Greedy algorithms for incremental design with guaranteed packing and covering performance

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Outline

1 Two space-filling criteria

$\mathscr{X}$ = a compact subset of $\mathbb{R}^d$, $\mathscr{X} = \mathrm{cl}(\mathrm{int}(\mathscr{X}))$ (often, $\mathscr{X} = [0,1]^d$)

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→ Use pairs $(\mathbf{x}_i, f(\mathbf{x}_i))$, $i = 1, \ldots, n$,
to approximate or integrate f over $\mathscr{X}$

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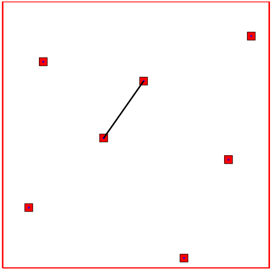
We shall consider two "classical" criteria:

1. Packing radius
2. Covering radius

(+ the mesh-ratio)

1/ Maximise the packing radius $\mathrm{PR}(\mathbf{X}_n) \triangleq \frac{1}{2}\min_{i\neq j}\|\mathbf{x}_i - \mathbf{x}_j\|$

$\mathrm{PR}(\mathbf{X}_n) =$ separation radius $= \frac{1}{2}$ Maximin distance criterion

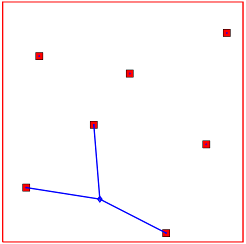


→ can often be related to numerical stability issues

→ easy to compute, but pushes points to the boundary of $\mathscr{X}$

2/ Minimise the covering radius $\mathrm{CR}(\mathbf{X}_n) \triangleq \max_{\mathbf{x}\in\mathscr{X}} \min_{\mathbf{x}_i} \|\mathbf{x} - \mathbf{x}_i\|$

$\mathrm{CR}(\mathbf{X}_n)$ = fill distance = dispersion = miniMax distance criterion



➞ any arbitrary point in never too far from a design point
➞ $\mathrm{CR}(\mathbf{X}_n)$ is more difficult to compute (and optimise) than $\mathrm{PR}(\mathbf{X}_n)$
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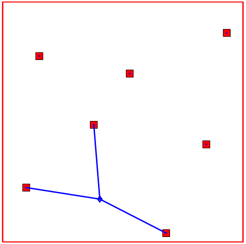

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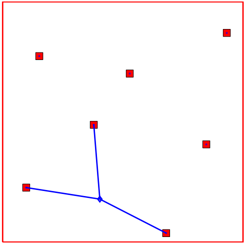

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3/ We may also **minimise the mesh-ratio:**

$$\mathrm{MR}(\mathbf{X}_n) \triangleq \frac{\mathrm{CR}(\mathbf{X}_n)}{\mathrm{PR}(\mathbf{X}_n)}$$ (with $\mathrm{MR}(\mathbf{X}_n) \geq 1$ when $\mathscr{X}$ is connected)

2 Incremental design: Greedy Packing

→ **sequence of points $\mathbf{x}_1, \mathbf{x}_2 \ldots$, i.e., $\mathbf{X}_{k+1} = \mathbf{X}_k \cup \{\mathbf{x}_{k+1}\}$, $k = 1, 2 \ldots$**

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We don't know in advance when the sequence will be stopped
(but before some maximum design size n)

We want all $\mathbf{X}_k$, $k \leq n$, reasonably space filling

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Greedy-Packing algorithm (= "coffee-house design" (Müller, 2007, Chap. 4))

$\mathbf{x}_1$ given (center of $\mathscr{X}$, or random), then
$\mathbf{x}_{k+1} \in \mathrm{Arg}\max_{\mathbf{x} \in \mathscr{X}} d(\mathbf{x}, \mathbf{X}_k)$, $\mathbf{X}_{k+1} = \mathbf{X}_k \cup \{\mathbf{x}_{k+1}\}$

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→ **at least 50% efficient**
(Gonzalez, 1985)
— simple proof by induction

$$\begin{cases} \mathrm{CR}(\mathbf{X}_k) & \leq & 2\,\mathrm{CR}_k^*\,, \ \forall k \geq 1 \\ \mathrm{PR}(\mathbf{X}_k) & \geq & \frac{1}{2}\,\mathrm{PR}_k^*\,, \ \forall k \geq 2 \\ \mathrm{MR}(\mathbf{X}_k) & \leq & 2\,, \qquad \forall k \geq 2 \end{cases}$$

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$\boxed{d(\mathbf{x}, \mathbf{X}_{k+1}) = \min\{d(\mathbf{x}, \mathbf{X}_k), \|\mathbf{x} - \mathbf{x}_{k+1}\|\}}$ → complexity grows linearly

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$\boxed{\limsup_{k\to\infty} \mathrm{MR}(\mathbf{X}_k) \geq 2}$ for any sequence of nested designs

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$\mathbf{x}_1$ given (center of $\mathscr{X}$, or random), then

$\mathbf{x}_{k+1} \in \boxed{\mathrm{Arg}\max_{\mathbf{x} \in \mathscr{X}_{\mathrm{cand}}}} \; d(\mathbf{x}, \mathbf{X}_k)$, $\mathbf{X}_{k+1} = \mathbf{X}_k \cup \{\mathbf{x}_{k+1}\}$

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In practice, $\mathbf{x}_{k+1} \in \mathscr{X}_{\mathrm{cand}}$ with $\boxed{\mathscr{X}_{\mathrm{cand}}}$ a finite set of candidates in $\mathscr{X}$

3 Relaxed Greedy Packing

Relaxed Greedy-Packing algorithm

$\mathbf{x}_1$ given (center of $\mathscr{X}$, or random), $\boxed{\alpha_k} \in (0,1]$ for all k, then
$\mathbf{x}_{k+1}$ such that $d(\mathbf{x}_{k+1}, \mathbf{X}_k) = \boxed{\alpha_k}\, \mathrm{CR}(\mathbf{X}_k)$, $\mathbf{X}_{k+1} = \mathbf{X}_k \cup \{\mathbf{x}_{k+1}\}$

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  Let $\mathbf{x}_k^*$ be such that $d(\mathbf{x}_k^*, \mathbf{X}_k) = \mathrm{CR}(\mathbf{X}_k)$ (furthest away point), $\alpha < 1$

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$$\mathbf{x}_{k+1} = (1-\alpha)\mathbf{x}_{j,k} + \alpha\, \mathbf{x}_k^*, \text{ with } \|\mathbf{x}_{j,k} - \mathbf{x}_k^*\| = \mathsf{CR}(\mathbf{X}_k)$$

