Design of Computer Experiments — (1) without model —

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Objectives

Computer experiments: based on simulations

➤ Usually, $\mathbf{x} \in \mathbb{R}^d$ ➠ observation $Y(\mathbf{x})$ (physical experiment)
➤ here, numerical simulation: $Y(\mathbf{x}) = f(\mathbf{x})$, observation = evaluation of an unknown function $f(\cdot)$
(no measurement error)

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from pairs $(\mathbf{x}_i, f(\mathbf{x}_i))$, $i = 1, 2, \ldots, n$

- optimization: find $\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathscr{X}} f(\mathbf{x})$
- inversion: construct $\{\mathbf{x} \in \mathscr{X} : f(\mathbf{x}) = T\}$
- estimation of a probability of failure: $\text{Prob}\{f(\mathbf{x}) > C\}$ when $\mathbf{x} \sim$ probability density $\varphi(\cdot)$
- sensitivity analysis
- **approximation/interpolation of $f(\cdot)$** by a predictor $\eta_n(\cdot)$, to be constructed

Objective = approximation/interpolation

$f(\mathbf{x})$ an unknown function, defined on $\mathscr{X} \subset \mathbb{R}^d$ (compact)
construct a "good" approximation $\eta_n(\cdot)$ of $f(\cdot)$ over $\mathscr{X}$ from pairs $(\mathbf{x}_i, f(\mathbf{x}_i))$, $i = 1, 2, \ldots, n$ (n not necessarily fixed *a priori*)

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- Since $f(\cdot)$ is unknown, we must observe everywhere!
- maximize the spread of the n points $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ in $\mathscr{X}$

(uniformly seems reasonable and can be properly justified (Biedermann and Dette, 2001))

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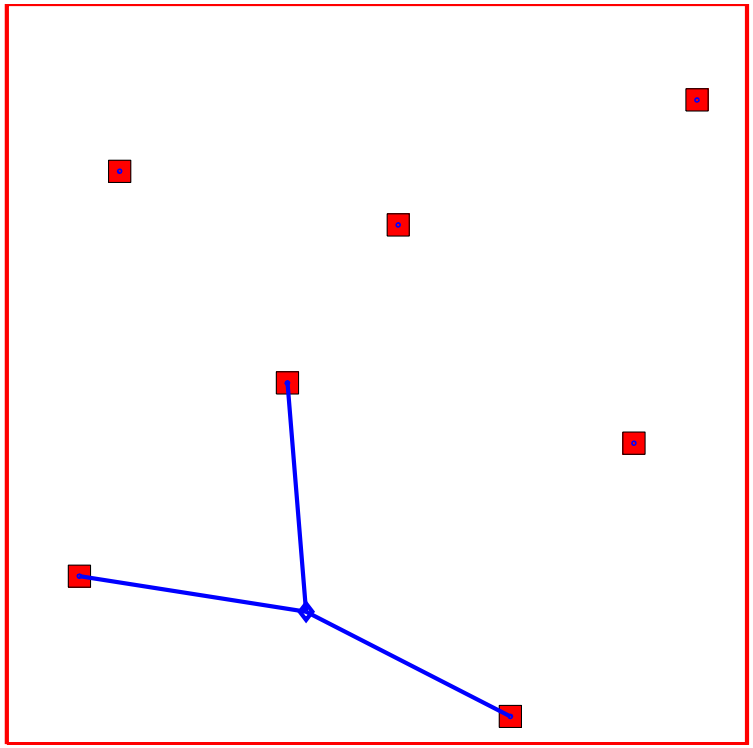
▷ $\mathbf{X}_n$ is the design (an n-point design) ◁

What does "observe everywhere" mean?

— very much based on (P., 2017)

General overview: 3 families of design criteria

1. Inter-distance: between $\mathbf{X}_n$ and $\mathscr{X}$ (miniMax, dispersion)



. . . a bit tricky
(but we are never far from a design point)

General overview: 3 families of design criteria

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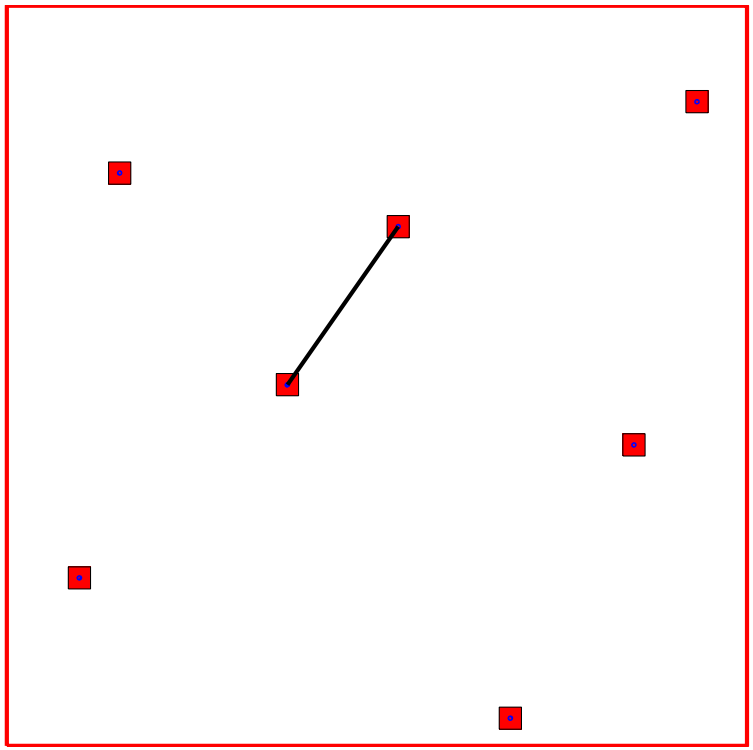
2. Intra-distances: within $\mathbf{X}_n$, between design points $\mathbf{x}_i$, $i = 1, \ldots, n$
   (Maximin, energy...)



. . . easier

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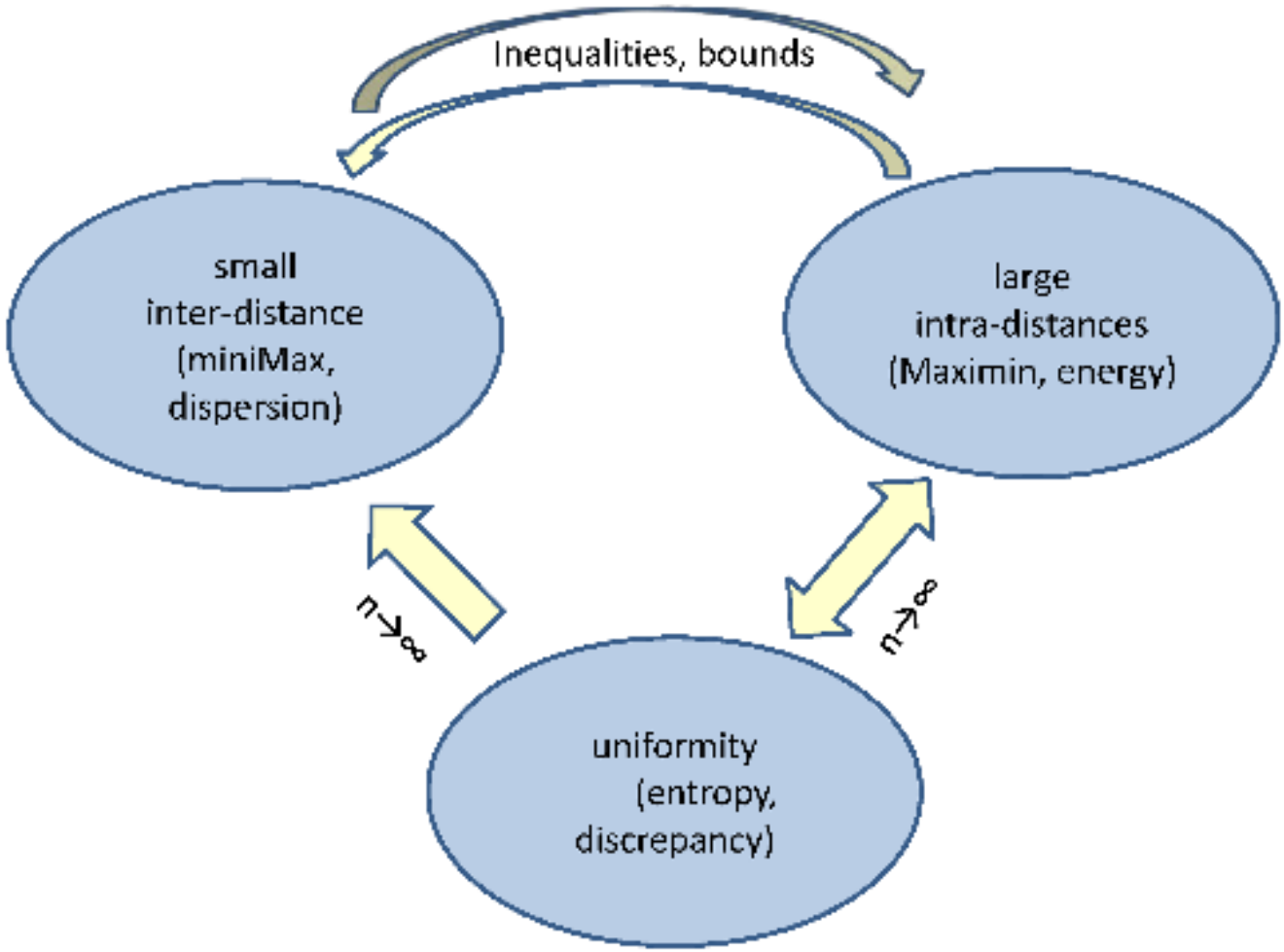
2. Intra-distances: within $\mathbf{X}_n$, between design points $\mathbf{x}_i$, $i = 1, \ldots, n$
   (Maximin, energy...)
3. Uniformity of the distribution of $\mathbf{x}_i$, $i = 1, \ldots, n$
   (entropy, discrepancy ➠ generate infinite sequences of points)


Inequalities, bounds
small
inter-distance
(miniMax,
dispersion)
large
intra-distances
(Maximin, energy)
$n \to \infty$
$n \to \infty$
uniformity
(entropy,
discrepancy)

Plan

1. Geometrical space-filling criteria
   - 1.1 miniMax & Maximin: generalities
   - 1.2 Latin hypercubes
   - 1.3 miniMax (inter-distance) criterion
   - 1.4 Maximin (intra-distances) criterion
   - 1.5 Relations between Φ_{Mm} and Φ_{mM} ($d \geq 2$)
   - 1.6 Regularized Maximin, energy
2. Uniformity: quasi Monte-Carlo, discrepancy
   - 2.1 Entropy, optimal graphs
   - 2.2 Discrepancy: motivation
   - 2.3 Discrepancy criteria
   - 2.4 Low discrepancy sequences
   - 2.5 (t, m, d)-nets & (t, d)-sequences
3. Dispersion & miniMax
   - 3.1 Dispersion
   - 3.2 Low dispersion sequences
4. Conclusions part (1)

1 Geometrical space-filling criteria

1.1 miniMax & Maximin: generalities (Johnson et al., 1990)

① **miniMax**: minimize $\Phi_{mM}(\mathbf{X}_n) = \max_{\mathbf{x}\in\mathscr{X}} \min_i \|\mathbf{x} - \mathbf{x}_i\|$

$$\Phi_{mM}(\mathbf{X}_n) = d_{\text{Hausdorff}}(\mathbf{X}_n, \mathscr{X}) = \max\{\max_{\mathbf{x}\in\mathscr{X}} d(x, \mathbf{X}_n), \underbrace{\max_{\mathbf{x}_i\in\mathbf{X}_n} d(\mathbf{x}_i, \mathscr{X})}_{=0 \ (\mathbf{X}_n\in\mathscr{X}^n)}\}$$

➠ **Inter-distance** between $\mathbf{X}_n$ and $\mathscr{X}$

$$d = 1 \Leftrightarrow x_i = (2i-1)/(2n),\ i = 1, \ldots, n$$
$$\Rightarrow \Phi^*_{mM,n} = 1/(2n)$$

$d > 1 \Leftrightarrow$ **sphere-covering**

② **Maximin**: maximize $\Phi_{Mm}(\mathbf{X}_n) = \min_{i \neq j} d_{ij} = \min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\|$

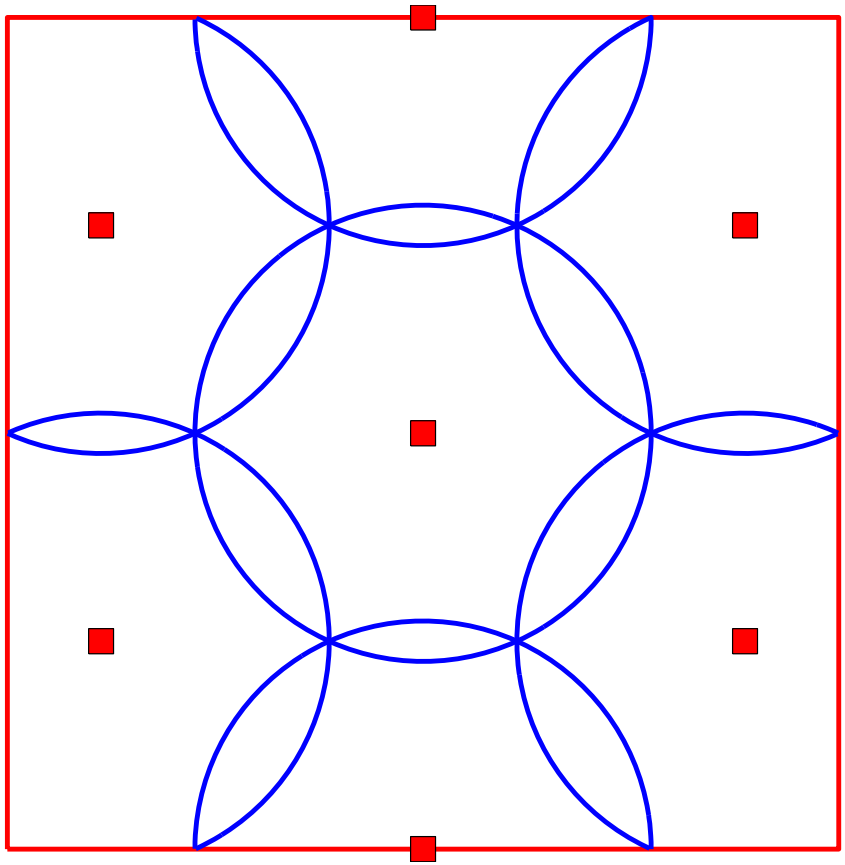
➠ **Intra-distances** for $\mathbf{X}_n$ (between points $\mathbf{x}_i$ in $\mathbf{X}_n$)

