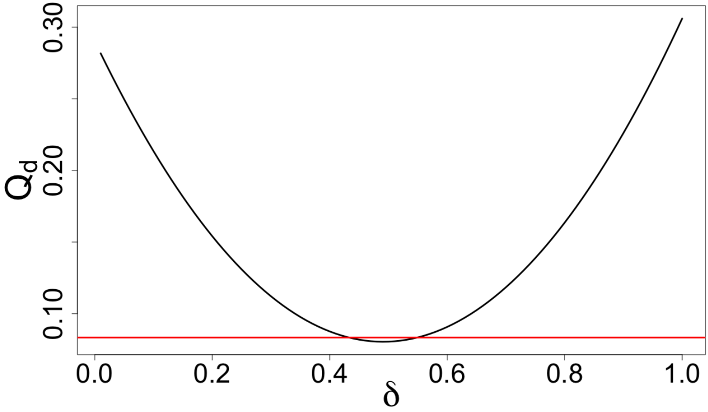



Figure 9: $Q_d(\mathbb{D}_{n,\delta})$ as a function of $\delta$ and $Q_d(\mathbb{D}_n^{(0)}) = 1/12$ with $d = 10$ ;

# Weak covering

For an $n$-point design $\mathbb{Z}_n = \{Z_1, \ldots, Z_n\}$, denote the proportion of the Voronoi cell around $Z_i$ covered by the ball $\mathcal{B}_d(Z_i, r)$ as:

$$V_{d,Z_i,r} := \mathrm{vol}(V(Z_i) \cap \mathcal{B}_d(Z_i, r))/\mathrm{vol}(V(Z_i))\,.$$

Then we can state the following simple lemma.

**Lemma**

*Consider a design $\mathbb{Z}_n = \{Z_1, \ldots, Z_n\}$ such that all Voronoi cells $V(Z_i)$ are congruent. Then for any $Z_i \in \mathbb{Z}_n$, $C_d(\mathbb{Z}_n, r) = V_{d,Z_i,r}$.*

## Theorem

*Depending on the values of $r$ and $\delta$, the quantity $C_d(\mathbb{D}_{n,\delta}, r)$ can be expressed through $C_{d,Z,r}$ for suitable $Z$ as follows.*

- *For $r \leq \delta$:*

$$C_d(\mathbb{D}_{n,\delta}, r) = \frac{1}{2} C_{d,\mathbf{2\delta-1},2r}$$

- *For $\delta \leq r \leq 1+\delta$:*

$$C_d(\mathbb{D}_{n,\delta}, r) = \frac{1}{2}\left[C_{d,\mathbf{2\delta-1},2r} + d\int_0^{r-\delta} C_{d-1,\frac{\mathbf{2\delta-1-x}}{\mathbf{1-x}},\frac{2\sqrt{r^2-(x+\delta)^2}}{1-x}} (1-x)^{d-1}\,dx\right]$$

- *For $r \geq 1+\delta$:*

$$C_d(\mathbb{D}_{n,\delta}, r) = \frac{1}{2}\left[C_{d,\mathbf{2\delta-1},2r} + d\int_0^{1} C_{d-1,\frac{\mathbf{2\delta-1-x}}{\mathbf{1-x}},\frac{2\sqrt{r^2-(x+\delta)^2}}{1-x}} (1-x)^{d-1}\,dx\right]$$

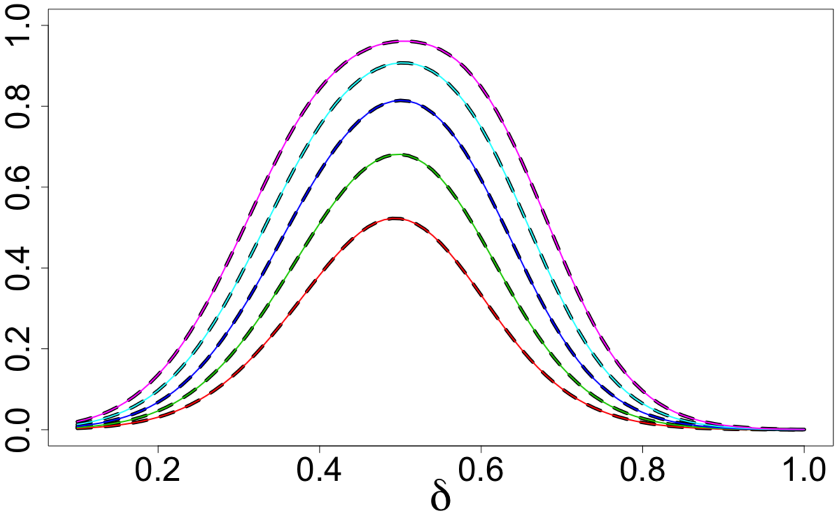



Figure 10: $C_d(\mathbb{D}_{n,\delta}, r)$ and its approximation: $d = 15$, $r$ from 1.15 to 1.35 increasing by 0.05

