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Incremental space-filling design based on coverings and spacings: improving upon low discrepancy sequences

UQSay

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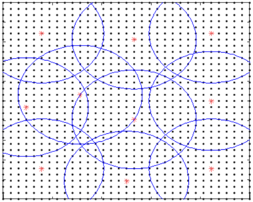
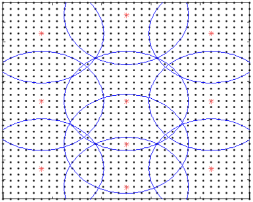
Objective

Find algorithmic constructions to define space-filling designs.

Given a compact subset $\mathscr{X} \subset \mathbb{R}^d$, we say that a finite subset $\mathbf{Z}_n \subset \mathscr{X}$ is a space-filling design if $\mathbf{Z}_n$ fills $\mathscr{X}$ evenly.





Objective

Ultimate aim

The definition of incremental algorithms that generate sequences $\mathbf{X}_n$ with small optimality gap, i.e., with a small increase in the maximum distance between points of $\mathscr{X}$ and the elements of $\mathbf{X}_n$ with respect to the optimal solution $\mathbf{X}_n^\star$.

Incremental space-filling design based on coverings and spacings: improving upon low discrepancy sequences, Nogales-Gómez, A., Pronzato, L., Rendas, M.J. Submitted, 2020. *https://hal.archives-ouvertes.fr/hal-02987983v1*

Basic definitions and notation

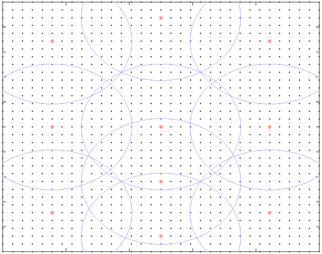
- $\mathscr{X} \subset \mathbb{R}^d$, compact: the hypercube $\mathscr{C}_d = [0,1]^d$ as typical example.
- $\mathbf{Z}_n = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ a n-point design in $\mathscr{X}$.
- $d(\mathbf{x}, \mathbf{Z}_n) = \min_{i=1,\ldots,n} \|\mathbf{x} - \mathbf{z}_i\|$, for $\mathbf{x} \in \mathscr{X}$ with $\|\cdot\|$ the ℓ_2 norm.

Covering radius

$$\mathsf{CR}(\mathbf{Z}_n) = \mathsf{CR}_{\mathscr{X}}(\mathbf{Z}_n) = \max_{\mathbf{x} \in \mathscr{X}} d(\mathbf{x}, \mathbf{Z}_n)$$

Packing radius

$$\mathsf{PR}(\mathbf{Z}_n) = \min_{\mathbf{z}_i \neq \mathbf{z}_j \in \mathbf{Z}_n} \frac{1}{2} \|\mathbf{z}_i - \mathbf{z}_j\| \; (n \geq 2)$$



Mesh-ratio

$$\rho(\mathbf{Z}_n) = \frac{\mathsf{CR}(\mathbf{Z}_n)}{\mathsf{PR}(\mathbf{Z}_n)} \; (n \geq 2)$$

Submodularity

- $\mathscr{X}_C$ a finite set with C elements.
- $f : 2^{\mathscr{X}_C} \to \mathbb{R}$ a set-function.

Diminishing returns property

A set-function $f : 2^{\mathscr{X}_C} \to \mathbb{R}$ is submodular if and only if

$$f(\mathbf{A} \cup \{\mathbf{x}\}) - f(\mathbf{A}) \geq f(\mathbf{B} \cup \{\mathbf{x}\}) - f(\mathbf{B}),$$

$$\forall \mathbf{A} \subset \mathbf{B} \in 2^{\mathscr{X}_C}, \ \mathbf{x} \in \mathscr{X}_C \setminus \mathbf{B}$$

2nd order diminishing returns property

$$f(\mathbf{A} \cup \{\mathbf{x}\}) - f(\mathbf{A}) \geq f(\mathbf{A} \cup \{\mathbf{x}, \mathbf{y}\}) - f(\mathbf{A} \cup \{\mathbf{y}\}),$$
$$\forall \mathbf{A}, \mathbf{B} \in 2^{\mathscr{X}_C}, \ \mathbf{x}, \mathbf{y} \in \mathscr{X}_C \setminus \mathbf{A}$$

Greedy Algorithm

Greedy Algorithm

set $\mathbf{X} = \emptyset$
while $|\mathbf{X}| < k$ **do**
    find $\mathbf{x}$ in $\mathscr{X}_C$ such that $f(\mathbf{X} \cup \{\mathbf{x}\})$ is maximal
    $\mathbf{X} \leftarrow \mathbf{X} \cup \{\mathbf{x}\}$
end while
return $\mathbf{X}$

Theorem (Nemhauser, Wolsey & Fisher, 1978)

Let f be a non-decreasing submodular function, then, for any given k, $1 \leq k \leq C$, the Greedy Algorithm returns a set $\mathbf{X}$ with bounded optimality gap

$$\frac{f^\star - f(\mathbf{X})}{f^\star - f(\emptyset)} \leq (1 - 1/k)^k \leq 1/\mathrm{e} < 0.3679\,, \tag{1}$$

where $f^\star = \max_{\mathbf{X} \subset \mathscr{X}_C : |\mathbf{X}| \leq k} f(\mathbf{X})$ and $\mathrm{e} = \exp(1)$.