$d = 1 \Leftrightarrow x_i = (i-1)/(n-1),\ i = 1, \ldots, n$
$\Rightarrow \Phi^*_{Mm,n} = 1/(n-1)$

$d > 1 \Leftrightarrow$ **sphere-packing**

Examples :

① miniMax $d = 2, n = 7$
(radius=$\phi_{mM}(\mathbf{X}_n)$)



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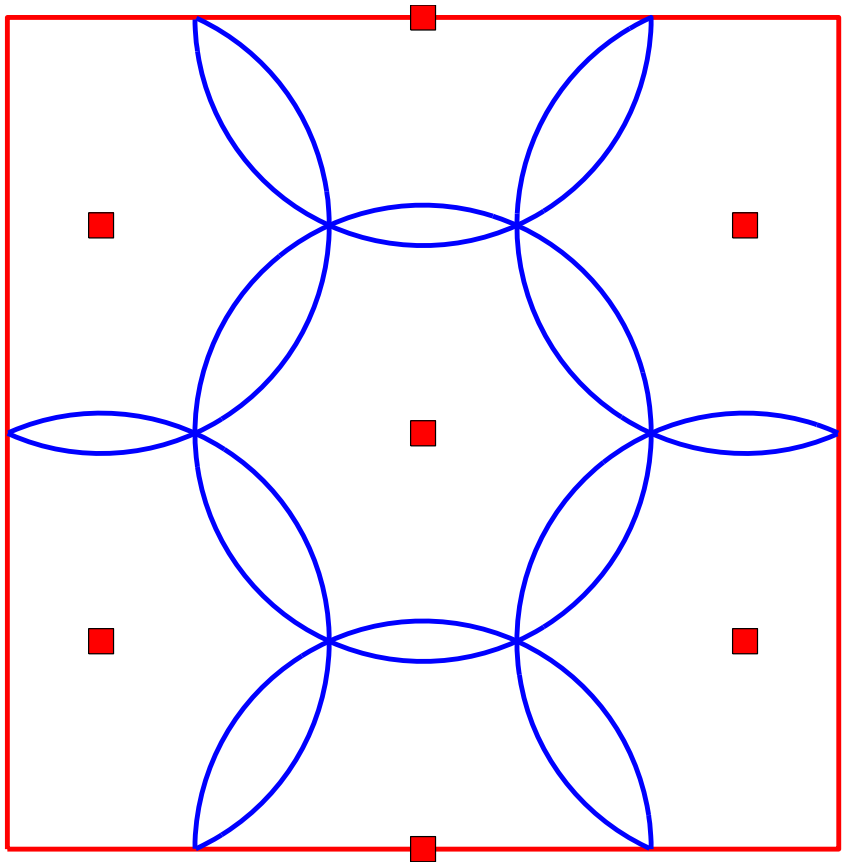
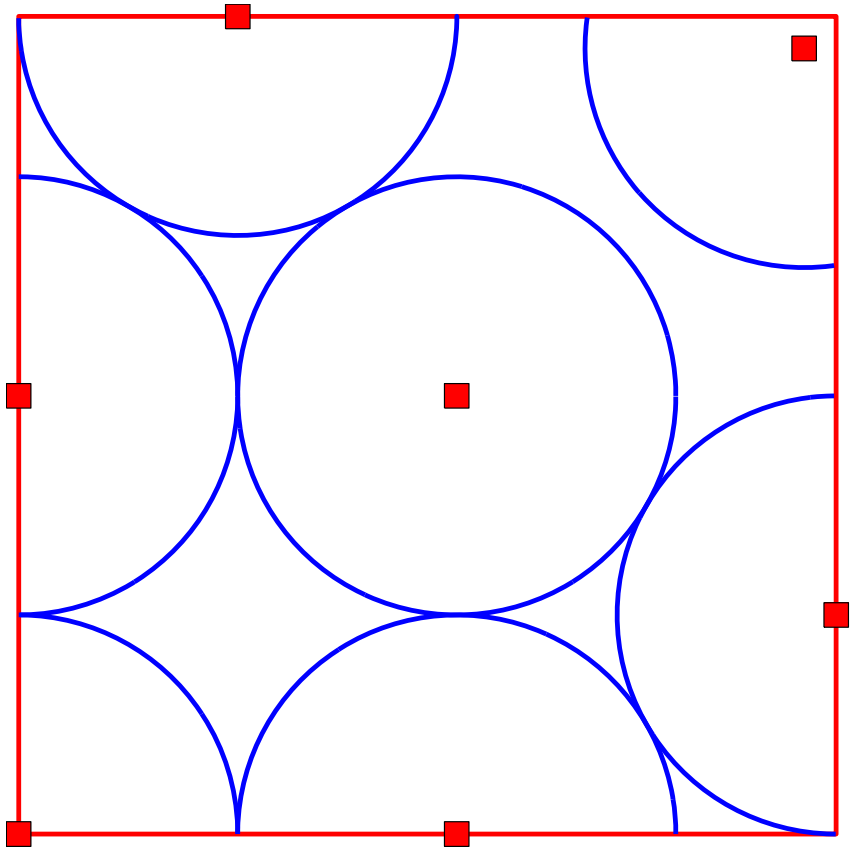


② Maximin $d = 2, n = 7$
(radius=$\phi_{Mm}(\mathbf{X}_n)/2$)



Why Maximin $\Leftrightarrow$ sphere-packing?

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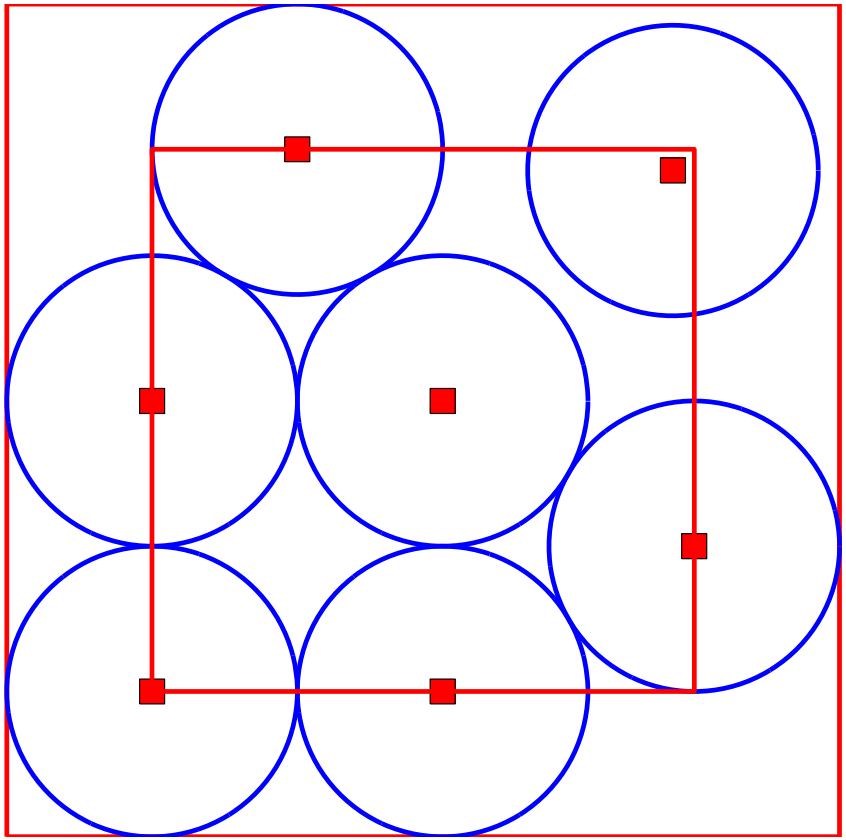

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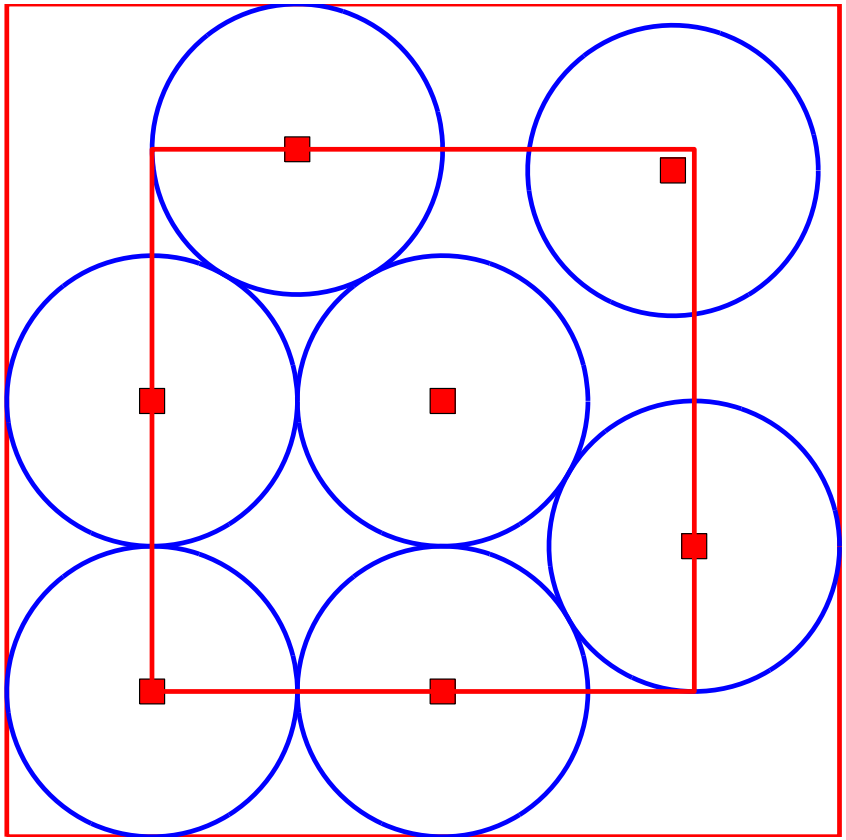
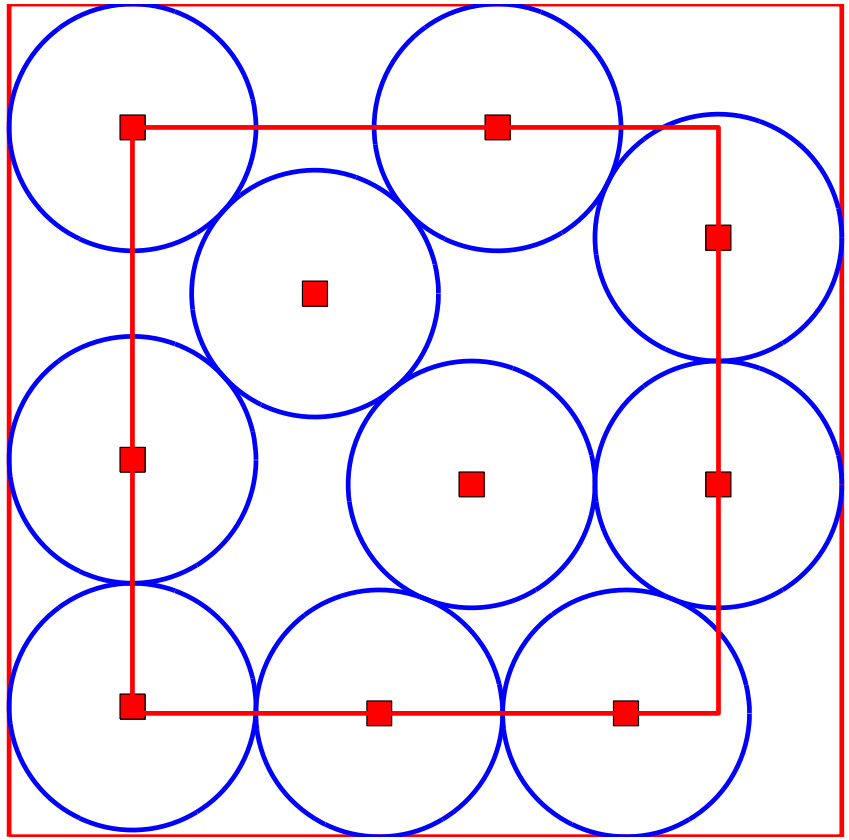


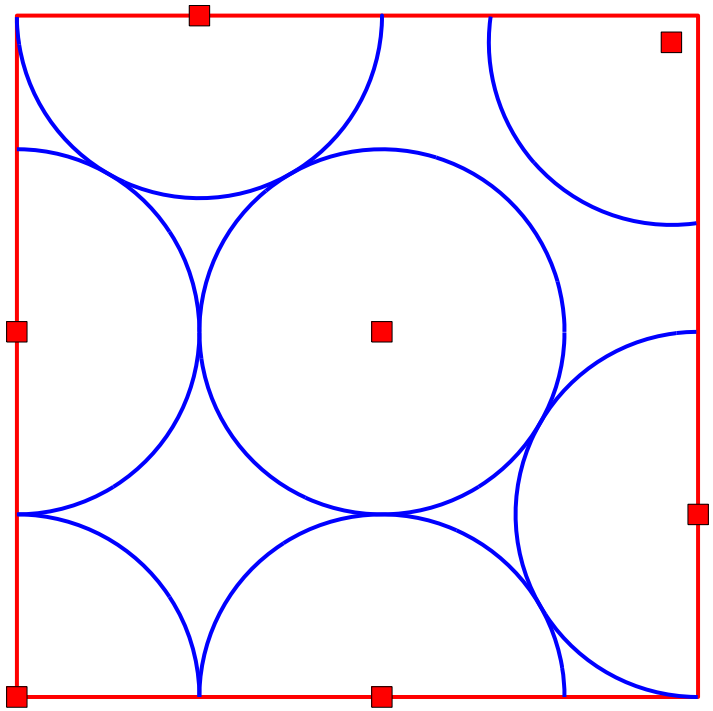
$d = 2, n = 10$



A few difficulties:

a) Local optima

Maximin $d = 2, n = 7$, global opt.