α can be random in $[a, 1]$, $0 < a < 1$

$$(\mathbf{x}_k^* \in \mathscr{X}_{\rm cand} \not\Rightarrow \mathbf{x}_{k+1} \in \mathscr{X}_{\rm cand})$$

Performance guarantees: (P and Zhigljavsky, 2023)

Define $a_0 \triangleq 1$, $a_k \triangleq \min\{\alpha_1, \ldots, \alpha_k\}$

→ at least $a_{k-1} \times$ 50% efficient

$$\begin{cases} \mathrm{CR}(\mathbf{X}_k) & \leq & (2/a_{k-1})\,\mathrm{CR}_k^*\,, & \forall k \geq 1 \\ \mathrm{PR}(\mathbf{X}_k) & \geq & (a_{k-1}/2)\,\mathrm{PR}_k^*\,, & \forall k \geq 2 \\ \mathrm{MR}(\mathbf{X}_k) & \leq & 2/a_{k-1}\,, & \forall k \geq 2 \end{cases}$$

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➠ random designs, of arbitrary size, with space-filling performance guarantees (not the case with determinantal point processes)

Asymptotic performance guarantees: (P and Zhigljavsky, 2023)

If $\alpha_k \geq a > 0$ for all k and $\liminf_{k\to\infty} \alpha_k = \alpha \in (0,1]$,

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$$\begin{cases} \limsup_{k\to\infty} \frac{\mathrm{CR}(\mathbf{X}_k)}{\mathrm{CR}_k^*} & \leq & \frac{2}{\alpha} \\ \liminf_{k\to\infty} \frac{\mathrm{PR}(\mathbf{X}_k)}{\mathrm{PR}_k^*} & \geq & \frac{\alpha}{2} \\ \limsup_{k\to\infty} \mathrm{MR}(\mathbf{X}_k) & \leq & \frac{2}{\alpha} \end{cases}$$

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➠ Connection with with **energy minimisation**

➠ Projections onto **lower dimensional subspaces** can be accounted for

▸▸ Boundary avoidance

Energy minimisation

K a symmetric PD kernel, $\mathbf{X}_n \rightarrow$ empirical measure $\xi_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{\mathbf{x}_i}$

discrete energy $$\mathscr{E}_K^{\neq}(\xi_n) = \frac{2}{n(n-1)} \sum_{1\leq i<j\leq n} K(\mathbf{x}_i, \mathbf{x}_j)$$

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Audze and Eglais (1977) $\rightarrow \mathscr{E}_{K_2}^{\neq}(\xi_n)$, with $K_2(\mathbf{x}, \mathbf{x}') = 1/\|\mathbf{x} - \mathbf{x}'\|^2$ (Riesz kernel)

➠ Optimal design $\mathbf{X}_n^*$ for $K_s(\mathbf{x}, \mathbf{x}') = 1/\|\mathbf{x} - \mathbf{x}'\|^s$ = set of s Fekete points asymptotically uniform in $\mathscr{X}$ ($\xi_n \stackrel{\mathrm{w}}{\rightarrow} \mu$) for $s \geq d$

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Greedy energy minimisation

$$\boxed{\mathbf{x}_{k+1} \in \operatorname{Arg\,min}_{\mathbf{x}\in\mathscr{X}} P_{K,\xi_k}(\mathbf{x})}$$ with

$P_{K,\xi_k}(\mathbf{x}) = \frac{1}{k}\sum_{i=1}^k K(\mathbf{x},\mathbf{x}_i)$ = potential of ξ_k at $\mathbf{x}$

➞ if K is "sharp" enough, $\mathbf{x}_{k+1}$ is far from $\mathbf{X}_k$

Let $K(k) = K_{s_k}$ (Riesz kernel) with $s_k/\log k \to \infty$ as $k \to \infty$,
or $K(k) = K_{\nu,\ell_k}$ (Matérn kernel, $\nu = p + 1/2$, $p \in N_0$)
with $k^{1/d}(\log k)^2\ell_k \to 0$ as $k \to \infty$,
(ℓ = correlation length, e.g., $K_{3/2,\ell}(\mathbf{x},\mathbf{x}') = (1+\sqrt{3}\|\mathbf{x}-\mathbf{x}'\|/\ell)e^{-\sqrt{3}\|\mathbf{x}-\mathbf{x}'\|/\ell}$)

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Greedy energy minimisation with $K(k)$: $\mathbf{x}_{k+1} \in \mathrm{Arg\,min}_{\mathbf{x}\in\mathscr{X}} P_{K(k),\xi_k}(\mathbf{x})$

$\iff$ a special case of relaxed greedy packing

→ $\alpha_k = \frac{d(\mathbf{x}_{k+1},\mathbf{X}_k)}{\mathrm{CR}(\mathbf{X}_k)} \to 1$ as $k \to \infty$

→ asymptotically, same performance as with Greedy Packing

$$\begin{cases} \limsup_{k\to\infty} \frac{\mathrm{CR}(\mathbf{X}_k)}{\mathrm{CR}_k^*} & \leq & 2 \\ \liminf_{k\to\infty} \frac{\mathrm{PR}(\mathbf{X}_k)}{\mathrm{PR}_k^*} & \geq & \frac{1}{2} \\ \limsup_{k\to\infty} \mathrm{MR}(\mathbf{X}_k) & \leq & 2 \end{cases}$$

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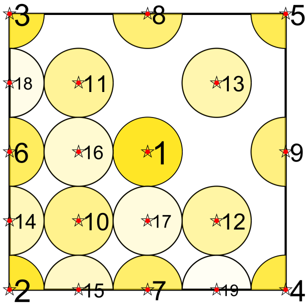
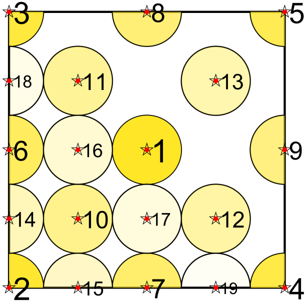
. . . but the sequence of design points is different from that of Greedy Packing!