Lazy Greedy Algorithm

- Improvement of f, $\delta_{\mathbf{X}}(\mathbf{x}) = f(\mathbf{X} \cup \{\mathbf{x}\}) - f(\mathbf{X}) \geq 0$
- $\max f(\mathbf{X}_n \cup \{\mathbf{x}\}) \Leftrightarrow \max \delta_{\mathbf{X}_n}(\mathbf{x})$
- By construction, $\mathbf{X}_i \subset \mathbf{X}_n$ for all $i < n$. Then, since f is submodular, for all $i < n$, $\delta_{\mathbf{X}_n}(\mathbf{x}) \leq \delta_{\mathbf{X}_i}(\mathbf{x})$

First iteration: compute all $\delta_{\mathbf{X}_0}(\mathbf{x})$ for all $\mathbf{x} \in \mathscr{X}_C$, and define it as the current upper bound $\overline{\delta}(\mathbf{x})$.

At iteration k: Initialize $\mathscr{L}_{k-1} = \mathscr{X}_C \setminus \mathbf{X}_{k-1}$
And let $\mathbf{x}_k^{\star\star}$ be its member with largest $\overline{\delta}(\mathbf{x})$.
While $\mathscr{L}_{k-1} \neq \emptyset$:
update $\overline{\delta}(\mathbf{x}_k^{\star\star}) = \delta_{\mathbf{X}_{k-1}}(\mathbf{x}_k^{\star\star})$,
remove from $\mathscr{L}_{k-1}$ all $\mathbf{x}$ s.t. $\overline{\delta}(\mathbf{x}) \leq \overline{\delta}(\mathbf{x}_k^{\star\star})$.
When $\mathscr{L}_{k-1} = \emptyset$, update $\mathbf{X}_{k-1}$ into $\mathbf{X}_k = \mathbf{X}_{k-1} \cup \{\mathbf{x}_k^{\star\star}\}$.

Covering measures

For any $r \geq 0$, we define the covering measure of $\mathbf{Z}_n$ by

$$\Phi_r(\mathbf{Z}_n) = \frac{\mathrm{vol}\{\mathscr{X} \cap [\cup_{i=1}^n \mathscr{B}(\mathbf{z}_i, r)]\}}{\mathrm{vol}(\mathscr{X})} \,.$$

For a given $\mathbf{Z}_n$, consider also the function $r \in \mathbb{R}^+ \to F_{\mathbf{Z}_n}(r) = \Phi_r(\mathbf{Z}_n)$.
$F_{\mathbf{Z}_n}$ is non-decreasing, $F_{\mathbf{Z}_n}(0) = 0$ and $F_{\mathbf{Z}_n}(r) = 1$ for any $r \geq \mathsf{CR}(\mathbf{Z}_n)$.
If X is distributed with the uniform probability measure μ on $\mathscr{X}$, we have

$$\mathrm{Prob}\,\{X \in \cup_{i=1}^n \mathscr{B}(\mathbf{z}_i, r)\} = \mathrm{Prob}\{d(X, \mathbf{Z}_n) \leq r\} = \int_{\{\mathbf{x} \in \mathscr{X}\,:\, d(\mathbf{x}, \mathbf{Z}_n) \leq r\}} \mu(\mathrm{d}\mathbf{x}) = F_{\mathbf{Z}_n}(r)\,,$$

and $F_{\mathbf{Z}_n}$ is the cumulative distribution function (c.d.f.) of the random variable $d(X, \mathbf{Z}_n)$, supported on $[0, \mathsf{CR}(\mathbf{Z}_n)]$.

Integrated covering measure

- $f_{\mathbf{Z}_n}$ the probability density function (p.d.f.) corresponding to $F_{\mathbf{Z}_n}$.
- For any b, B, $0 \le b < B$, $q > -1$ and $\mathbf{Z}_n \neq \emptyset$:

Integrated covering measure

$$I_{b,B,q}(\mathbf{Z}_n) = \int_b^B r^q \, F_{\mathbf{Z}_n}(r) \, \mathrm{d}r$$

$$= \frac{1}{q+1} \left\{ \left[B^{q+1} F_{\mathbf{Z}_n}(B) - b^{q+1} F_{\mathbf{Z}_n}(b) \right] - \int_b^B r^{q+1} \, f_{\mathbf{Z}_n}(r) \, \mathrm{d}r \right\} ,$$

with $I_{b,B,q}(\mathbf{Z}_n) = 0$ for $\mathbf{Z}_n = \emptyset$.