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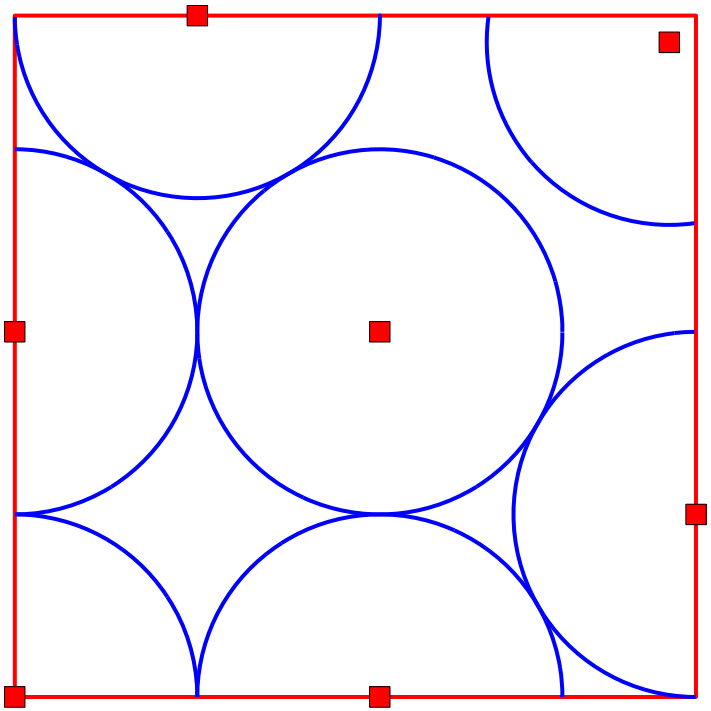

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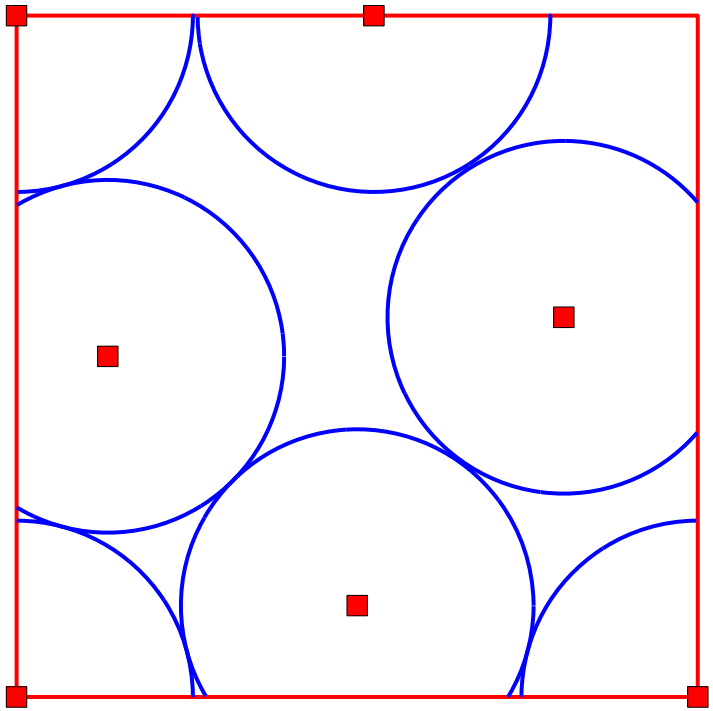

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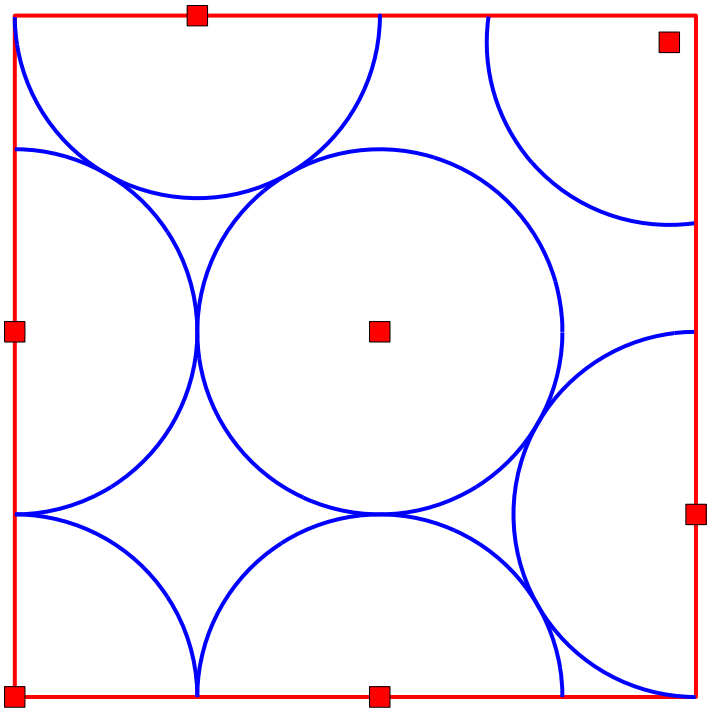

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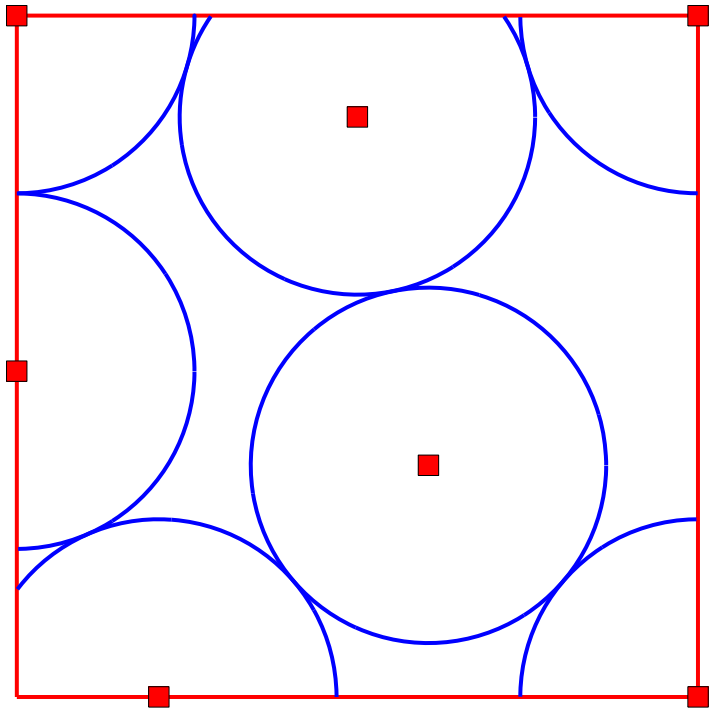

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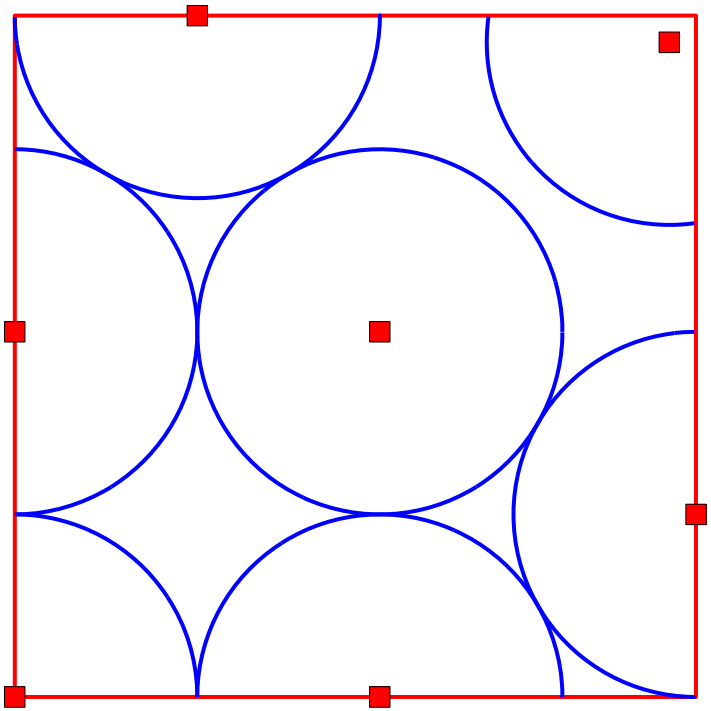

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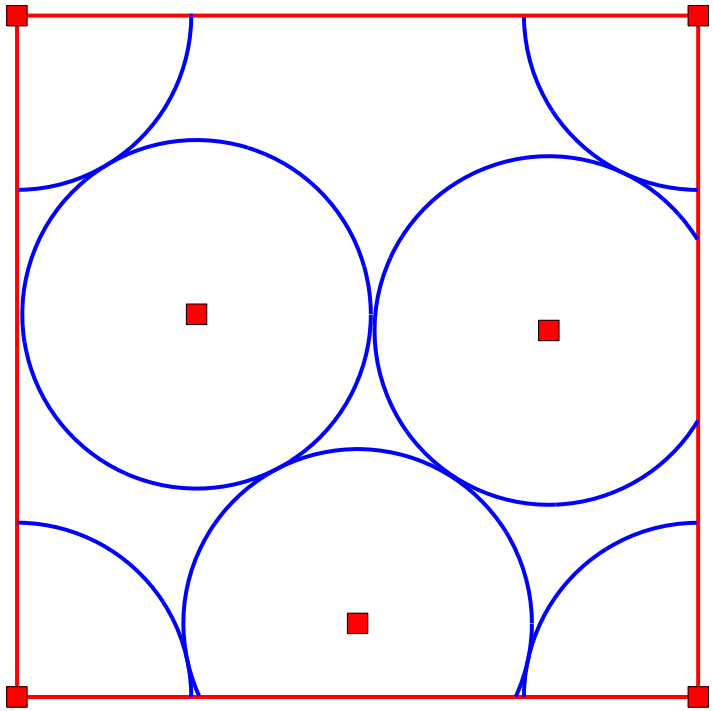

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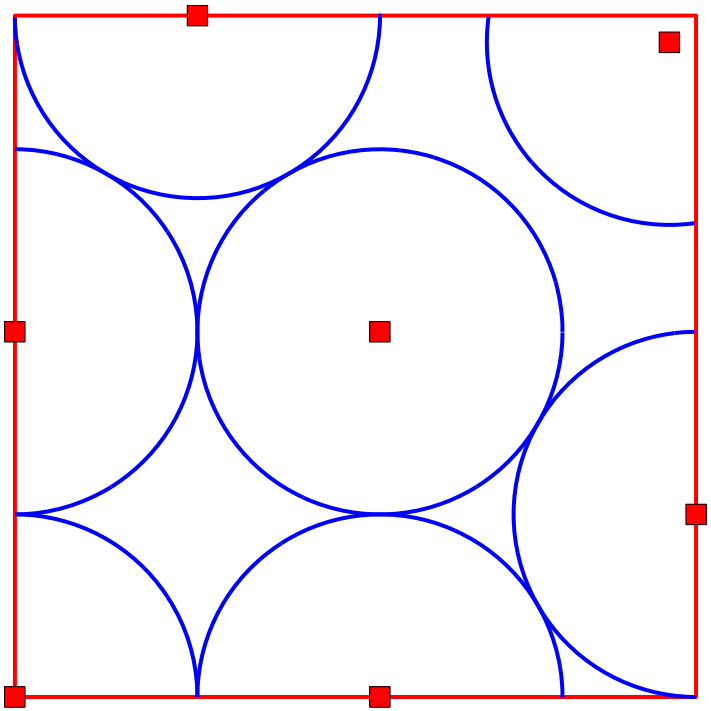

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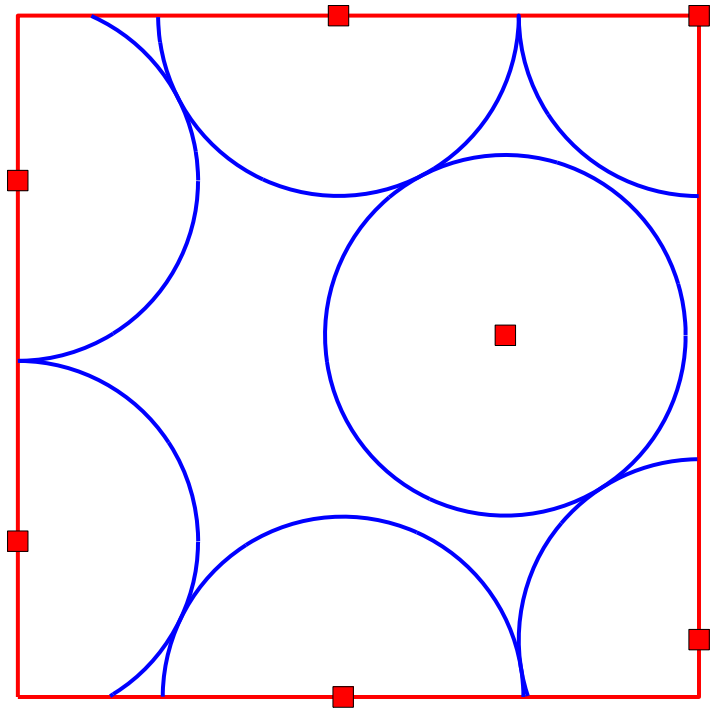
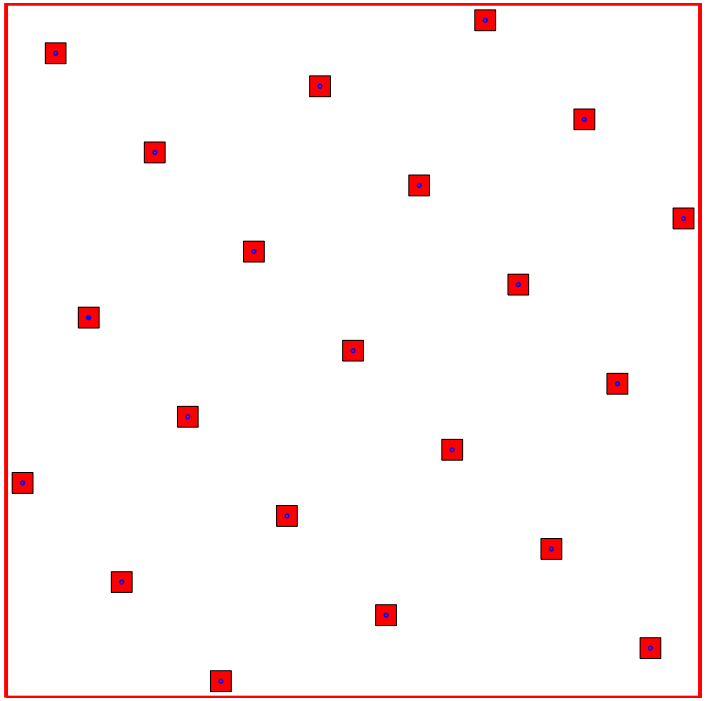
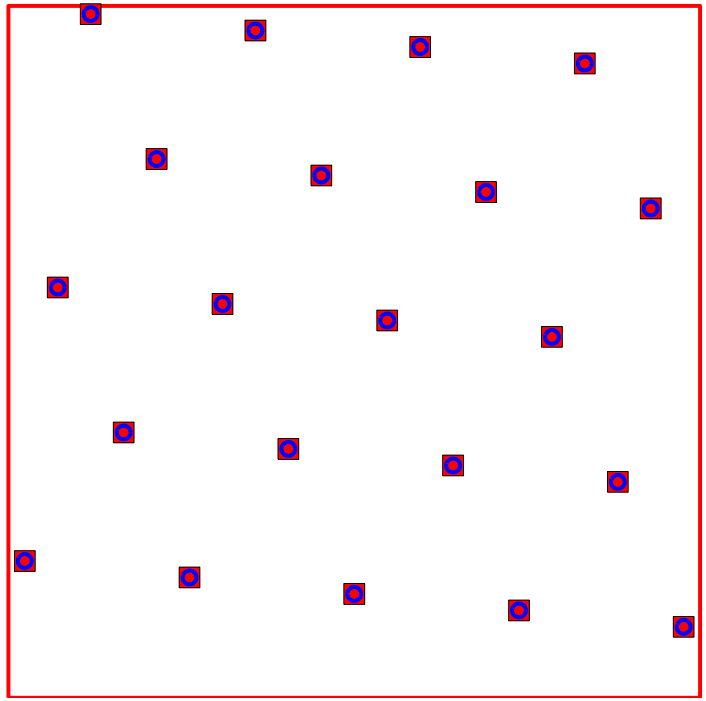