Example: $\mathscr{X} = [0,1]^d$, $d = 2$, $n = 19$

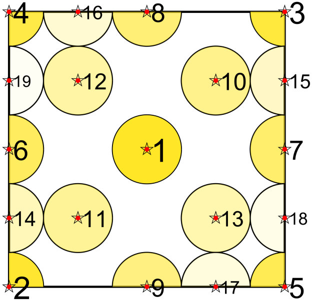


→ standard GP

Example: $\mathscr{X} = [0,1]^d$, $d = 2$, $n = 19$



→ standard GP



→ Riesz kernel K_5

Greedy Packing with projections

$\mathscr{X} = [0,1]^d$, $\mathcal{J}_i \subseteq \{1,\ldots,d\}$ = coordinates of a subspace of interest (e.g., $\mathcal{J}_i = (1,3,5)$ for $d = 5$)

$w(|\mathcal{J}_i|)$ = weight (importance) of subset $\mathcal{J}_i$ (only depends on its dimension)

$\mathbb{J}$ the set of all such index sets of interest

$$\mathbf{x}_{k+1} \in \mathrm{Arg}\max_{\mathbf{x}\in\mathscr{X}} \min_{\mathcal{J}\in\mathbb{J}} \underbrace{\left\{ \frac{d(\{\mathbf{x}\}_{\mathcal{J}}, \{\mathbf{X}_k\}_{\mathcal{J}})}{w(|\mathcal{J}|)\,\mathsf{CR}_{\mathcal{J}}(\mathbf{X}_k)} \right\}}_{\text{concerns projections onto } \mathcal{J}}$$

→ performance guarantees on projections

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→ performance guarantees on projections

Lh (random) design with d **(very) small (2 or 3)**:
$\mathscr{X}$ = regular grid = $\{\frac{i-1}{n-1},\ i = 1,\ldots,n\}^d$, $\mathbf{x}_1$ random in $\mathscr{X}$
$w(d) \gg w(1) > 0$ ($\Rightarrow \mathbf{X}_n$ is a Lh), randomise if equivalent choices for $\mathbf{x}_{k+1}$

Example: $\mathscr{X} = [0,1]^d$, $d = 5$, $n = 200$
full space (weight $w(5)$) + 10 subspaces of dimension 2 (weight $w(2)$)

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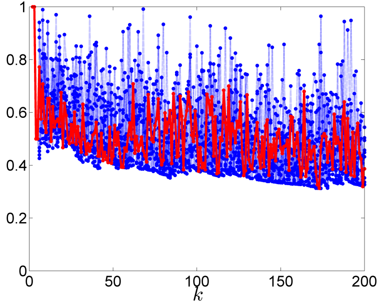
→ plot $\alpha_{k,\mathcal{J}} = \frac{d(\{\mathbf{x}_{k+1}\}_{\mathcal{J}},\{\mathbf{X}_k\}_{\mathcal{J}})}{\mathrm{CR}_{\mathcal{J}}(\mathbf{X}_k)}$ for $|\mathcal{J}| = 2$ and $|\mathcal{J}| = 5$



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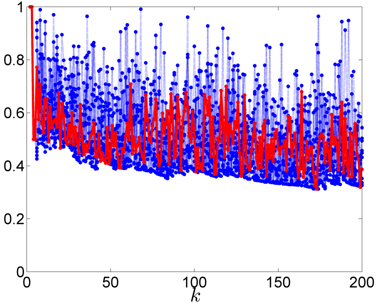

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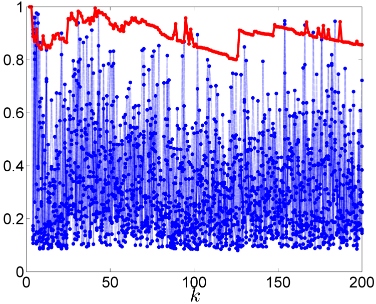
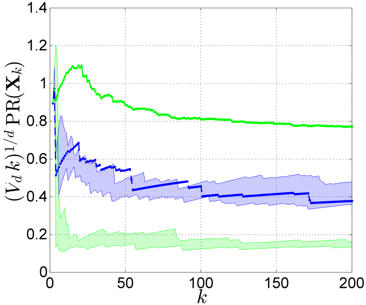


for $w(5) = 10$, $w(2) = 1$

$a_{\mathcal{J}} = \min_k \alpha_{k,\mathcal{J}}$ ➞ $a_{\mathcal{J}} \times 50\%$ guaranteed PR and CR efficiency for subspace $\mathcal{J}$

$w(5) = w(2) = 1$, $w(5) = 10$, $w(2) = 1$

Packing: $(V_d\, k)^{1/d} \mathrm{PR}(\mathbf{X}_k)$



(with $V_d = \mathrm{vol}\, [\mathscr{B}_d(\mathbf{0}, 1)]$)

envelope for 10 projections in dimension 2 and **full space** ($d = 5$)

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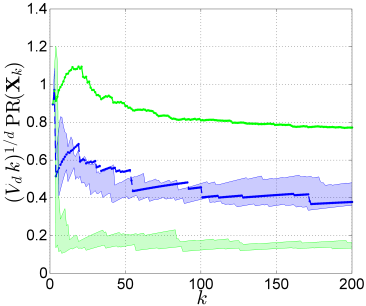
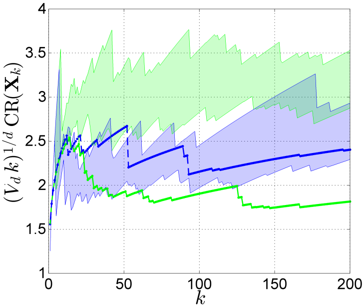


Covering: $(V_d\, k)^{1/d}\mathrm{CR}(\mathbf{X}_k)$



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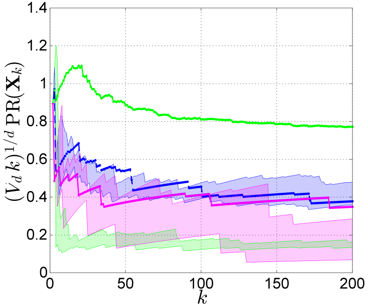

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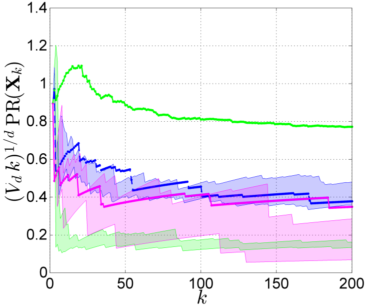

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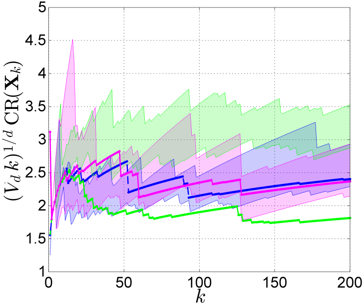

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envelope for 10 projections in dimension 2 and **full space** ($d = 5$)