The set function $I_{b,B,q} : \mathbf{Z}_n \to I_{b,B,q}(\mathbf{Z}_n)$ is non-decreasing and submodular, and satisfies $I_{b,B,q}(\emptyset) = 0$.

Maximizing $I_{0,B,q}(\mathbf{Z}_n)$ for $B \ge diam(\mathscr{X}) \leftrightarrow$ minimizing $\int_0^B r^{q+1} \, f_{\mathbf{Z}_n}(r) \, \mathrm{d}r$

Integrated covering measure (continuation)

$$\left(\int_0^B r^{q+1}\, f_{\mathbf{Z}_n}(r)\,\mathrm{d}r\right)^{1/(q+1)} = E_{q+1}(\mathbf{Z}_n)$$

$E_{q+1}(\mathbf{Z}_n) \to \mathsf{CR}(\mathbf{Z}_n)$ as $q \to \infty$

- For B and q large enough, maximizing $I_{0,B,q}(\mathbf{Z}_n)$ should therefore provide designs with small values of $\mathsf{CR}(\mathbf{Z}_n)$.

Greedy maximization of $I_{0,B,q}(\mathbf{Z}_n) \leftrightarrow$ greedy minimization of $E_{q+1}(\mathbf{Z}_n)$.

Choice of b and B

Choices of b and B relate to lower and upper bounds on $\mathsf{CR}_n^\star$, the optimal (minimum) value of $\mathsf{CR}(\mathbf{Z}_n)$, for designs of size n_1 and n_2, for $n \in \{n_1, n_1+1, \ldots, n_2\}$.

Since the n balls $\mathscr{B}(\mathbf{x}_i, \mathsf{CR}_n^\star)$ centered at the optimal design points cover $\mathscr{X}$, $nV_d(\mathsf{CR}_n^\star)^d \geq \mathrm{vol}(\mathscr{X}) = 1$, with V_d the volume of the d-dimensional unit ball $\mathscr{B}(\mathbf{0}, 1)$, $V_d = \pi^{d/2}/\Gamma(d/2+1)$.

$$\mathsf{CR}_n^\star \geq R_\star(n,d) = (nV_d)^{-1/d}\,.$$

$\mathscr{X}$ can be covered by m^d hypercubes with side $1/m$ $\rightarrow$ by m^d balls with radius $\sqrt{d}/(2m)$. Taking $m = \lfloor n^{1/d} \rfloor$, we have $n \geq m^d$ and:

$$\mathsf{CR}_n^\star \leq \mathsf{CR}_{m^d}^\star \leq R^\star(n,d) = \frac{\sqrt{d}}{2\,\lfloor n^{1/d} \rfloor}\,.$$

A reasonable choice when $n \in [n_1, n_2]$ is then $b = b_\star = R_\star(n_2, d)$ and $B = B^\star = R^\star(n_1, d)$.

Implementation: $\widehat{I}^{A}_{b,B,q}(\mathbf{Z}_n)$

- To evaluate $I_{b,B,q}(\mathbf{Z}_n)$, we substitute the empirical c.d.f. $\widehat{F}_{\mathbf{Z}_n}$, obtained by replacing μ by the uniform measure μ_Q supported on a finite subset $\mathscr{X}_Q$ of $\mathscr{X}$.
- $\mathscr{X}_Q = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(Q)}\}$, well spread over $\mathscr{X}$.
- $d_j(\mathbf{Z}_n) = d(\mathbf{x}^{(j)}, \mathbf{Z}_n)$, $j = 1, \dots, Q$.
- $\overline{d}_j(\mathbf{Z}_n) = \min\{\max\{d_j(\mathbf{Z}_n), b\}, B\}$, $j = 1, \dots, Q$.
- $\overline{d}_{j:Q}$ the $\overline{d}_j$ sorted by increasing values, with $\overline{d}_{1:Q}(\mathbf{Z}_n) \le \overline{d}_{2:Q}(\mathbf{Z}_n) \le \cdots \le \overline{d}_{2:Q}(\mathbf{Z}_n) \le \overline{d}_{Q+1:Q}(\mathbf{Z}_n) = B$,

we obtain:

$$I_{b,B,q}(\mathbf{Z}_n) \approx \widehat{I}^{A}_{b,B,q}(\mathbf{Z}_n) = \frac{1}{Q(q+1)} \sum_{j=1}^{Q} j \left[\overline{d}^{\,q+1}_{j+1:Q}(\mathbf{Z}_n) - \overline{d}^{\,q+1}_{j:Q}(\mathbf{Z}_n) \right]$$

An alternative approach: $\widehat{I}^{B}_{b,B,q}(\mathbf{Z}_n)$

Discrete approximation

Taking m radii r_i well spread over $[b, B]$, with $b = r_1 < r_2 < \cdots < r_m = B$, the trapezoidal rule gives

$$I_{b,B,q}(\mathbf{Z}_n) \approx \widehat{I}^{B}_{b,B,q}(\mathbf{Z}_n) = \sum_{i=1}^{m-1} \frac{r_{i+1}^q \, \widehat{F}_{\mathbf{Z}_n}(r_{i+1}) + r_i^q \, \widehat{F}_{\mathbf{Z}_n}(r_i)}{2} \, (r_{i+1} - r_i) \, .$$