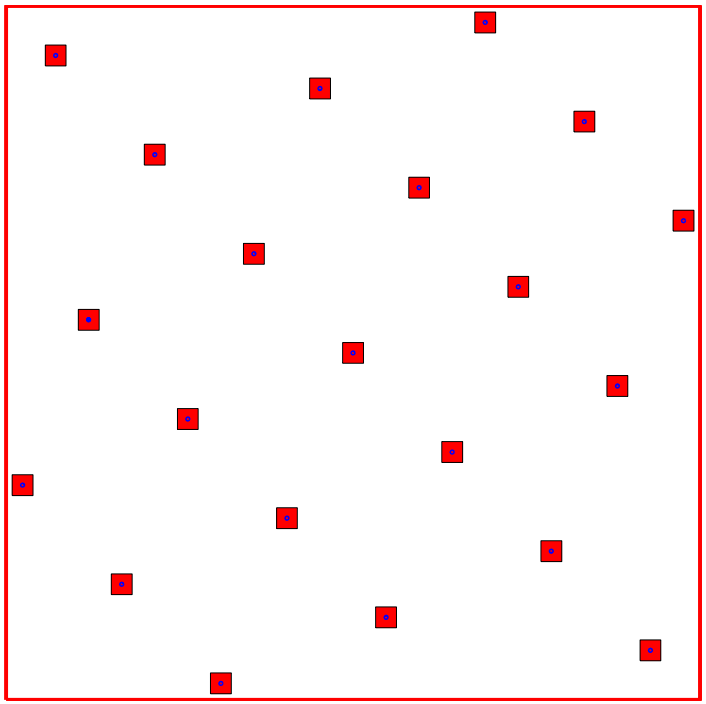
b) Misleading intuition



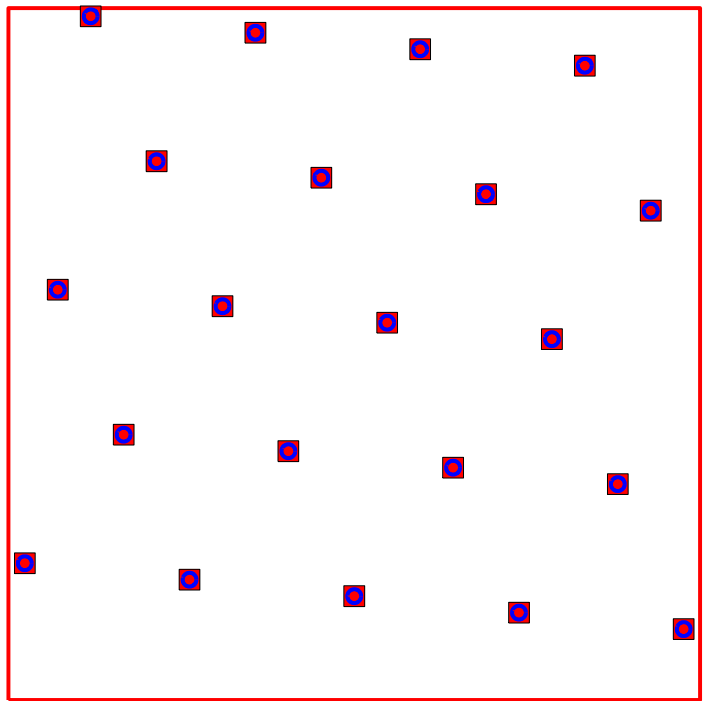


Which one is better?

b) Misleading intuition



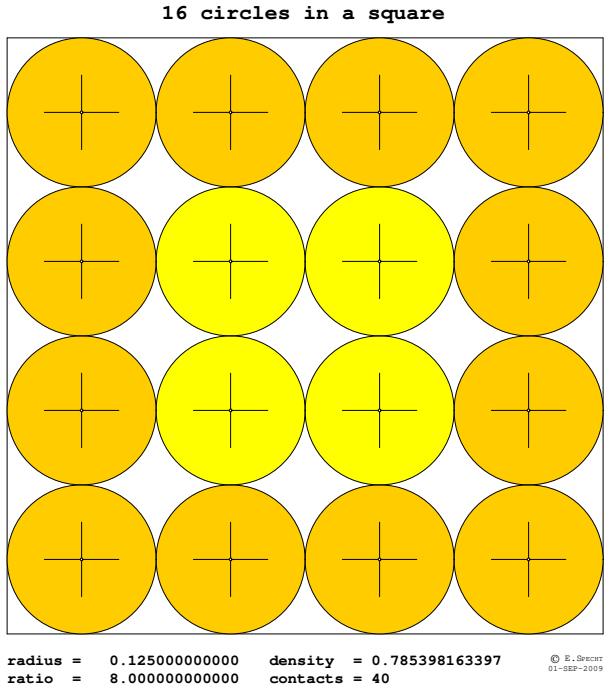
Geometry : $\Phi_{Mm}(\mathbf{X}_n) = 0.2020$
$\Phi_{mM}(\mathbf{X}_n) = 0.2357$
Uniformity : $D_{Cent,L_2}(\mathbf{X}_n) = 0.0280$
$D_{WA,L_2}(\mathbf{X}_n) = 0.0388$



Geometry : $\Phi_{Mm}(\mathbf{X}_n) = 0.2302$
$\Phi_{mM}(\mathbf{X}_n) = 0.2217$
Uniformity : $D_{Cent,L_2}(\mathbf{X}_n) = 0.0536$
$D_{WA,L_2}(\mathbf{X}_n) = 0.0633$

c) Sphere-packing: no trivial solution,
see `http://www.packomania.com/`

$$d = 2, n = 16$$



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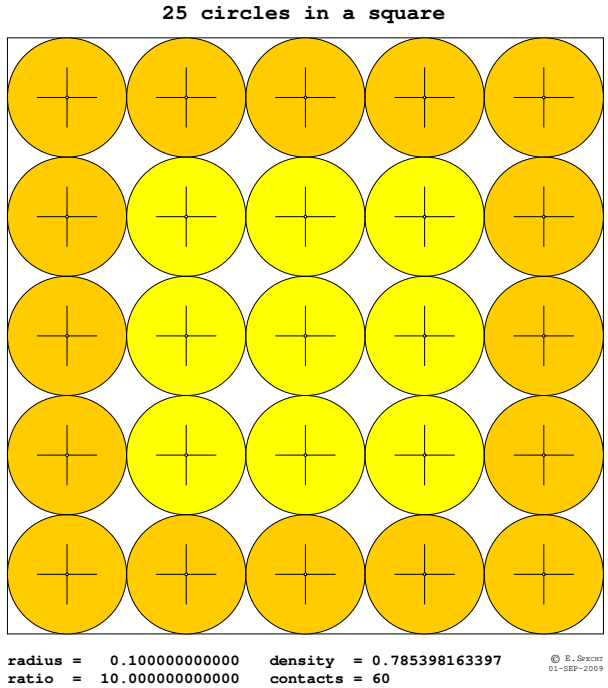
$$d = 2, n = 25$$



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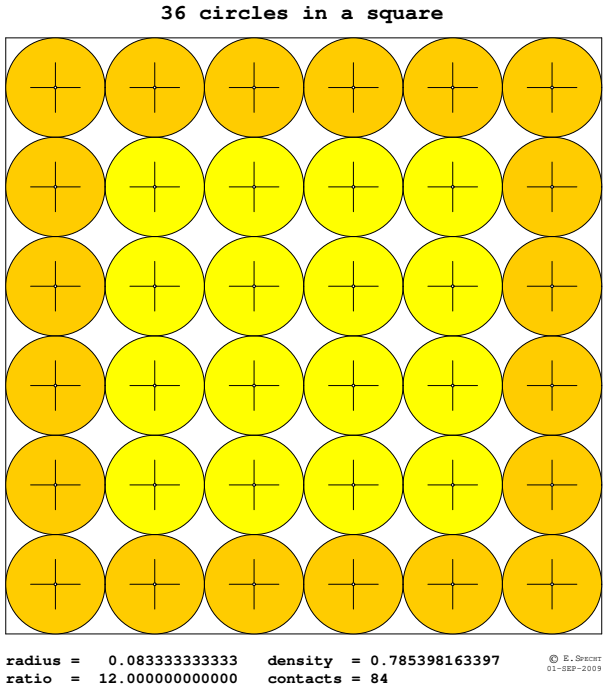

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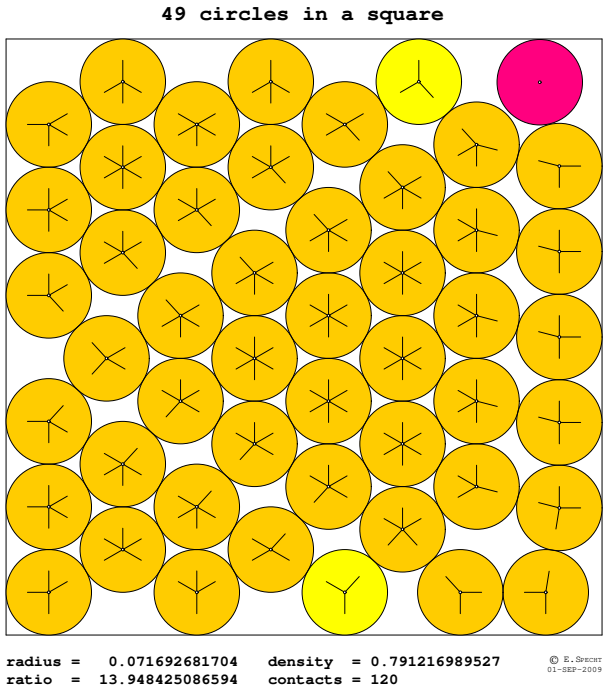
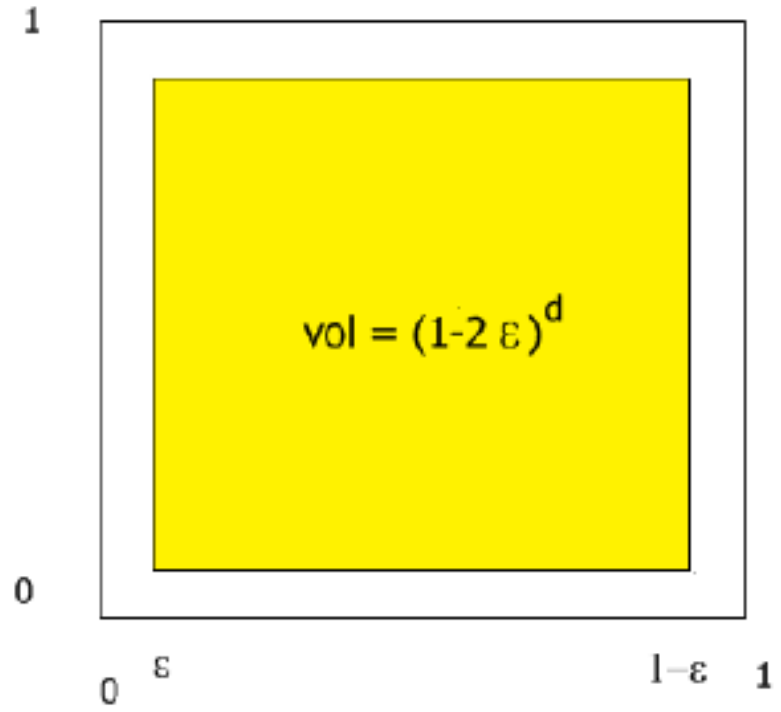
$$d = 2, n = 49$$



Cube packing is much easier! (see § 3.1)

d) Curse of dimensionality: when $d \to \infty$, all volume of $[0,1]^d$ is along the boundary

$$\mathcal{X} = \mathbb{I}_d \triangleq [0,1]^d$$



For ϵ given, volume of central part $= (1-2\epsilon)^d \to 0$ when $d \to \infty$

Ex: 64 balls in a cube, in 4 regular layers of 16 balls

$\to$ 56 touch the boundary!

e) Another issue related to dimension: big difference between a cube and a ball for large d (see (Blum et al., 2016, Chap. 2))

➤ Unit cube $\mathcal{K}_d(\mathbf{0}, 1) = [-1/2, 1/2]^d$: volume $= 1$, max distance between 2 points $= \sqrt{d}$

➤ Unit ball $\mathscr{B}_d(\mathbf{0}, 1)$: volume $= \pi^{d/2}/\Gamma(d/2+1) \to 0$ (quickly) as $d \to \infty$, max distance between 2 points $= 2$

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$\text{vol}[\mathcal{K}_d(\mathbf{0}, 1) \setminus \mathscr{B}_(\mathbf{0}, 1)] \to 1$ as $d \to \infty$, but $\mathscr{B}_d(\mathbf{0}, 1) \not\subset \mathcal{K}_d(\mathbf{0}, 1)$! (the centers of faces are always at distance $1/2$ from$\mathbf{0}$)

$\Longrightarrow$ For large d, working within a cube is much more difficult than working within a ball

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We shall lower our ambitions: finding an optimal design is extremely difficult, we shall only try to find "reasonable" designs