4 Boundary avoidance

GP puts many points on the boundary of $\mathscr{X}$

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$$\rightarrow \mathbf{x}_{k+1} \in \mathrm{Arg}\max_{\mathbf{x}\in\mathscr{X}} \min \left\{ d(\mathbf{x}, \mathbf{X}_n),\ \beta \underbrace{d(\mathbf{x}, \partial\mathscr{X})}_{\text{distance to boundary}} \right\}$$

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Shang and Apley (2021) recommend $\beta = 2\sqrt{2d}$

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$$\beta = \beta(n_{\max,d}) = \frac{d}{2\,(n_{\max} V_d)^{-1/d}} - \sqrt{d} \ \text{(with } V_d = \mathrm{vol}\,[\mathscr{B}_d(\mathbf{0},1)])$$

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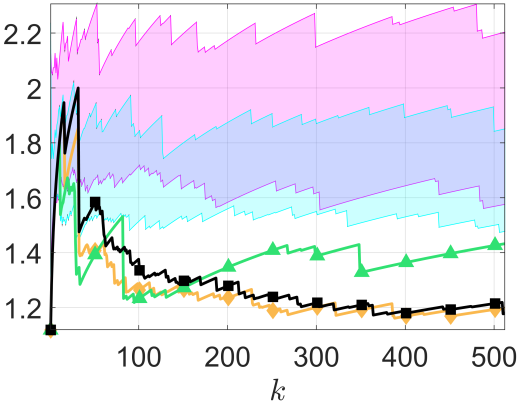
Comparison between: random points, (scrambled) Sobol' points, greedy packing ($\beta = \infty$), greedy packing with boundary avoidance ($\beta = 2\sqrt{2d}$), relaxed greedy packing with $\alpha = \alpha(n_{\max,d}) = 1 - \frac{2\,(n_{\max} V_d)^{-1/d}}{\sqrt{d}}$

$\mathscr{X} = [0,1]^d$, $d = 5$, $n_{max} = 2^9 = 512$

Covering radius $\text{CR}(\mathbf{X}_k)$ (as it decreases like $k^{-1/d}$, we plot $k^{1/d}\text{CR}(\mathbf{X}_k)$)



Random designs

(scrambled) Sobol'

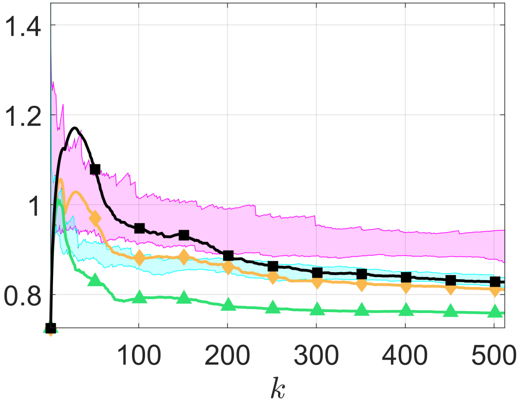
▲ — $\beta = 2\sqrt{2d}$

■ — $\beta = +\infty$ (standard GP)

♦ — $\alpha = \alpha(n_{max,d})$

$\mathscr{X} = [0,1]^d$, $d = 5$, $n_{\max} = 2^9 = 512$, μ uniform

Quantisation error: $k^{1/d} E_{10,\mu}(\mathbf{X}_k) = k^{1/d} \left\{\int [d(\mathbf{x},\mathbf{X}_k)]^{10} \mu(\mathrm{d}\mathbf{x})\right\}^{1/10}$



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Distance c.d.f. $F_{\mathbf{X}_n}(r)$

Consider $d(U,\mathbf{X}_n) = \min_{\mathbf{x}_i \in \mathbf{X}_n} \|U - \mathbf{x}_i\|$ with $U \overset{d}{\sim} \mu$ uniform on $\mathscr{X}$ $(= [0,1]^d)$

define $F_{\mathbf{X}_n}(r) = \mathrm{Prob}\{U \in \cup_{i=1}^n \mathscr{B}_d(\mathbf{x}_i, r)\} = \mathrm{Prob}\{d(U,\mathbf{X}_n) \le r\}$

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→ contains all the information about the filling of $\mathscr{X}$ by $\mathbf{X}_n$

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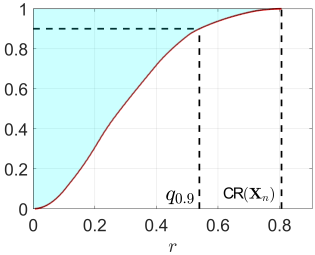

$F_{\mathbf{X}_n}(r)$ ➞ $E_{1,\mu}(\mathbf{X}_n)$

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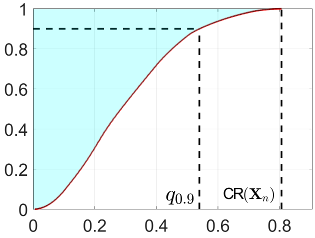
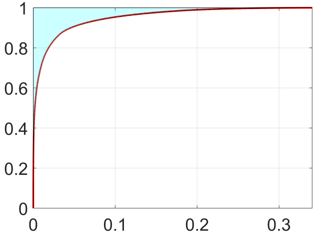


$F_{\mathbf{X}_n}(r) \xrightarrow{r} E_{1,\mu}(\mathbf{X}_n)$



$F_{\mathbf{X}_n}(r^{1/5}) \xrightarrow{r} E_{5,\mu}^5(\mathbf{X}_n)$

Distance c.d.f. for random designs and Sobol' points

(normalised) $F_{\mathbf{X}_n}(r)$ for a random design $\mathbf{R}_n$ with $\mathbf{x}_i \overset{d}{\sim} \mu$ and for Sobol' points $\mathbf{S}_n$

$F_{\mathbf{S}_n}(n^{-1/d} r)$ ●—●, $F_{\mathbf{R}_n}(n^{-1/d} r)$ ▲—▲ (and ★—★)

Asymptotically $F_{\mathbf{R}_n}(n^{-1/d} r) \to 1 - \exp(-V_d r^d)$ (Weibull) as $n \to \infty$ ■- - -■

with $V_d = \pi^{d/2}/\Gamma(d/2+1)$ volume of $\mathscr{B}_d(\mathbf{0}, 1)$

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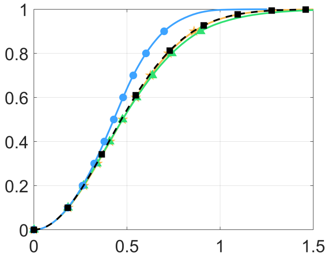