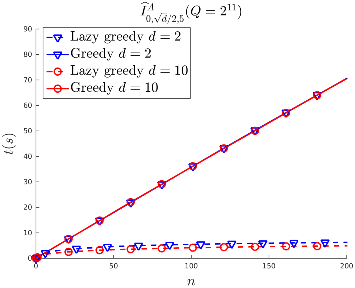
When the r_i are regularly spaced, with $r_{i+1} - r_i = \delta_r$ for all i, the expression simplifies into

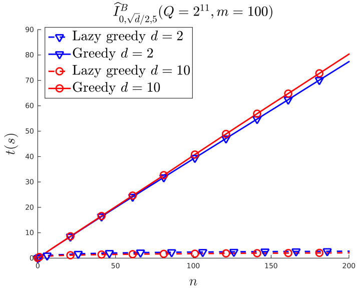
$$\widehat{I}^{B}_{b,B,q}(\mathbf{Z}_n) = \delta_r \left[\frac{r_1^q \, \widehat{F}_{\mathbf{Z}_n}(r_1) + r_m^q \, \widehat{F}_{\mathbf{Z}_n}(r_m)}{2} + \sum_{i=2}^{m-1} r_i^q \, \widehat{F}_{\mathbf{Z}_n}(r_i) \right] .$$

Approximations $\widehat{I}^A_{b,B,q}$ and $\widehat{I}^B_{b,B,q}$

- We compare the designs obtained by maximizing $\widehat{I}^A_{b,B,q}(\mathbf{Z}_n)$ and $\widehat{I}^B_{b,B,q}(\mathbf{Z}_n)$, with $m = 100$, in terms of CR($\mathbf{Z}_n$).
- The set $\mathscr{X}_C$ of candidate points coincides with $\mathscr{X}_Q$ and corresponds to the first $2^{11} = 2\,048$ elements of Sobol' sequence in $\mathscr{X} = \mathscr{C}_d$.
- We consider the two cases $d = 2$ and $d = 10$ and take $q = 5$.
- The covering radius CR($\mathbf{Z}_n$) is approximated by CR$_{\mathscr{X}_N}(\mathbf{Z}_n)$, with $\mathscr{X}_N$ given by 2^{18} points of a scrambled Sobol' sequence complemented by a 2^d full factorial design, which gives $N = 262\,176$ for $d = 5$ and $N = 263\,168$ for $d = 10$.
- We consider the two cases where $b = b_\star = R_\star(n_2, d)$ and $B = B^\star = R^\star(n_1, d)$, with $n_1 = 50$ and $n_2 = 100$ and $b = 0$, $B = \sqrt{d}/2$

Computational times of the greedy and lazy-greedy maximizations of $\widehat{I}^A_{0,\sqrt{d}/2,5}(\mathbf{Z}_n)$ and $\widehat{I}^B_{0,\sqrt{d}/2,5}(\mathbf{Z}_n)$.





- Linear increase of computational cost with n for the greedy version: acceleration provided by the lazy-greedy implementation.
- For the lazy-greedy algorithm, maximization of $\widehat{I}^B_{0,\sqrt{d}/2,5}(\mathbf{Z}_n)$ (with $m = 100 \ll Q$) is faster than maximization of $\widehat{I}^A_{0,\sqrt{d}/2,5}(\mathbf{Z}_n)$.
- The effect of d is negligible.

Effect of b, B

- We apply Greedy algorithm to the maximization of $\widehat{I}^{A}_{b,B,q}(\mathbf{Z}_n)$.
- $\mathscr{X}_C = \mathscr{X}_Q$ corresponds to the first $2^{10} = 1\,024$ elements of Sobol' sequence in $\mathscr{X} = \mathscr{C}_2$.
- We compare $b = 0$, $B = \sqrt{d}/2$ and $b = R_\star(n_2, d)$, $B = R^\star(n_1, d)$ for $q = 5$, with $n_1 = 10$ and $n_2 = 20$.

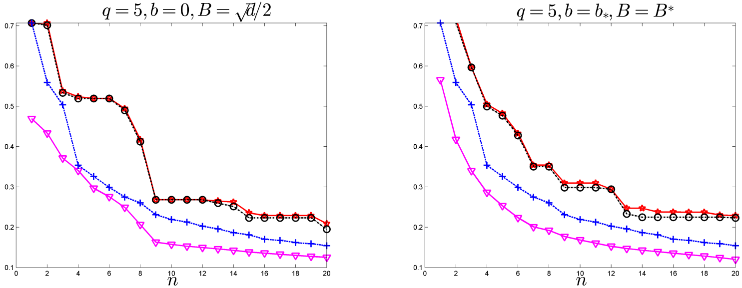


Figure: CR($\mathbf{X}_n$) (red solid line and ★), CR$_{\mathscr{X}_Q}(\mathbf{X}_n)$ (black dashed curve and ○), CR$^\star_n$ (blue dashed curve and $+$), empirical value of $E_{q+1}(\mathbf{X}_n)$ (magenta curve and ▽), for $\mathbf{X}_n$ obtained by greedy maximization of $\widehat{I}^{A}_{b,B,q}(\mathbf{X}_n)$.