# ‘Do not try to cover the vertices’

## Theorem

*Let $\gamma$ be fixed, $0 \le \gamma \le 1$. Consider $(1-\gamma)$-coverings of $[-1,1]^d$ generated by the designs $\mathbb{D}_{n,\delta}$ and the associated normalized radii $R_{1-\gamma}(\mathbb{D}_{n,\delta})$. For any $0 < \gamma < 1$ and $0 \le \delta \le 1$, the limit of $R_{1-\gamma}(\mathbb{D}_{n,\delta})$, as $d \to \infty$, exits and achieves minimal value for $\delta = 1/2$. Moreover, $R_{1-\gamma}(\mathbb{D}_{n,1/2})/R_1(\mathbb{D}_{n,1/2}) \to 1/\sqrt{3}$ as $d \to \infty$, for any $0 < \gamma < 1$.*

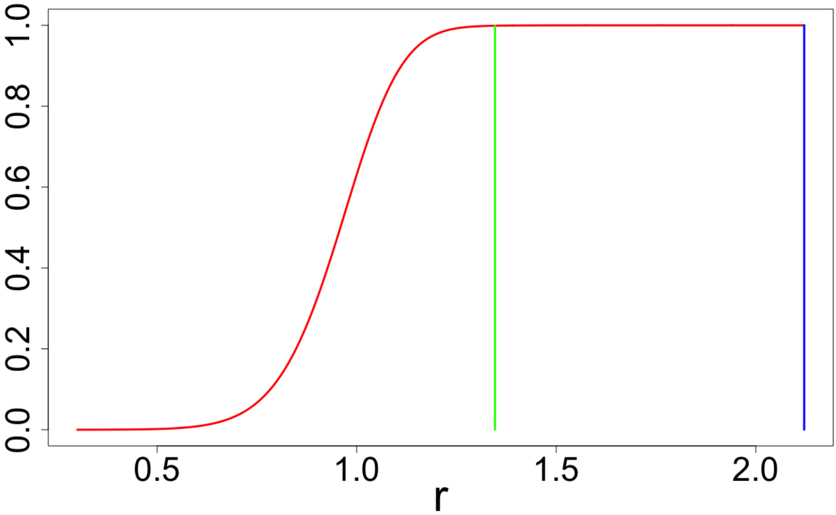



Figure 11: $C_d(\mathbb{D}_{n,\delta}, r)$ with $r_{0.999}$ and $r_1$: $d = 10$

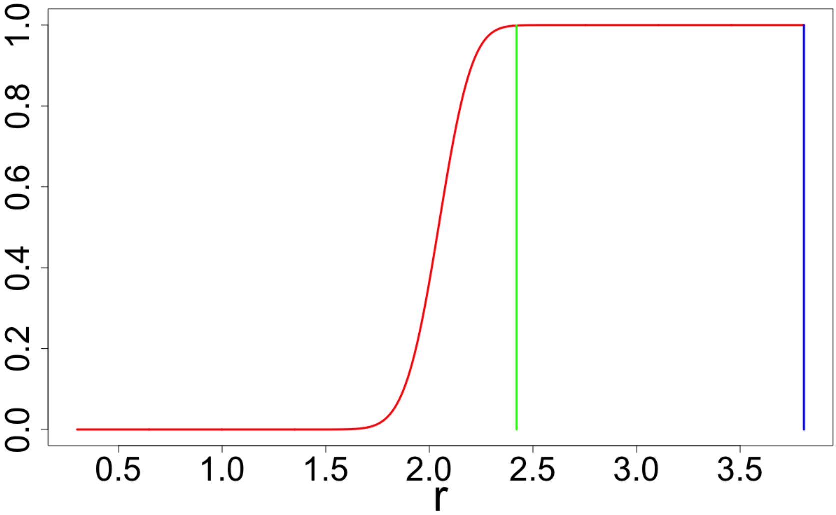



Figure 12: $C_d(\mathbb{D}_{n,\delta}, r)$ with $r_{0.999}$ and $r_1$: $d = 50$

Thank you for your attention!