$\mathscr{X} = [0,1]^d$, $d = 2$, $n = 512$

Consider the queue of the distribution rather than its support

$(E_{s,\mu}(\mathbf{X}_n) \to \mathrm{CR}(\mathbf{X}_n)$ as $s \to \infty)$

d small:
Good agreement with the asymptotic behaviour for $\mathbf{R}_n$

$\mathbf{S}_n$ much preferable to $\mathbf{R}_n$

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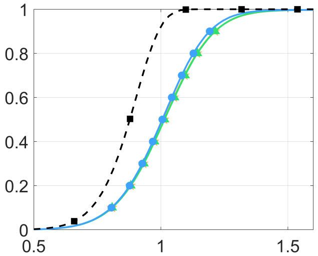

$\mathscr{X} = [0,1]^d$, $d = 10$, $n = 10^3$

d large:

$\mathbf{S}_n$ and $\mathbf{R}_n$ perform similarly

$\mathbf{R}_n$ far from the asymptotic behaviour

Asymptotic distribution:

neglect the boundary effect

→ strong boundary effect for large d

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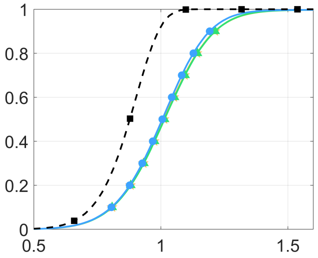

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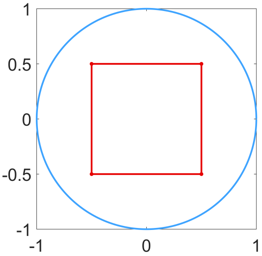
Random (uniform) designs in $\mathscr{X} = [-1,1]^d$ for large d: X and Y i.i.d. $\overset{d}{\sim} \mu$

$$\text{Prob}\left\{\left|\|X\|^2 - \frac{d}{3}\right| > t\right\} \leq 2\,\exp\left(-\frac{2\,t^2}{d}\right)$$

$$\text{Prob}\left\{\left|\|X-Y\|^2 - \frac{2d}{3}\right| > t\right\} \leq 2\,\exp\left(-\frac{t^2}{8\,d}\right)$$

Other difficulties with high dimensional cubes

$\mathscr{B}_d(\mathbf{0},1)$: volume $V_d = \pi^{d/2}/\Gamma(d/2+1) \rightarrow 0$ (quickly) as $d \rightarrow \infty$
$[-1/2, 1/2]^d$: volume $=1$



→ a 2d projection

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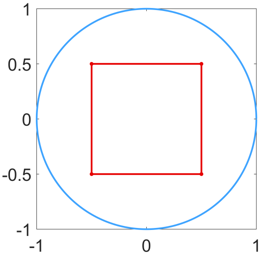

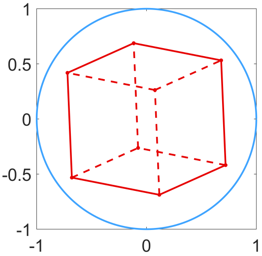

$d = 3$

➞ a 2d projection

➞ a random 2d projection

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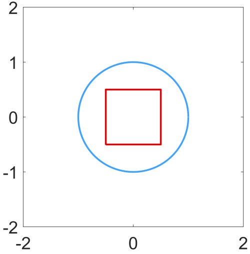

➞ a particular 2d projection

Other difficulties with high dimensional cubes

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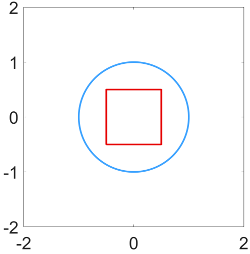
$[-1/2,1/2]^d$: volume $=1$



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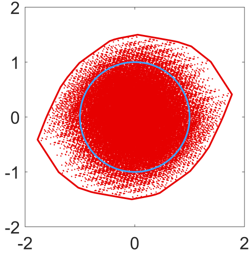

$d=16$ (65 536 vertices)

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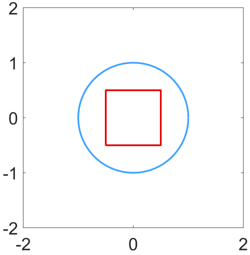

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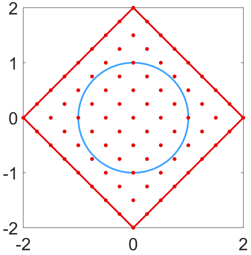

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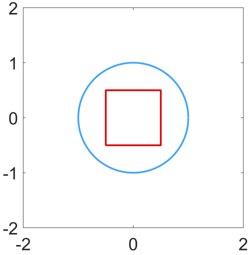

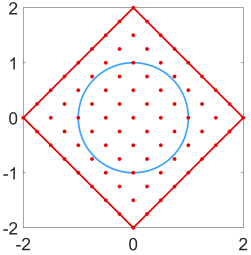

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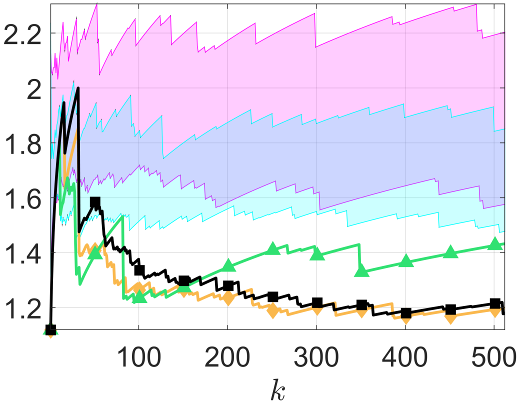
large d ➠ many vertices, far away, difficult to cover

$d = 5$, $n_{\max} = 2^9 = 512$

Covering radius $k^{1/d}\,\mathrm{CR}(\mathbf{X}_k)$



Random designs

(scrambled) Sobol'

▲ — $\beta = 2\sqrt{2d}$

■ — $\beta = +\infty$ (standard GP)

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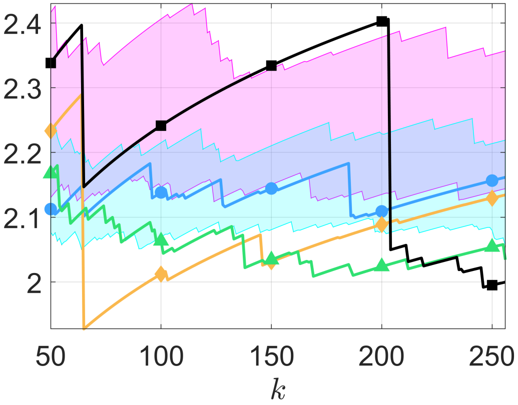