1.2 Latin hypercubes

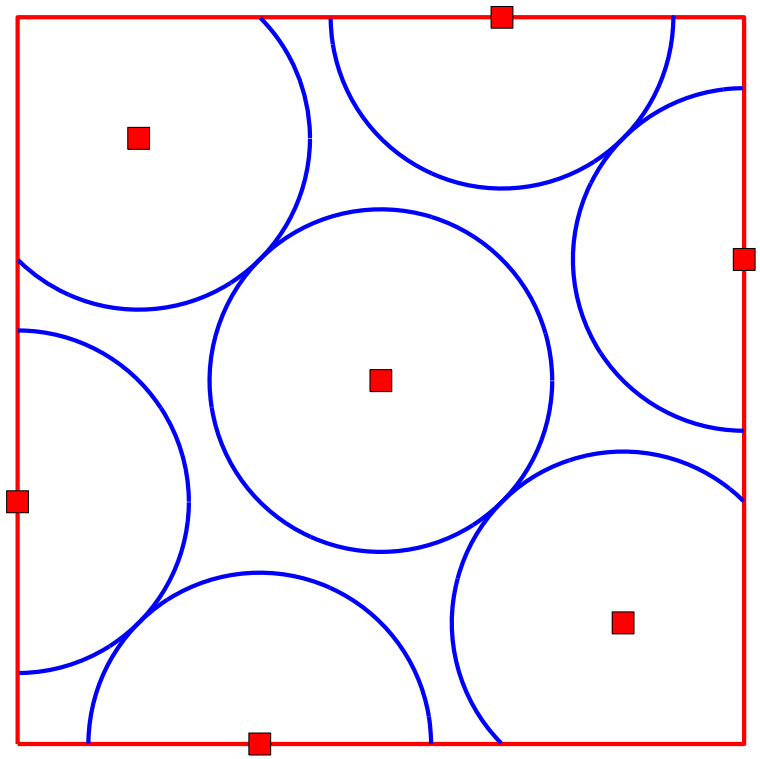
Objective: ensure good projection properties along each principal axis

each 1d projection is Maximin-optimal

$\{\mathbf{x}_i\}_\ell \in \{0, \frac{1}{n-1}, \ldots, \frac{k-1}{n-1}, \ldots, 1\}$ for all $\ell = 1, \ldots, d$

➠ only $(n!)^{d-1}$ possible designs

Maximin-optimal Lh ($d = 2, n = 7$, radius=$\phi_{Mm}(\mathbf{X}_n)/2$)



1.2 Latin hypercubes

Objective: ensure good projection properties along each principal axis

each 1d projection is Maximin-optimal

$\{\mathbf{x}_i\}_\ell \in \{0, \frac{1}{n-1}, \ldots, \frac{k-1}{n-1}, \ldots, 1\}$ for all $\ell = 1, \ldots, d$

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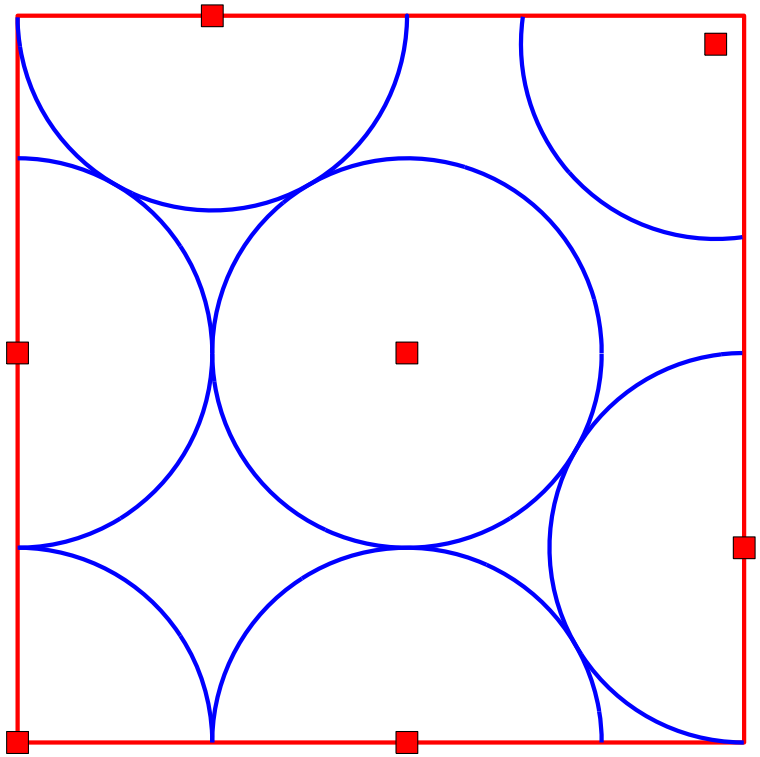
Maximin-optimal, not Lh, ($d = 2, n = 7$, radius=$\phi_{Mm}(\mathbf{X}_n)/2$)



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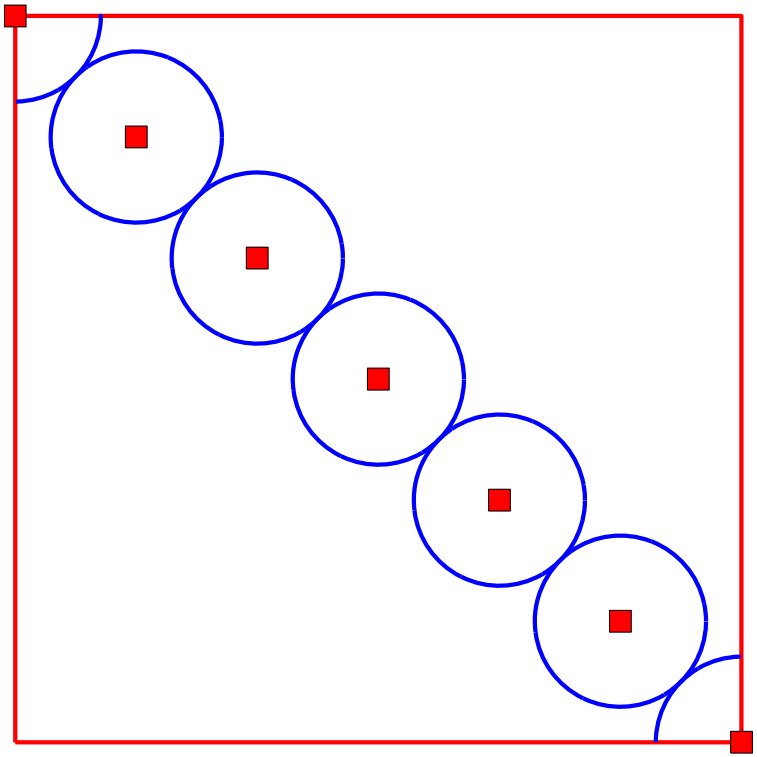

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➠ Optimizing within the class of Lh designs ensures good 1d projection properties

Important when $f(\cdot)$ may possibly not depend on some input factors $\{\mathbf{x}\}_\ell$:

➤ no repetition of points a factor is removed
➤ the projection on $d' < d$ components is still a Lh
(but not necessarily with a good distribution of points if $d' > 1$)

Abundant literature since (McKay et al., 1979), see (Viana, 2013)
The Lh constraint worsens the space-filling property

⏩ miniMax

Optimization within the class of Lh designs:

Let $\mathbf{X}_n$ be a n-point Lh design:

- choose a coordinate ℓ (among d)
- choose a pair of points $\mathbf{x}_i$ and $\mathbf{x}_j$ in $\mathbf{X}_n$
- exchange their ℓ-th coordinate
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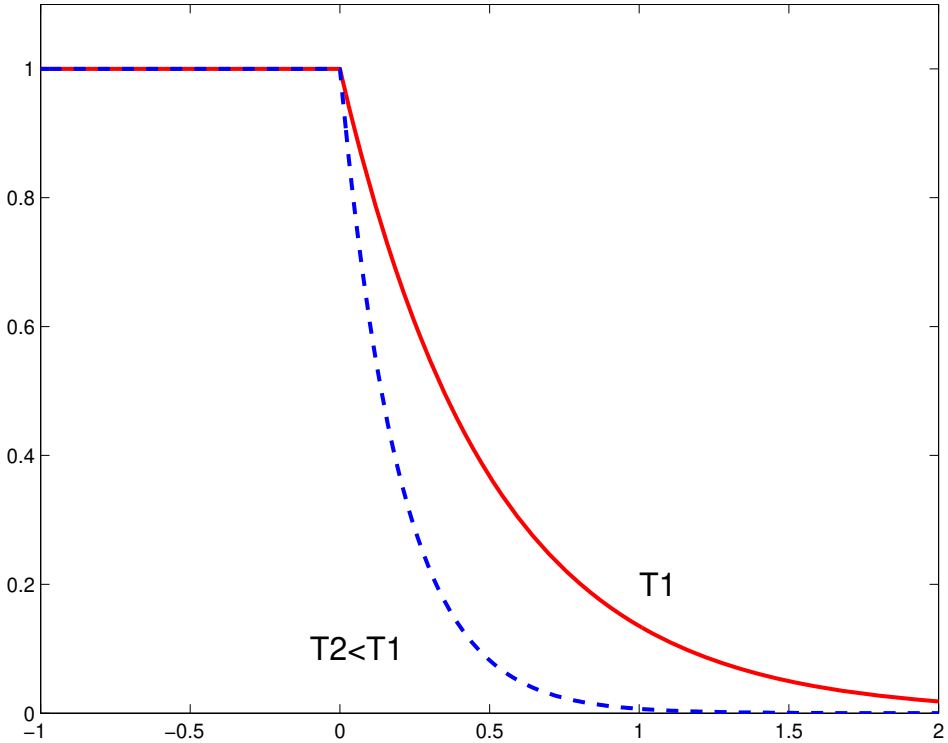
Simulated annealing (minimization of $\Phi(\cdot)$) — principle:

- 0) start from a Lh design $\mathbf{X}_n^0$, set $k = 0$
- 1) generate a Lh design $\mathbf{X}_n^{k+}$ from $\mathbf{X}_n^k$
- 2) calculate $\Delta\Phi_k = \Phi(\mathbf{X}_n^{k+}) - \Phi(\mathbf{X}_n^k)$
- 3) Accept $\mathbf{X}_n^{k+}$, i.e., do $\mathbf{X}_n^{k+1} = \mathbf{X}_n^{k+}$ with probability $P_k = \min\left\{1, \exp\left(-\frac{\Delta\Phi_k}{T_k}\right)\right\}$, keep $\mathbf{X}_n^{k+1} = \mathbf{X}_n^k$ with prob. $1 - P_k$
  $k \leftarrow k+1$, return to 1

$\mathbf{X}_n^{k+}$ such that $\Delta\Phi_k < 0$ is always accepted
$\mathbf{X}_n^{k+}$ such that $\Delta\Phi_k > 0$ is more often accepted for T_1 than for $T_2 < T_1$



➠ Take T_0 large enough (to escape from local optimas),
then decrease T_k (slowly enough)
(for instance, $T_k = \frac{T_0}{\log(k+1)}$,
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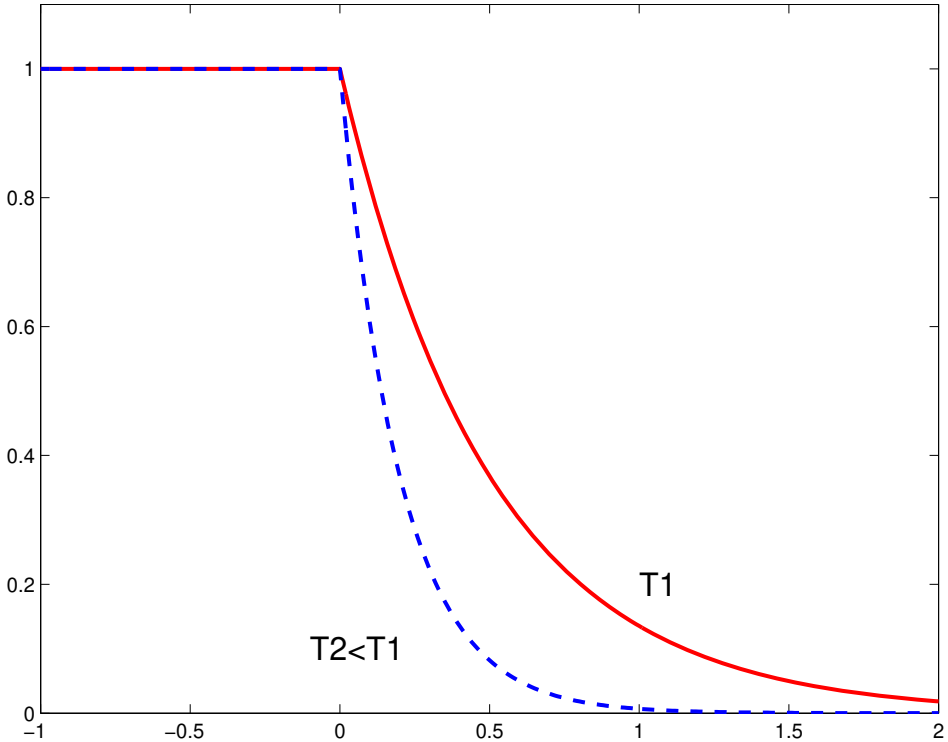

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Many variants, abundant literature...

Always store the best $\mathbf{X}_n^k$ found along the trajectory of the algorithm!!!