Effect of b, B

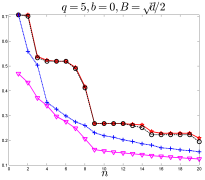


Figure: $\mathrm{CR}(\mathbf{X}_n)$ (red solid line and $\bigstar$), $\mathrm{CR}_{\mathscr{X}_Q}(\mathbf{X}_n)$ (black dashed curve and $\circ$), $\mathrm{CR}_n^\star$ (blue dashed curve and $+$), empirical value of $E_{q+1}(\mathbf{X}_n)$ (magenta curve and $\triangledown$).

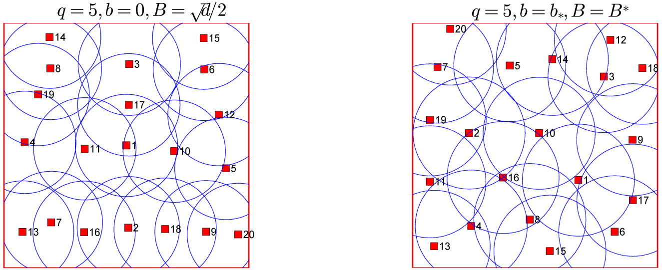


Figure: $\mathbf{X}_{20}$ and circles centered at design points with radius $\mathrm{CR}(\mathbf{X}_{20})$; the order of selection of the points is indicated.

Effect of q

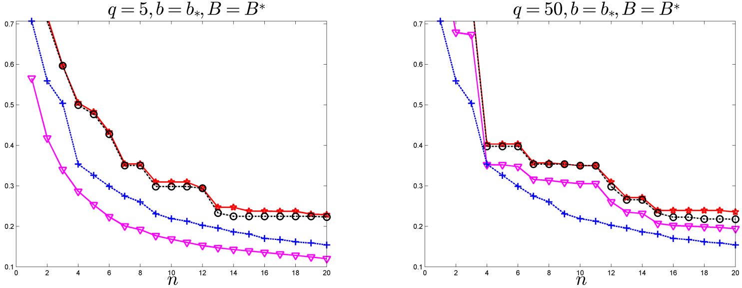


Figure: $\mathrm{CR}(\mathbf{X}_n)$ (red solid line and ★), $\mathrm{CR}_{\mathscr{X}_Q}(\mathbf{X}_n)$ (black dashed curve and ○), $\mathrm{CR}_n^\star$ (blue dashed curve and +), empirical value of $E_{q+1}(\mathbf{X}_n)$ (magenta curve and ▽), for $\mathbf{X}_n$ obtained by greedy maximization of $\widehat{I}^A_{b,B,q}(\mathbf{X}_n)$.

- The approximation $E_{q+1}(\mathbf{X}_n)$ is closer to $\mathrm{CR}(\mathbf{X}_n)$ for $q = 50$, but when $q = 5$ $\mathrm{CR}(\mathbf{X}_n)$ is smaller for $n \in \{1, 2, 3, 7, \ldots, 12, 14, \ldots, 20\}$.
- Best performances are not necessarily achieved with high values of q.

Maximization of $\widehat{I}^A_{b,B,q}$ and $\widehat{I}^B_{b,B,q}$: covering radii and computational times

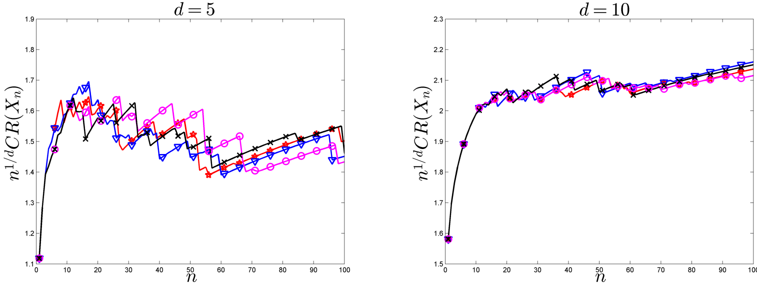


Figure: $\widehat{I}^A_{b_\star,B^\star,5}$ (red ★), $\widehat{I}^B_{b_\star,B^\star,5}$ (blue ▽), $\widehat{I}^A_{0,\sqrt{d}/2,5}$ (magenta ○) and $\widehat{I}^B_{0,\sqrt{d}/2,5}$ (black ×); $m = 100$ for $\widehat{I}^B_{b,B,q}$, $C = Q = 2^{11}$.