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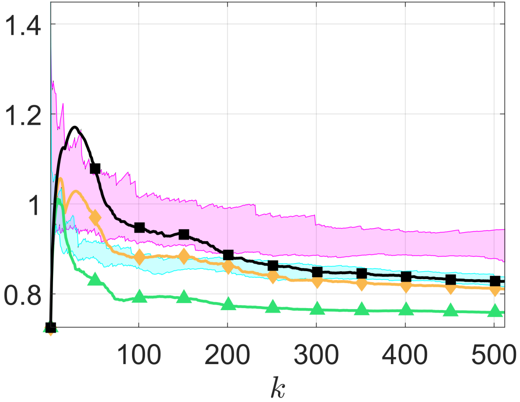

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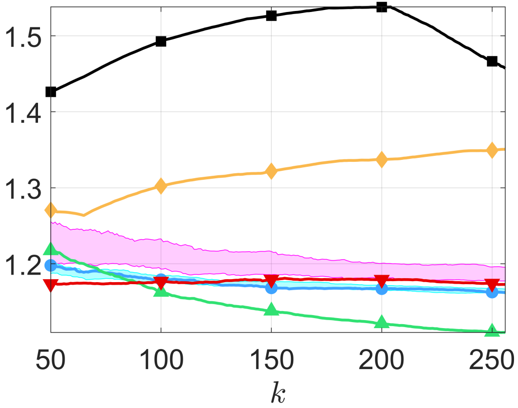

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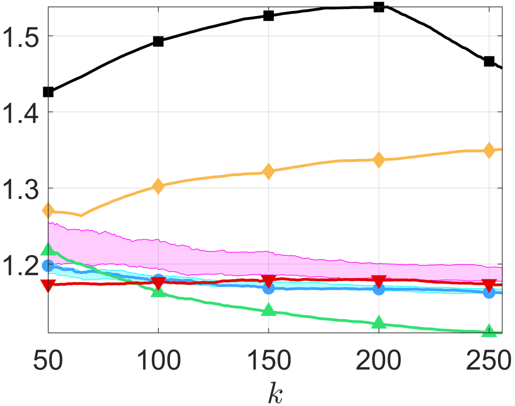

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Greedy quantisation: choose $\mathbf{x}_{k+1}$ within a finite set of candidates $\mathscr{X}_{\rm cand}$

approximate $\int [d(\mathbf{x}, \mathbf{X}_n)]^s \mu(\mathrm{d}\mathbf{x})$ by a finite sum

→ a second finite set $\mathscr{X}_{\rm eval}$ (Nogales Gómez, P and Rendas, 2021)

➠ $\mathscr{X}_{\rm cand}$ and $\mathscr{X}_{\rm eval}$ necessarily much smaller than $\mathscr{X}_{\rm cand}$ for greedy packing

6 Designs in a high dimensional cube

Based on (Karvonen, P and Zhigljavsky, 2026)

- Forget about $\mathrm{CR}(\mathbf{X}_n)$, consider $E_{s,\mu}(\mathbf{X}_n)$, μ uniform
- Consider **random designs** $\mathbf{R}_n$ with the $\mathbf{x}_i$ i.i.d. $\overset{d}{\sim} \mathbb{P}$ for some $\mathbb{P}$
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We have $E^s_{s,\mu}(\mathbf{R}_n) = \mathsf{E}_U\{d^s(U,\mathbf{R}_n)\} = s\int_{r\geq 0} r^{s-1}[1-F_{\mathbf{R}_n}(r)]\,\mathrm{d}r$

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Therefore, $\mathsf{E}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\} = s\int_{r\geq 0} r^{s-1}[1 - F_n(r;\mathbb{P})]\,\mathrm{d}r$

with $F_n(t;\mathbb{P}) = \mathsf{E}_{\mathbf{R}_n}\{F_{\mathbf{R}_n}(t)\}$ the **mean distance c.d.f.**
(Jensen inequality $\Rightarrow \mathsf{E}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\} > [\mathsf{E}_{\mathbf{R}_n}\{E_{s,\mu}(\mathbf{R}_n)\}]^s$ for $s > 1$)

→ compute/approximate $F_n(t;\mathbb{P})$

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$$\mathrm{Prob}_{\mathbf{R}_n}\left\{d(\mathbf{u},\mathbf{R}_n)\leq t\right\} = 1 - \left(1-\mathbb{P}\left\{\|\mathbf{u}-X\|\leq t\right\}\right)^n,\ \ X \overset{d}{\sim} \mathbb{P}$$

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→ approximate $\mathbb{P}\left\{\|\mathbf{u} - X\| \leq t\right\}$ (Noonan and Zhigljavsky, 2024)

When $\mathbb{P}$ is spherically symmetric with center $\mathbf{0}$, $\mathbb{P}\left\{\|\mathbf{u} - X\| \leq t\right\} = \mathcal{I}(\|\mathbf{u}\|, t)$, a one dimensional integral involving the regularised incomplete beta-function

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Calculation of $F_n(t;\mathbb{P})$ ➟ integration with respect to the distribution of $\|U\|$

If $\mathscr{X}$ is a ball we are done: three nested one-dimensional integrals

- one for $\mathcal{I}(\|\mathbf{u}\|, t)$
- one for $F_n(t;\mathbb{P})$ (with respect to distribution of $\|U\|$ with $U \overset{d}{\sim} \mu$)
- one for $\mathsf{E}_{\mathbf{R}_n}\{E_{s,\mu}^s(\mathbf{R}_n)\} = s\int_{r\geq 0} r^{s-1}[1 - F_n(r;\mathbb{P})]\,\mathrm{d}r$

➞ minimise $\mathsf{E}_{\mathbf{R}_n}\{E_{s,\mu}^s(\mathbf{R}_n)\}$ with respect to $\mathbb{P}$ (parameterised)

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1. Use a parametric distribution for the $\mathbf{x}_i$ in $\mathscr{X}$

$\mathbb{P}_{\alpha,\delta}(d\mathbf{x}) = \prod_{i=1}^d p_{\alpha,\delta}(x_i)\mathrm{d}x_i$
$= \text{product of symmetric Beta}_\delta(\alpha,\alpha)$ distributions on $[-\delta,\delta]$, $\alpha,\delta \geq 0$

$$p_{\alpha,\delta}(t) = \frac{(2\delta)^{1-2\alpha}}{\mathrm{B}(\alpha,\alpha)}[\delta^2 - t^2]^{\alpha-1}\,, \;\; -\delta < t < \delta$$

$\delta \leq 1$ for designs in $\mathscr{X} = [-1,1]^d$; for $\alpha = 0$ each $\mathbf{x}_i = \pm\delta$ with prob. 1/2;
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2. Approximate $\mathbb{P}_{\alpha,\delta}$ by a spherically symmetric distribution