➠ Ensures convergence to the optimum when $k \to \infty$ under rather general conditions

1.3 miniMax criterion $\Phi_{mM}(\mathbf{X}_n) = \max_{\mathbf{x}\in\mathscr{X}} \min_i \|\mathbf{x} - \mathbf{x}_i\|$

Φ_{mM} is interesting for approximation:

Any $\mathbf{x}$ in $\mathscr{X}$ is at most at distance Φ_{mM} from a design point $\mathbf{x}_i$

Evaluation of $\Phi_{mM}(X_n) = \max_{\mathbf{x}\in\mathscr{X}} \min_{i=1,\ldots,n} \|\mathbf{x} - \mathbf{x}_i\| = \max_{\mathbf{x}\in\mathscr{X}} d(\mathbf{x}, X_n)$:

we need to find a $\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathscr{X}} d(\mathbf{x}, X_n)$

Key idea: replace $\arg\max_{\mathbf{x}\in\mathscr{X}} d(\mathbf{x}, X_n)$ by $\arg\max_{\mathbf{x}\in\mathscr{X}_Q} d(\mathbf{x}, X_n)$ for a suitable finite $\mathscr{X}_Q \subset \mathscr{X}$

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A/ & B/ Tools from **algorithmic geometry** ($d \lesssim 5$) ➔ exact result through the construction of a suitable $\mathcal{X}_Q$

C/ MCMC $\mathcal{X}_Q =$ adaptive grid

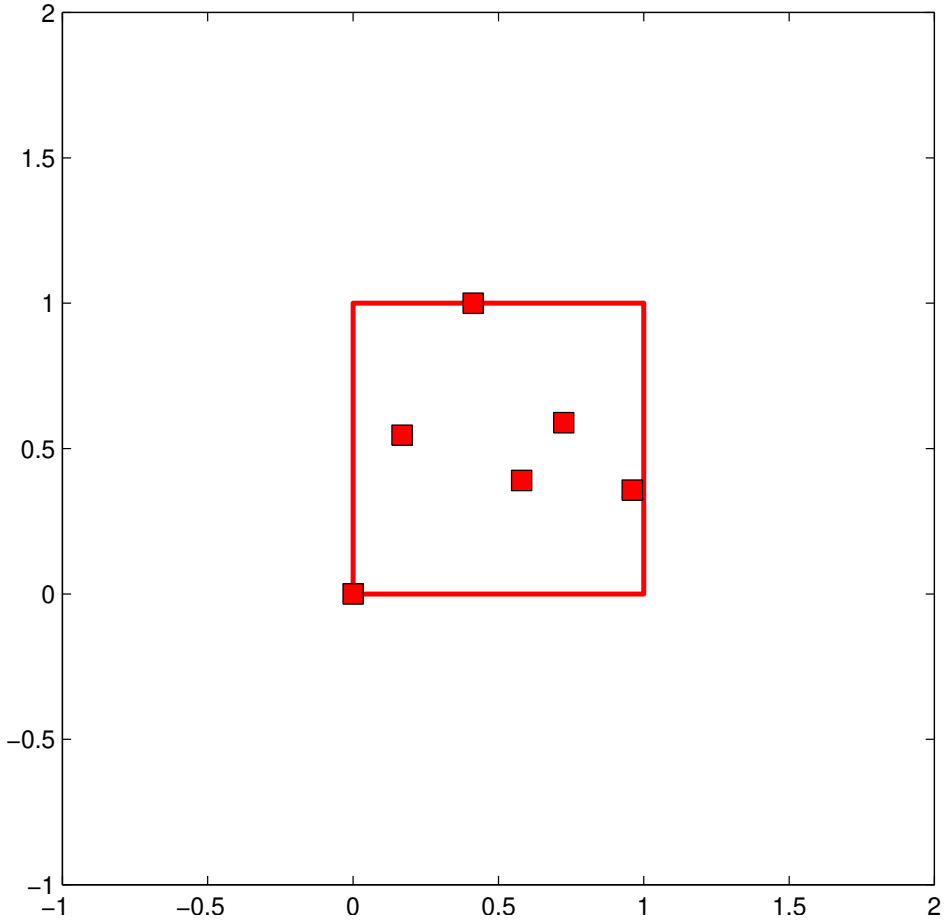
A/ Delaunay triangulation

$\mathscr{X}$ = **hypercube**, see (P. and Müller, 2012)

Delaunay

- $\mathbf{X}_n$ ($= n$ points in $\mathscr{X} = [0,1]^d$), consider X'_m, with $m = (2d+1)n$ points, formed by X_n and its $2d$ reflections through the $(d-1)$-dimensional faces of $\mathscr{X}$
- Compute the Delaunay triangulation of $X'_m \rightarrow$ d-dimensional simplices (each one having $d+1$ vertices), with circumscribed spheres $\mathcal{S}_j$ not containing any point of X'_m in their interior
- $\max_{\mathbf{x} \in \mathscr{X}} d(\mathbf{x}, X_n)$ is attained for $\mathbf{x}$ = centre of one $\mathcal{S}_j$
- Take $\mathscr{X}_Q$ = finite set given by centres of $\mathcal{S}_j$ that belong to $\mathscr{X}$
- $Q = |\mathscr{X}_Q| = \mathcal{O}(m^{\lceil d/2 \rceil})$, computational time $= \mathcal{O}(m^{1+\lceil d/2 \rceil}) \rightarrow$ small d only

$\mathscr{X}_Q = \{$ centres of circumscribed spheres to Delaunay simplices $\}$



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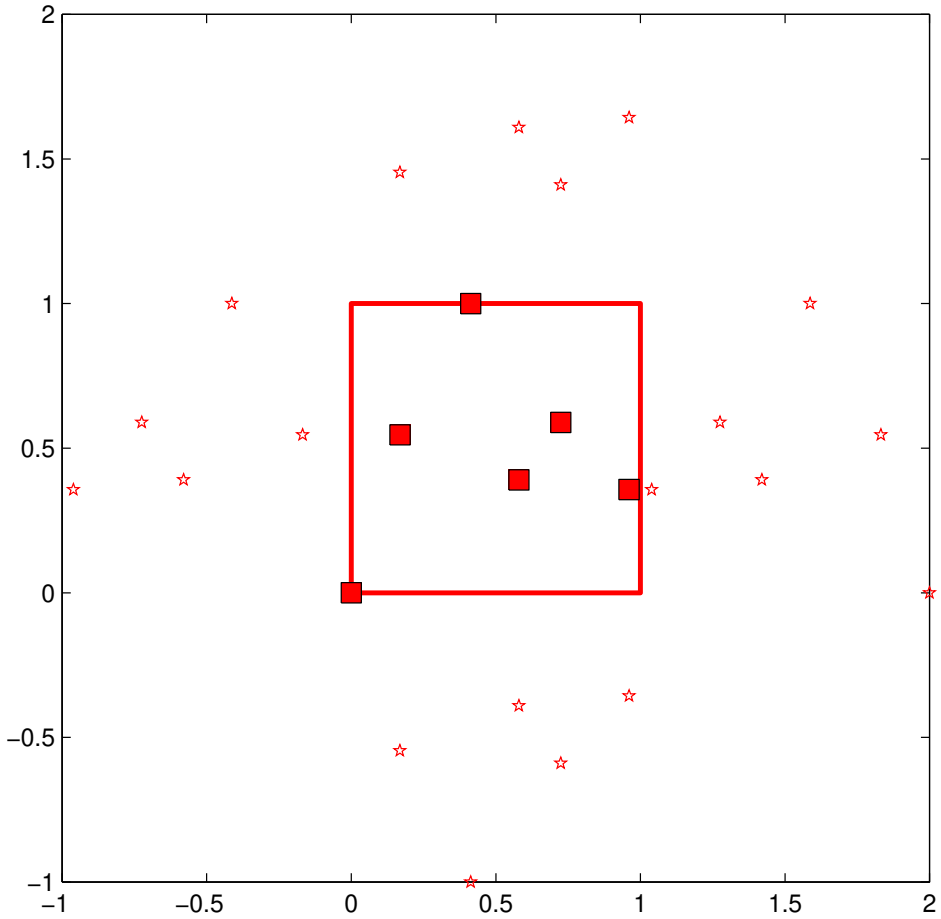

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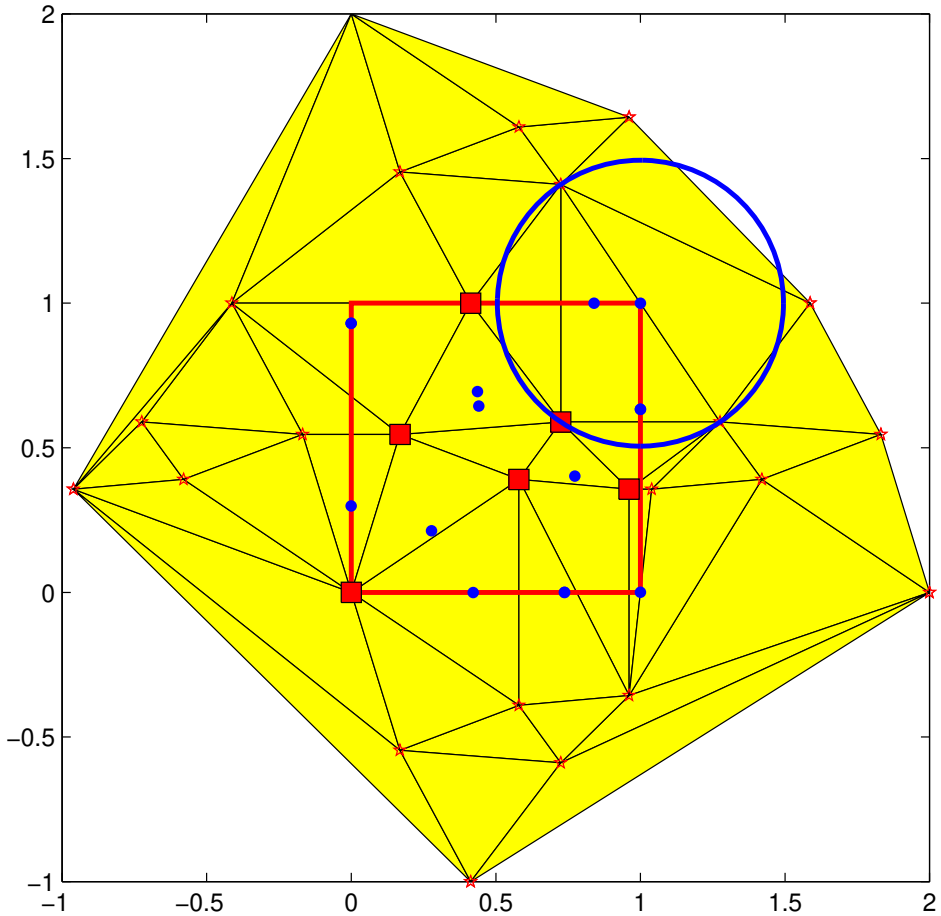


$n = 6$ points, 45 triangles, 12 circles (the largest one is plotted)

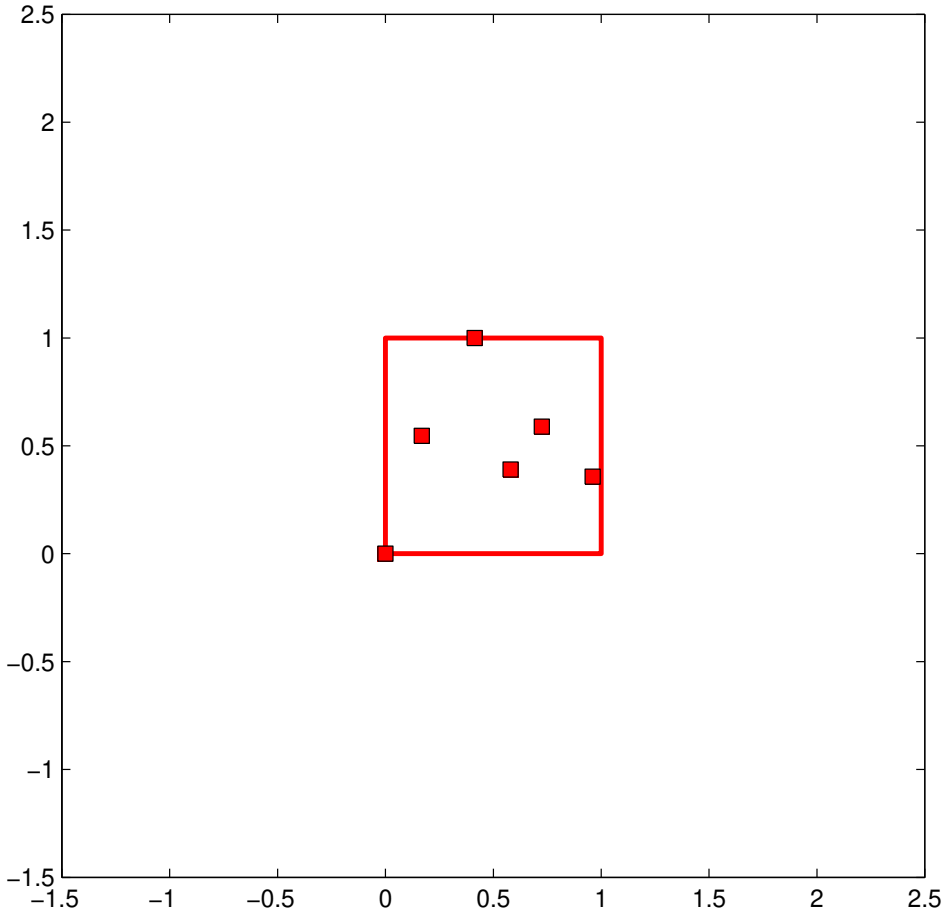
B/ Voronoï tessellation

Voronoï

$\mathscr{X}$ = **polytope in** $\mathbb{R}^d$, see Cortés and Bullo (2005, 2009)

- Partition $\mathbb{R}^d$ into n cells $\mathcal{C}_i$ containing points closest to $\mathbf{x}_i$ than to any other site in X_n
- Each $\mathcal{C}_i$ = convex polyhedron in $\mathbb{R}^d$ (some are open and infinite)
- $\mathscr{X}$ is a polytope of $\mathbb{R}^d \Rightarrow \mathcal{C}_i \cap \mathscr{X}$ = polytope $\rightarrow$ tessellation of $\mathscr{X}$ into n bounded convex polyhedra
- $\max_{\mathbf{x}\in\mathscr{X}} d(\mathbf{x}, X_n)$ is attained when $\mathbf{x}$ is a vertex of one of these polyhedra
- Take $\mathscr{X}_Q$ = collection of these vertices
- $Q = \mathcal{O}(n^{\lceil d/2 \rceil}) \rightarrow$ small d only
- Avoid infinite cells by adding a few (at least $d+1$) generators $\mathbf{x}'_j$ out of $\mathscr{X}$, far enough from $\mathscr{X}$ to ensure that the corresponding cells do not intersect $\mathscr{X}$