	$\widehat{I}^A_{b_\star,B^\star,5}$	$\widehat{I}^A_{0,\sqrt{d}/2,5}$	$\widehat{I}^B_{b_\star,B^\star,5}$	$\widehat{I}^B_{0,\sqrt{d}/2,5}$
$d = 2$	2.4	5.3	0.8	2.3
$d = 5$	3.8	5.2	1.4	2.2
$d = 10$	4.1	4.1	1.8	1.8

Coffee-house design

Coffee-house designs

- Obtained by greedy maximization of $\mathsf{PR}(\mathbf{Z}_n)$ for $n > 1$.
- $\mathbf{x}_1$ is usually the Chebyshev center of $\mathscr{X}$.
- $\mathbf{x}_{n+1} \in \operatorname{Arg\,max}_{\mathbf{x}\in\mathscr{X}} d(\mathbf{x}, \mathbf{X}_n)$.

The simple greedy coffee-house construction ensures:

$$\frac{1}{2} \leq \frac{\mathsf{CR}_n^\star}{\mathsf{CR}(\mathbf{X}_n)} \leq 1 \ (n \geq 1) \quad \text{and} \quad \frac{1}{2} \leq \frac{\mathsf{PR}(\mathbf{X}_n)}{\mathsf{PR}_n^\star} \leq 1 \ (n \geq 2)\,,$$

with $\mathsf{PR}_n^\star$, $\mathsf{CR}_n^\star$ the optimal (maximum) value of $\mathsf{PR}(\mathbf{Z}_n)$, $\mathsf{CR}(\mathbf{Z}_n)$ respectively.

Clustering to minimize the maximum intercluster distance, Gonzalez, T., *Theoretical Computer Science*, 38: 293-306, 1985.

Enhancing the coffee-house design

- Places design points on the boundary of $\mathscr{X}$: not favourable to obtain low CR($\mathbf{Z}_n$).
- We consider a modified method that forces design points to stay away from the boundary of $\mathscr{X}$.
- Parameter β that controls the ratio between the distance to the design and the distance to the boundary $\partial\mathscr{X}$ of the compact set $\mathscr{X}$.

β-spacing of $\mathbf{Z}_n$, for $\beta > 0$

$$S_\beta(\mathbf{Z}_n) = \sup\left\{r : \exists \mathbf{x} \in \mathscr{X} \text{ such that } d(\mathbf{x}, \mathbf{Z}_n) \geq r \text{ and } d(\mathbf{x}, \partial\mathscr{X}) \geq \frac{r}{\beta}\right\} =$$

$$\sup_{\mathbf{x}\in\mathscr{X}} D_\beta(\mathbf{x}, \mathbf{Z}_n)\,,$$

where $D_\beta(\mathbf{x}, \mathbf{Z}_n) = \min\{d(\mathbf{x}, \mathbf{Z}_n),\ \beta\, d(\mathbf{x}, \partial\mathscr{X})\}$, $\mathbf{x} \in \mathscr{X}$, and $d(\mathbf{x}, \partial\mathscr{X}) = \inf_{\mathbf{z}\in\partial\mathscr{X}} \|\mathbf{x} - \mathbf{z}\|$.

Enhancing the coffee-house design (continuation)

The coffee-house algorithm can be extended to:

The greedy maximization of $P_\beta(\mathbf{Z}_n)$, $\beta > 0$, where

$$P_\beta(\mathbf{Z}_n) = \min_{\mathbf{z}_i \neq \mathbf{z}_j \in \mathbf{Z}_n} \frac{1}{2} \min\{\|\mathbf{z}_i - \mathbf{z}_j\|\,,\ \beta\, d(\mathbf{z}_i, \partial\mathscr{X})\}$$

using $\mathbf{x}_{n+1} \in \operatorname{Arg\,max}_{\mathbf{x}\in\mathscr{X}} D_\beta(\mathbf{x}, \mathbf{X}_n)$ for any $n \geq 1$, where
$D_\beta(\mathbf{x}, \mathbf{Z}_n) = \min\{d(\mathbf{x}, \mathbf{Z}_n)\,,\ \beta\, d(\mathbf{x}, \partial\mathscr{X})\}\ ,\ \mathbf{x} \in \mathscr{X}$, and
$d(\mathbf{x}, \partial\mathscr{X}) = \inf_{\mathbf{z}\in\partial\mathscr{X}} \|\mathbf{x} - \mathbf{z}\|$.