Replace $X \overset{d}{\sim} \mathbb{P}_{\alpha,\delta}$ by $X' \overset{d}{\sim} \mathbb{Q}_{\alpha,\delta}$ spherically symmetric, with
$\|X'\|^2 \overset{d}{\sim} \mathrm{B}(t;a,b|M) = \frac{t^{a-1}(M-t)^{b-1}}{M^{a+b-1}\mathrm{B}(a,b)}$, $t \in (0,M)$, $a,b > 0$,
and a,b,M such that the first three moments of $\|X\|^2$ and $\|X'\|^2$ coincide
$\rightarrow$ explicit expressions for a,b,M as functions of α and δ (and d)
(Noonan and Zhigljavsky, 2024)

3. Approximation of $\mathsf{E}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$

3.1: approximate $F_n(t;\mathbb{P}_{\alpha,\delta})$ by $F_n(t;\mathbb{Q}_{\alpha,\delta})$:

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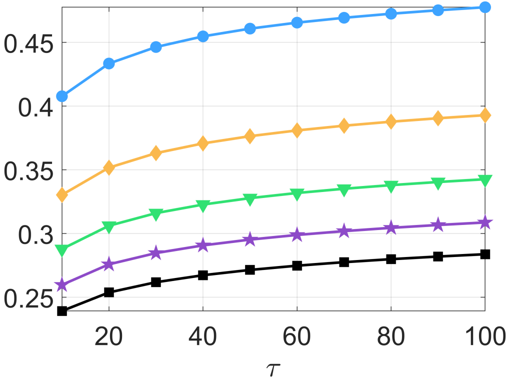
3.3 approximate $\mathsf{E}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\} = s\int_{r\geq 0} r^{s-1}[1-F_n(r;\mathbb{P}_{\alpha,\delta})]\,\mathrm{d}r$ by
$$\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\} = s\int_{r\geq 0} r^{s-1}[1-\widehat{F}_n(r;\mathbb{Q}_{\alpha,\delta})]\,\mathrm{d}r$$

➠ Minimise $\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$ with respect to α and δ

For all $d \gtrsim 10$, unless n is astronomically large, the optimal α equals zero!
(i.e., the $\mathbf{x}_i$ are at vertices of a cube $[-\delta_0, \delta_0]^d$)

$\delta_0(\tau)$ for $n = \tau d$, with
$d = 10$ (●), $d = 20$ (♦), $d = 30$ (▼), $d = 40$ (★), and $d = 50$ (■)



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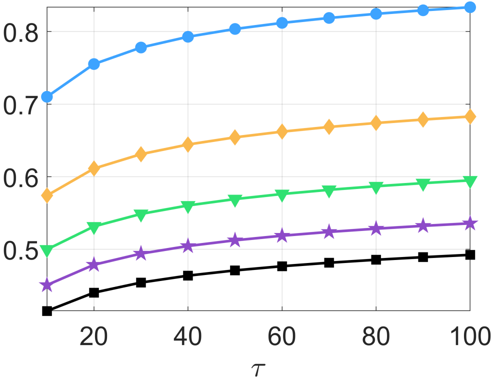

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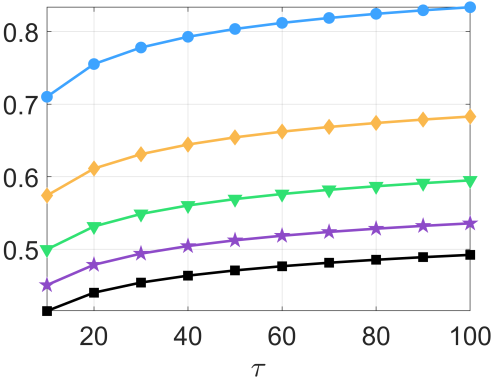
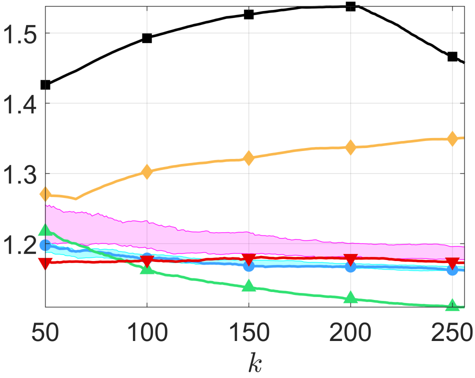


Small influence of n and s on δ_0 and δ_1 (small increase when $n \nearrow$ and/or $s \nearrow$)

$d = 10$, $n_{\max} = 2^8 = 256$, μ uniform

Quantisation error: $k^{1/d} E_{10,\mu}(\mathbf{X}_k)$



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Random designs

▼ — greedy quantisation

(scrambled) Sobol' in $[0, 1]^d$

▲ — $\beta = 2\sqrt{2d}$

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Minimisation of $\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$ for $s = 2$: $\alpha = 0 \rightarrow \delta_0 \simeq 0.446$

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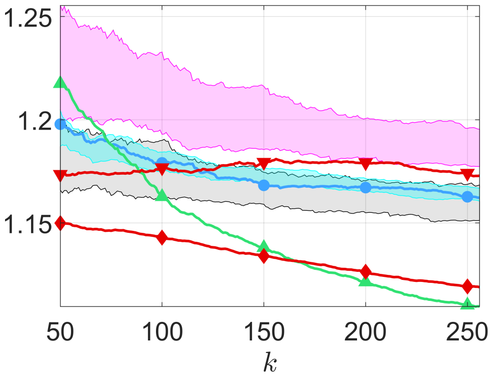

Random designs

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(scrambled) Sobol' in $[0,1]^d$

random sampling of vertices $\pm\delta_0$ without replacement

♦ — greedy quantisation ($s = 2$)

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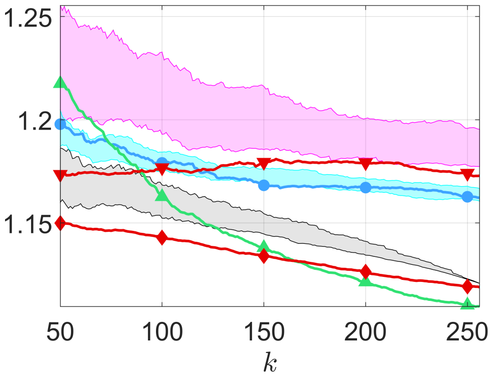

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in a 2^{d-2} fractional-factorial design

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2^{d-2} fractional-factorial design = subset of the 2^d vertices with max. PR (Box and Hunter, 1961a,b)