$\mathscr{X}_Q = \{$ vertices of Voronoï cells truncated to $\mathscr{X}$ $\}$



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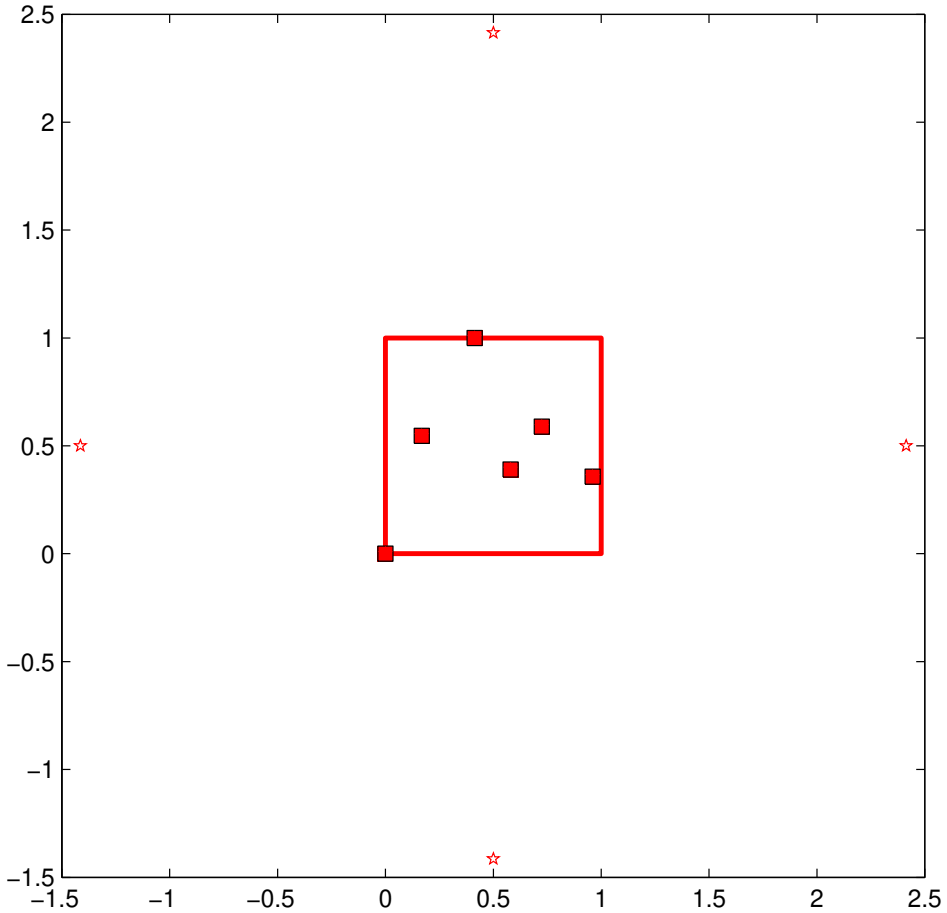

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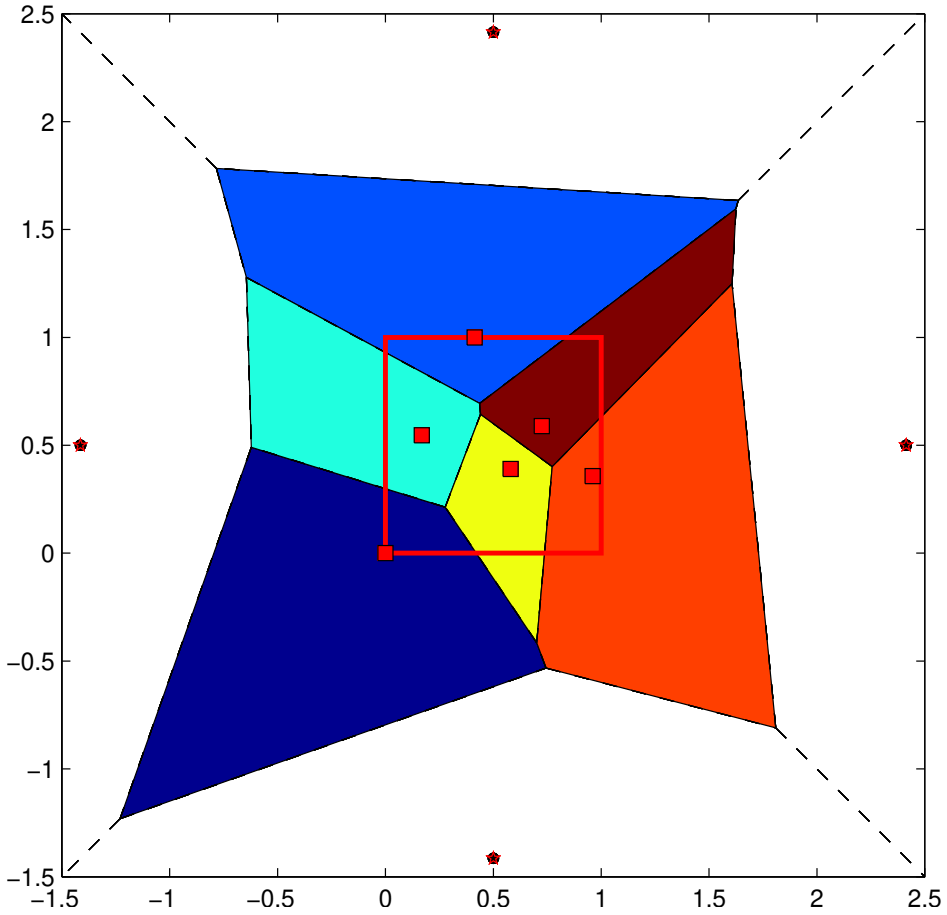

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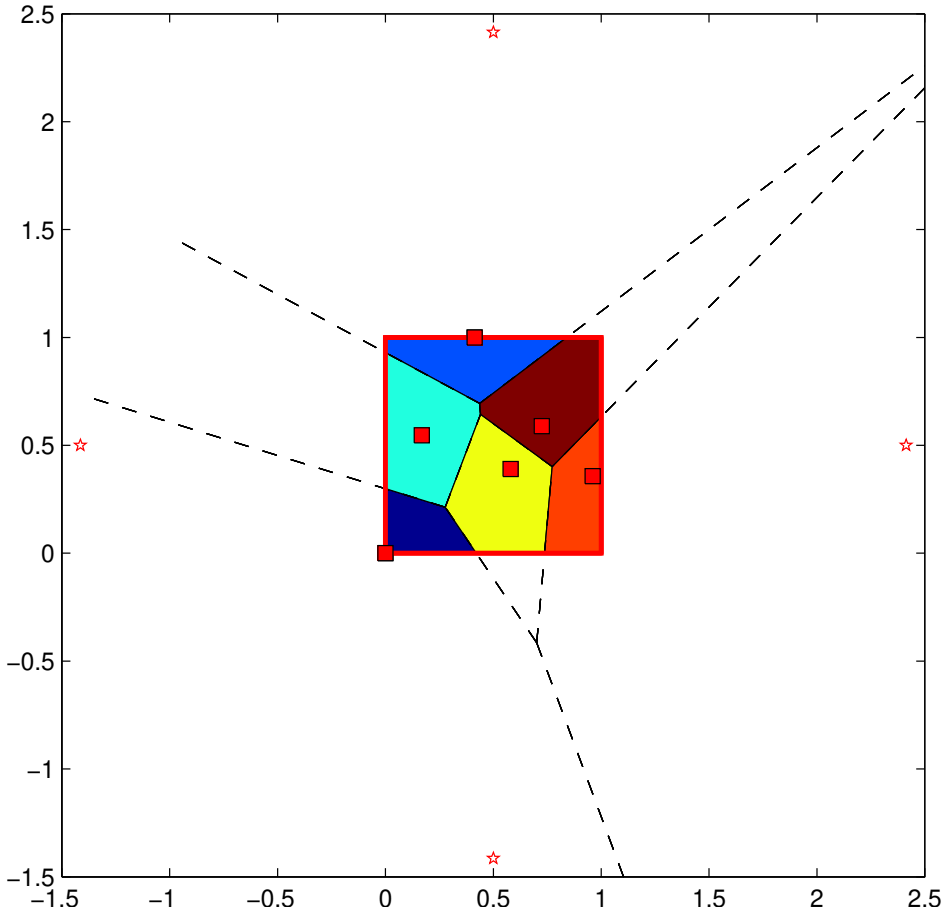

$n = 6$ points, 6 cells, $Q = 14$ vertices $\mathbf{x}^{(k)}$ tested for $\min_i \|\mathbf{x}^{(k)} - \mathbf{x}_i\|$

C/ Estimation via MCMC

2 ideas: extreme-value theory + multilevel splitting

C.a) Borrow results from extreme-value theory used in global optimization (Zhigljavsky and Žilinskas, 2007, Chap. 2), (Zhigljavsky and Hamilton, 2010)

- Q points $\mathbf{x}^{(j)}$ i.i.d. in $\mathscr{X}$, compute the Q distances $d_j = d(\mathbf{x}^{(j)}, X_n)$, associated order statistics $d_{1:Q} \geq d_{2:Q} \geq \cdots \geq d_{Q:Q}$

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$$\widehat{\Phi}_{mM}(X_n) = d_{1:Q} + C_k(d_{1:Q} - d_{k:Q})$$

where $C_k = b_1/(b_k - b_1)$ with $b_i = \Gamma(i + 1/d)/\Gamma(i)$.
Also, the asymptotic confidence level of

$$I_{k,\delta} = \left[d_{1:Q}, d_{1:Q} + \frac{d_{1:Q} - d_{k:Q}}{(1 - \delta^{1/k})^{-1/d} - 1} \right]$$

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- Precise estimation only for very large Q ➠ 2nd idea

C.b) the order statistics $d_{j:Q}$ for large j (small $d_{j:Q}$) are useless

➠ multilevel splitting algorithm

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- Replace all $\mathbf{x}^{(j)}$ at distance d_j from X_n less than some L_ℓ by points sampled independently (and uniformly) in the set $\mathscr{X}(L_\ell) = \{\mathbf{x} \in \mathscr{X} : d(\mathbf{x}, X_n) > L_\ell\}$, for an increasing sequence of levels L_ℓ

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  $\mathbf{x}_{j^*}$ (unique with probability one) such that $d_{j^*} = L_{\ell+1}$ is replaced by a new point sampled in $\mathscr{X}(L_{\ell+1})$
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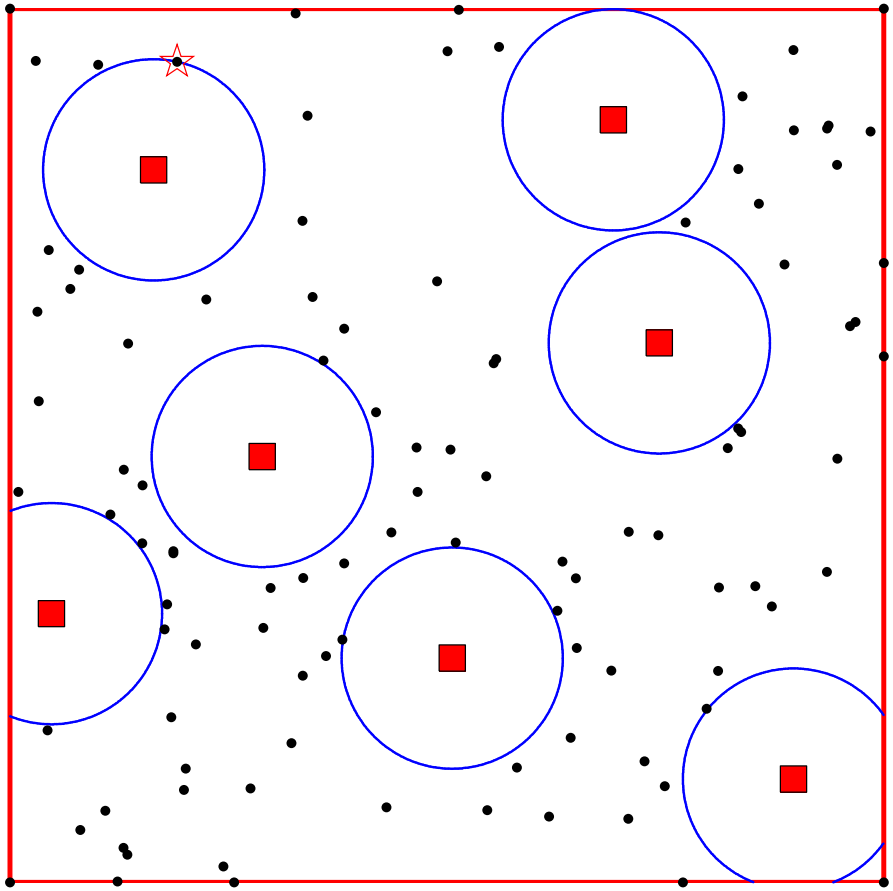
- Sampling ("uniformly") in $\mathscr{X}(L)$ is difficult when L is large: use a MCMC method with Metropolis-Hastings transitions as in (Guyader et al., 2011):
  - first replace $\mathbf{x}_{j^*}$ by a $\mathbf{x}_{j^{**}}$ chosen at random among the other $\mathbf{x}_j$
  - second, perform K successive steps of a random walk $\mathbf{x} \to \text{Proj}_{\mathscr{X}}(\mathbf{x} + \mathbf{z})$, with $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \sigma \mathbf{I}_d)$, accept transition if and only if $d(\mathbf{x} + \mathbf{z}, X_n) > L_{\ell+1} = d_{j^*}$