Choice of β

- Depending on n_2, such that $\mathbf{x}_2$ be at distance $R_\star(n_2, d)$ from a vertex of $\mathscr{X}$, with $R_\star(n_2, d)$ the lower bound on $\mathsf{CR}^\star_{n_2}$.
- This implies $d(\mathbf{x}_2, \partial\mathscr{X}) = R_\star(n_2, d)/\sqrt{d} = \|\mathbf{x}_2 - \mathbf{x}_1\|/\beta$ and gives

$$\beta = \beta_\star(n_2, d) = \frac{d}{2\, R_\star(n_2, d)} - \sqrt{d}\,.$$

Enhancing the coffee-house design (continuation)

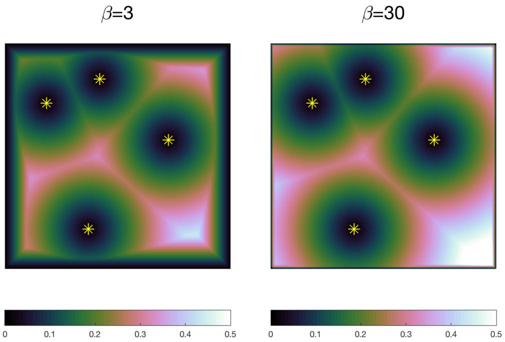


Figure: Edgephobe compromise distance $D_\beta(\mathbf{x}, \mathbf{Z}_n)$ for a 4-point design (yellow stars) in $\mathscr{X} = [0,1]^2$.

Numerical study

We compare the performance of

- Designs $\mathbf{X}_n^A$ that incrementally maximize the covering measure $\widehat{I}^A_{b_\star, B^\star, q}(\mathbf{X}_n)$.
- Nested subsequences $\mathbf{X}_n^H$ and $\mathbf{X}_n^S$ of low discrepancy Halton and Sobol' sequences.
- $\mathbf{X}_n^{CH,\beta}$ obtained by greedy maximization of the criteria $P_\beta(\mathbf{Z}_n)$ based on pairwise distances.
- Incremental constructions:
  - $\mathbf{X}_n^{VD}$, Wynn's Vertex-Direction method[1].
  - $\mathbf{X}_n^{RD}$, a relaxed version[2] of the covering criterion.

[1] The sequential generation of D-optimum experimental designs, Wynn, H., *Annals of Math. Stat.*, 41: 1655-1664, 1970.

[2] An algorithm for the construction of spatial coverage designs with implementation in SPLUS, Royle, J., Nychka, D., *Computers and Geosciences*, 24(5): 479-488, 1998.

Covering radii for $d = 10$, $q = 5$

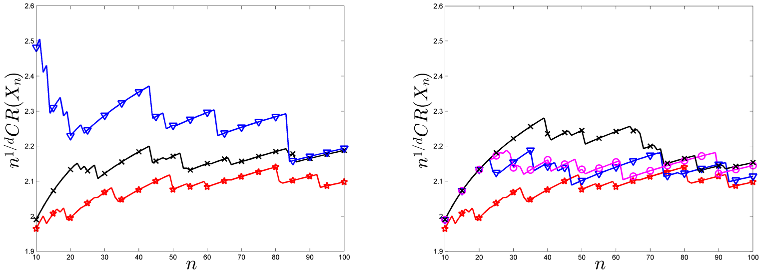


Figure: Left: $\mathbf{X}_n^A$ (red ★), $\mathbf{X}_n^H$ (blue ▽) and $\mathbf{X}_n^S$ Sobol' sequence (black ×). Right: $\mathbf{X}_n^A$ (red ★), $\mathbf{X}_n^{CH,\infty}$ (black ×), $\mathbf{X}_n^{CH,2\sqrt{2\,d}}$ (magenta ∘) and $\mathbf{X}_n^{CH,\beta_\star(100,d)}$, (blue ▽).

- $\mathbf{X}_n^A$ best overall performance.
- $\mathbf{X}_n^{CH,\beta_\star(100,d)}$ yields smaller covering radii for a few values of n.
- $\mathbf{X}_n^{CH,\infty}$ is almost always outperformed by the two other variants.

Mesh-ratio for $d = 10$

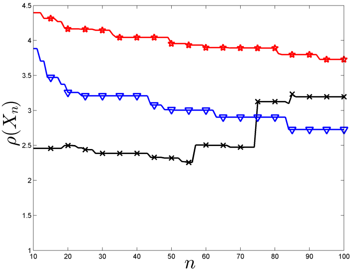


Figure: Left: $\mathbf{X}_n^A$ (red $\bigstar$), $\mathbf{X}_n^H$ (blue $\triangledown$) and $\mathbf{X}_n^S$ Sobol' sequence (black $\times$). Right: $\mathbf{X}_n^A$ (red $\bigstar$), $\mathbf{X}_n^{CH,\infty}$ (black $\times$), $\mathbf{X}_n^{CH,2\sqrt{2\,d}}$ (magenta $\circ$) and $\mathbf{X}_n^{CH,\beta_\star(100,d)}$, (blue $\triangledown$).

- Minimizing covering radius$\rightarrow$ reduces packing radius.
- $\mathbf{X}_n^A$ (red $\bigstar$) worse than other designs.
- The best mesh-ratios are observed for $\mathbf{X}_n^{CH,\infty}$, which greedily maximizes $\mathrm{PR}(\mathbf{X}_n)$.