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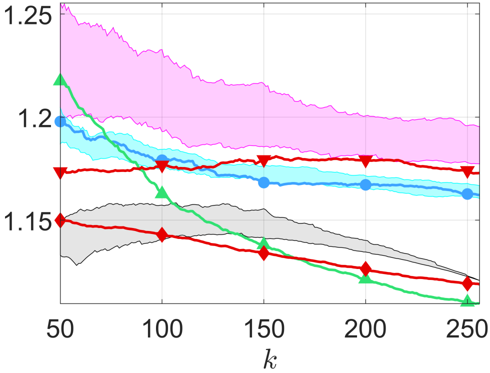

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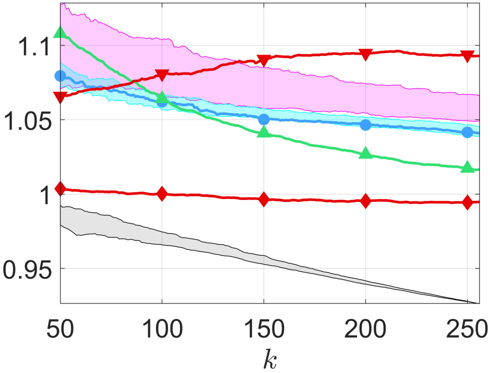

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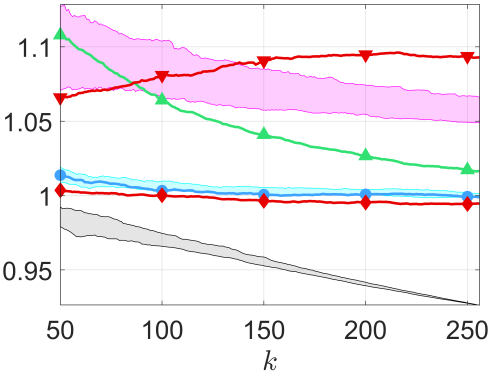
Minimisation of $\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$ for $s = 2$: $\alpha = 0 \to \delta_0 \simeq 0.446$
$\alpha = 1 \to \delta_1 \simeq 0.769$

Quantisation error: $k^{1/d} E_{2,\mu}(\mathbf{X}_k)$



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Random designs
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(scrambled) Sobol' in $[(1-\delta_1)/2, (1+\delta_1)/2]^d$
♦ — greedy quantisation ($s = 2$)

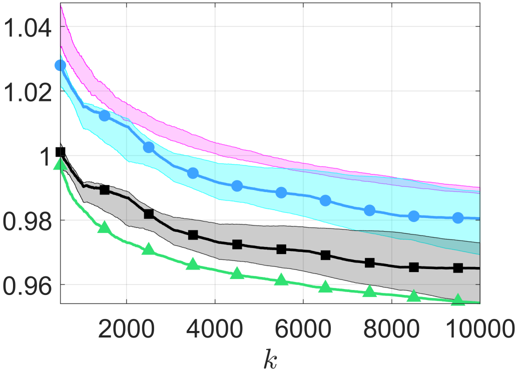
greedy packing on vertices $\pm\delta_0$
in a 2^{d-2} fractional-factorial design

fractional-factorial design $\Rightarrow n < 2^d$
(scrambled) Sobol' points in $[(1-\delta_1)/2, (1+\delta_1)/2]^d$: any n is allowed

$d = 10$, $n_{\max} = 10\,000$, μ uniform

Minimisation of $\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$ for $s = 2$: $\alpha = 1 \rightarrow \delta_1 \simeq 0.905$

Quantisation error: $k^{1/d} E_{2,\mu}(\mathbf{X}_k)$



Random designs

(scrambled) Sobol' in $[0,1]^d$

(scrambled) Sobol' in $[(1-\delta_1)/2, (1+\delta_1)/2]^d$

▲ — $\beta = 2\sqrt{2d}$

fractional-factorial design $\Rightarrow n < 2^d$

(scrambled) Sobol' points in $[(1-\delta_1)/2, (1+\delta_1)/2]^d$: any n is allowed

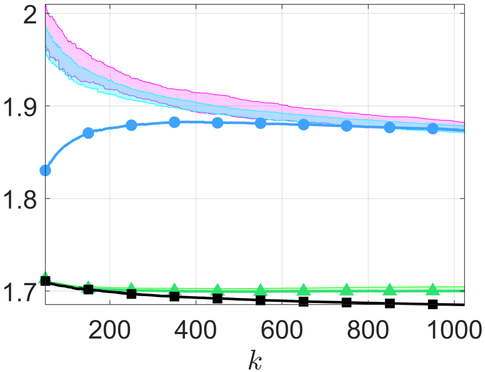
$d = 30$, $n_{max} = 2^{10} = 1\,024$, μ uniform

➠ "very high dimension": $\mathscr{X}$ has more than 10^9 vertices ($\gg n$)

Minimisation of $\widehat{\mathsf{E}}_{\mathbf{R}_n}\{E^s_{s,\mu}(\mathbf{R}_n)\}$ for $s = 2$: $\alpha = 0 \rightarrow \delta_0 \simeq 0.319$

$\alpha = 1 \rightarrow \delta_1 \simeq 0.554$

Quantisation error: $k^{1/d} E_{10,\mu}(\mathbf{X}_k)$



Random designs

(scrambled) Sobol' in $[0,1]^d$

(scrambled) Sobol' in $[(1-\delta_1)/2, (1+\delta_1)/2]^d$

greedy packing on vertices $\pm\delta_0$

in a 2^{d-20} fractional-factorial design

2^{d-20} fractional-factorial design = subset of the 2^{30} vertices with max. PR

7 Conclusions

- Greedy packing algorithm: an extremely useful too for the incremental construction of nested designs
- → space-filling designs in small dimension
  (with boundary avoidance when $\mathscr{X}$ is a cube)
- For large d (already starts at $d \gtrsim 10$), consider the quantisation error rather than the covering radius

- When $\mathscr{X} = [-1,1]^d$, design points should be in a smaller cube $\mathcal{C}_\delta = [-\delta, \delta]^d$ (with $\delta \searrow$ as $d \nearrow$)
- Use either random (or Sobol') points in $\mathcal{C}_\delta$, or a subset of vertices of $\mathcal{C}_\delta$
  Using a subset given by a 2^{d-m} fractional-factorial design with maximum packing radius is advisable (≠ minimum-aberration design)
- The greedy-packing algorithm can be used to sample vertices from this 2^{d-m} design
- As the design belongs to $\mathcal{C}_\delta = [-\delta, \delta]^d$, its projections in small dimensions have poor filling properties (but this can be corrected...)

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Thank you for your attention !

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