Covering radius and mesh-ratio for $d = 10$, $\mathscr{X}_{100} = \mathbf{Z}_{Lh,100}$

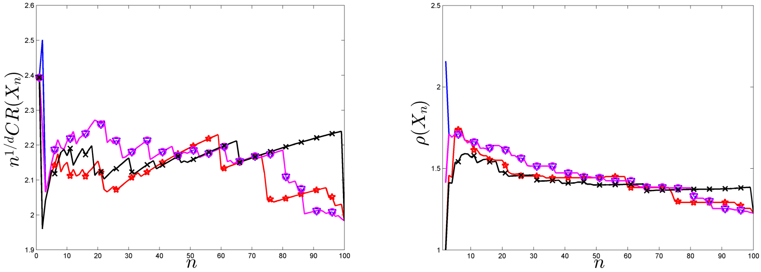


Figure: Greedy maximization of $\widehat{I}^{A}_{b_n,B_n,5}(\mathbf{Z}_n)$ (red ★) and of $P_\beta(\mathbf{Z}_n)$ with $\beta = \infty$ (black $\times$), $\beta = 2\sqrt{2\,d}$ (magenta $\circ$) and $\beta = \beta_\star(n_2, d)$ (blue $\triangledown$).

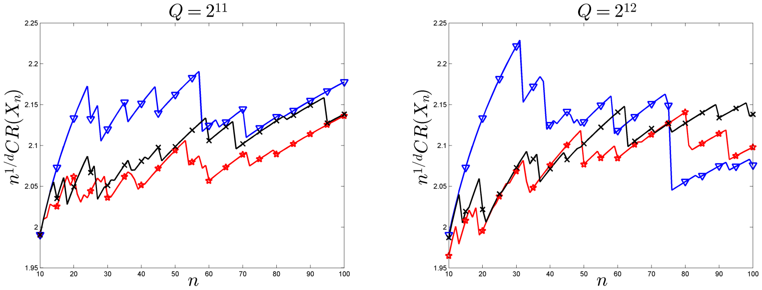


Figure: $\mathbf{X}_n^A$ (red ★), $\mathbf{X}_n^{VD}$ (blue ▽) and $\mathbf{X}_n^{RD}$ (black $\times$).

- $\mathbf{X}_n^A$ (red ★) and $\mathbf{X}_n^{RD}$ (black $\times$) perform rather similarly, with a small advantage to $\mathbf{X}_n^A$.
- $\mathbf{X}_n^{VD}$more sensitive to Q.

	$\mathbf{X}_n^A$	$\mathbf{X}_n^{VD}$	$\mathbf{X}_n^{RD}$	$\mathbf{X}_n^{LRD}$	$\mathbf{X}_n^{CH,\infty}$	$\mathbf{X}_n^{CH,2\sqrt{2d}}$	$\mathbf{X}_n^{CH,\beta_\star(100,d)}$
$Q = 2^{11}$	4.1	0.7	5.6	4.4	0.3	0.6	0.6
$Q = 2^{12}$	15.8	2.8	21.4	17.6	0.3	0.6	0.6

Designs in non-convex domain: annular geometry

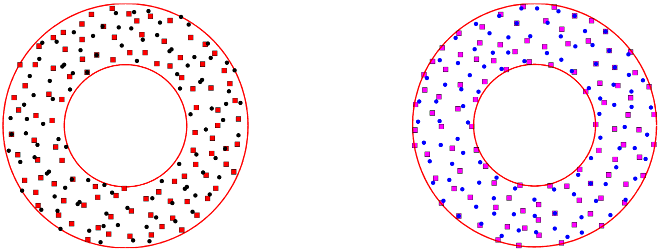


Figure: Left: $\mathbf{X}_n^A$ obtained by greedy maximization of $\widehat{I}^A_{b_\star,B^\star,5}(\mathbf{Z}_n)$ (red ■) and points $\mathbf{X}_n^S$ from Sobol' sequence (black dots). Right: coffee-house designs $\mathbf{X}_n^{CH,\infty}$ in $\mathscr{X}$ (magenta ■) and $\mathbf{X}_n^{CH',\infty}$ in $\mathscr{X}' \subset \mathscr{X}$ (blue dots).

Conclusion

- $\mathbf{X}_n^A$ attractive alternative to classic incremental constructions:
  - outperforms low discrepancy sequences.
  - better overall performance than best coffee-house versions.
  - stability advantage over $\mathbf{X}_n^{VD}$ and $\mathbf{X}_n^{RD}$.
- Different design methods $\rightarrow$ significantly different computational load.
- Coffee-house design hard to outperform in mesh-ratio since $\rho(\mathbf{X}_n) \leq 2$, but
- Highly sensitive to design packing (or separating) radius.

- $I_{b,B,q}(\mathbf{Z}_n)$ proposed in the paper is able to guarantee small covering radius.
- its incremental maximization is an attractive alternative, leading to small covering radii designs.
- Computationally efficient implementations: finite set $\mathscr{X}_C$ + lazy-greedy.
- Limitation: approximation of the uniform measure on $\mathscr{X}$, poor when the dimension d is very large.