$\mathbf{x}_{j*}$ such that $d_{j*} = \min_j d_j$



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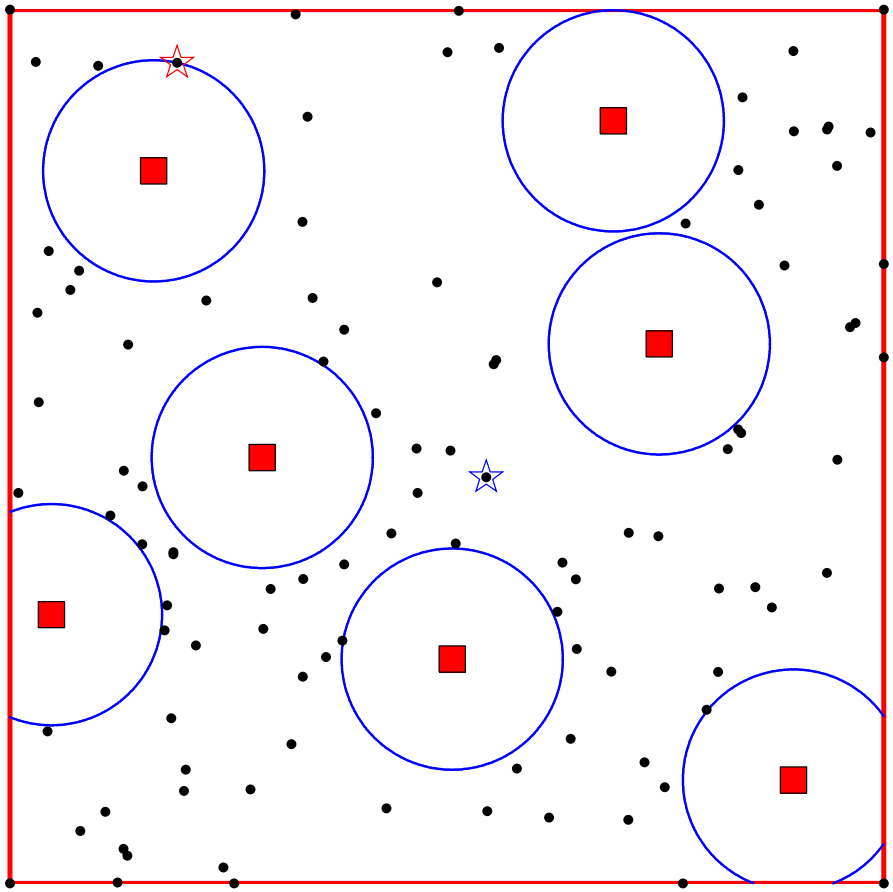
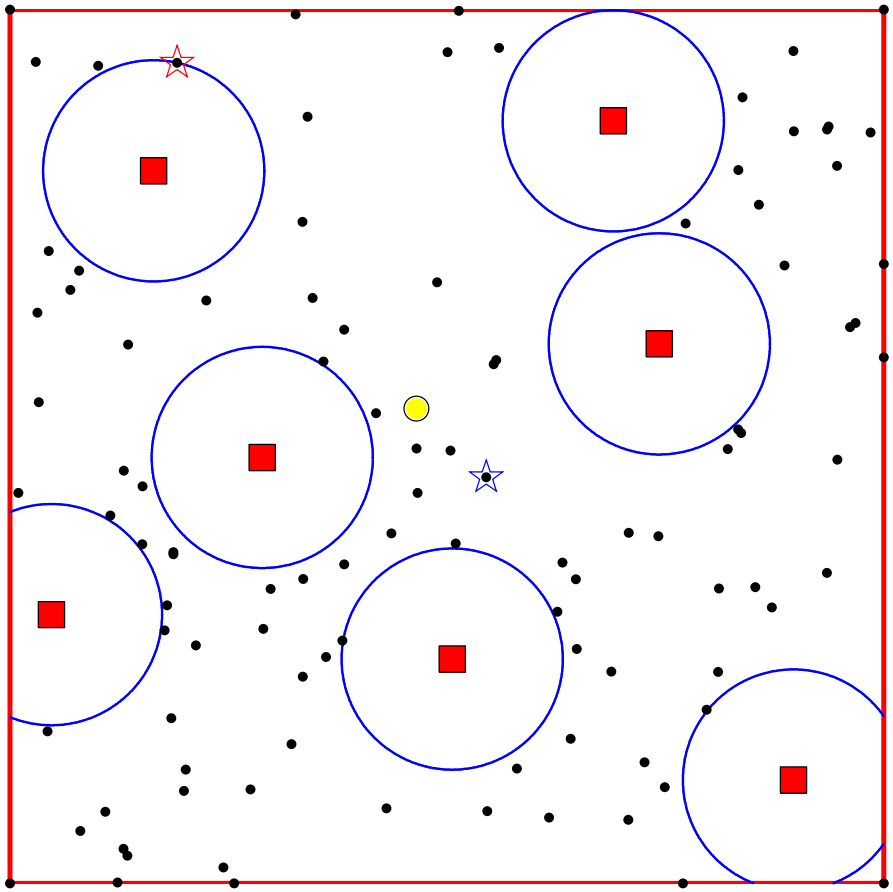
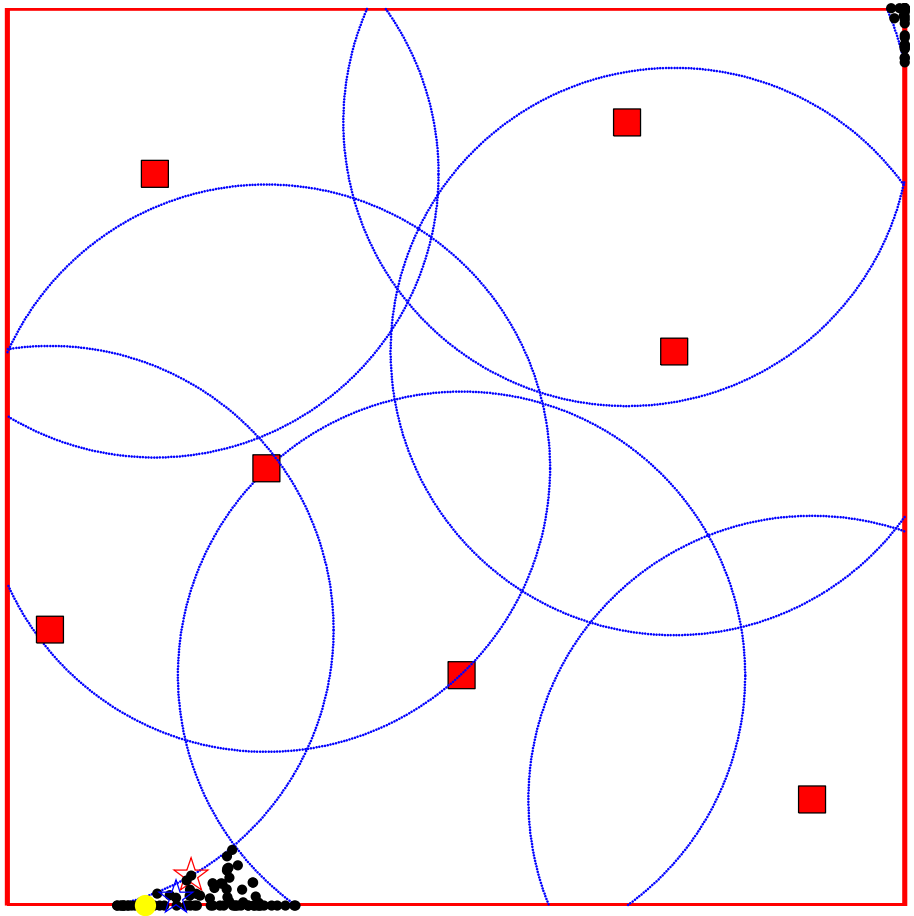


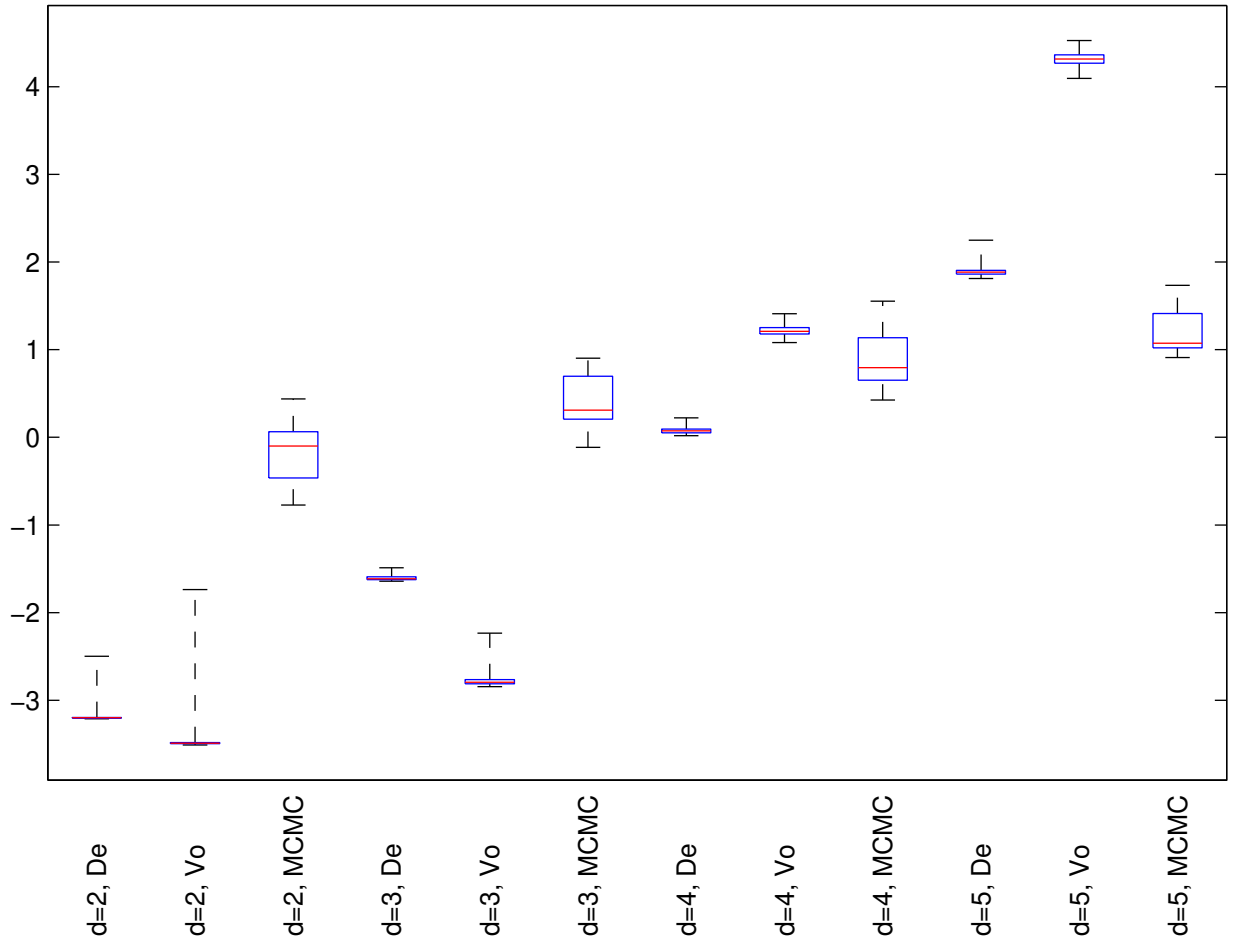
perform K successive steps of random walk



. . . after enough iterations



log(computing time)
$\mathscr{X} = [0,1]^d$, $n = 50$ ($\delta = 0.05$, $\epsilon = 0.001$, $K = 10$, $Q = nd$ for MCMC)



Minimization of $\Phi_{mM}(\mathbf{X}_n) = \max_{\mathbf{x}\in\mathscr{X}} \min_i \|\mathbf{x} - \mathbf{x}_i\|$?

(not convex, non differentiable)

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(not convex, non differentiable)

- 0/ General global optimization method (e.g., simulated annealing): not promising
- A/ Voronoï tessellation + generalized gradient
- B/ `k-means` and centroids
- C/ Stochastic gradient

A/ d (very) small: Voronoï tessellation + generalized gradient
($\Phi_{mM}(\cdot)$ not differentiable, but Lipschitz, with constant 1)

$$X_n^{(k+1)} = X_n^{(k)} - \gamma_k \, \tilde{\nabla}_{\Phi_{mM}}(X_n^{(k)})$$

- $\gamma_k > 0$, $\lim_{k\to\infty} \gamma_k = 0$ and $\sum_k \gamma_k = \infty$
- all columns of $\tilde{\nabla}_{\Phi_{mM}}(X_n^{(k)})$ equal $\mathbf{0}$, except the i-th one equal to $(\mathbf{x}_i - \mathbf{x}^*)/\|\mathbf{x}_i - \mathbf{x}^*\|$, where $\|\mathbf{x}_i - \mathbf{x}^*\| = \Phi_{mM}(X_n)$
  ➠ move $\mathbf{x}_i$ towards $\mathbf{x}^*$

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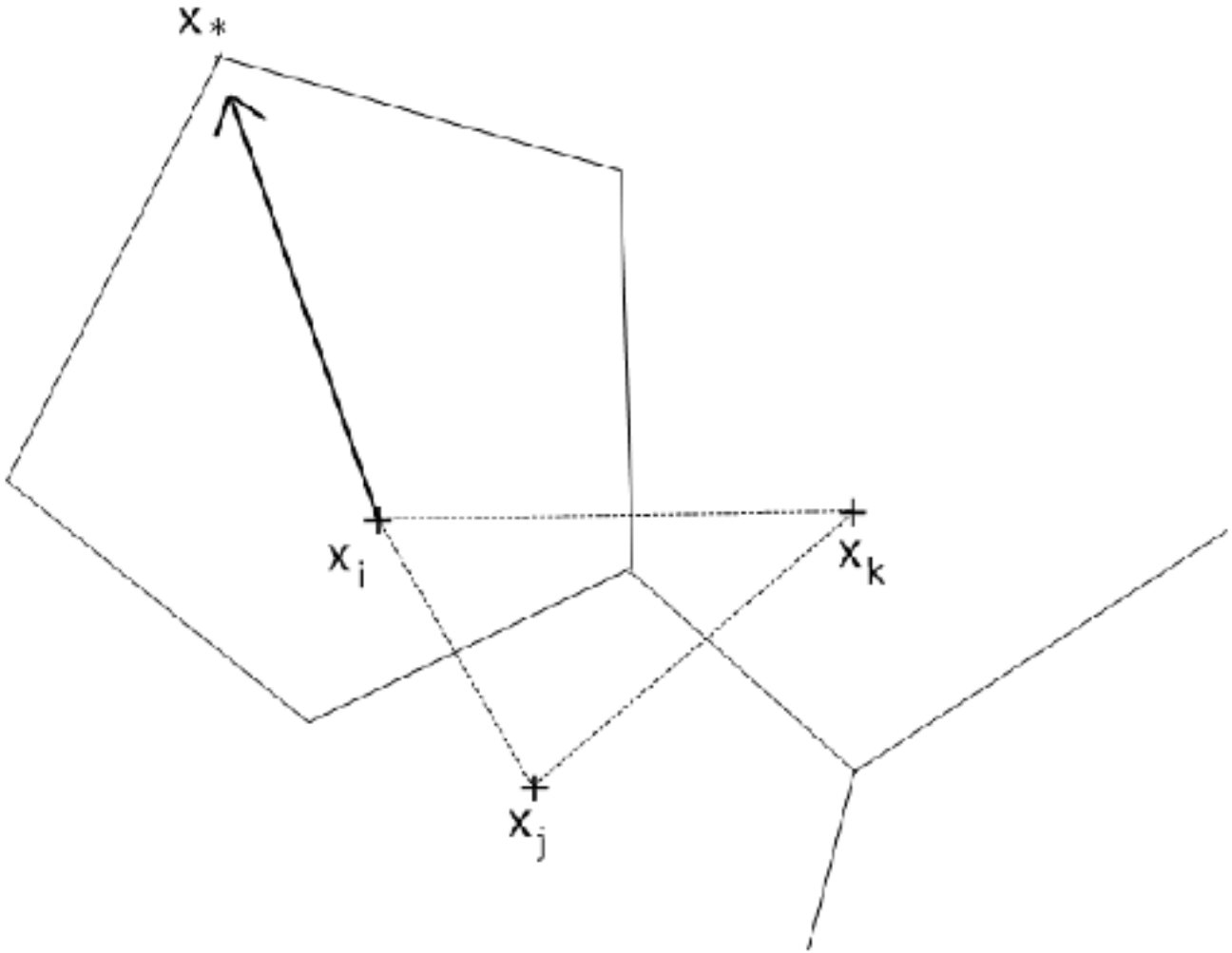
  ➠ move $\mathbf{x}_i$ towards $\mathbf{x}^*$

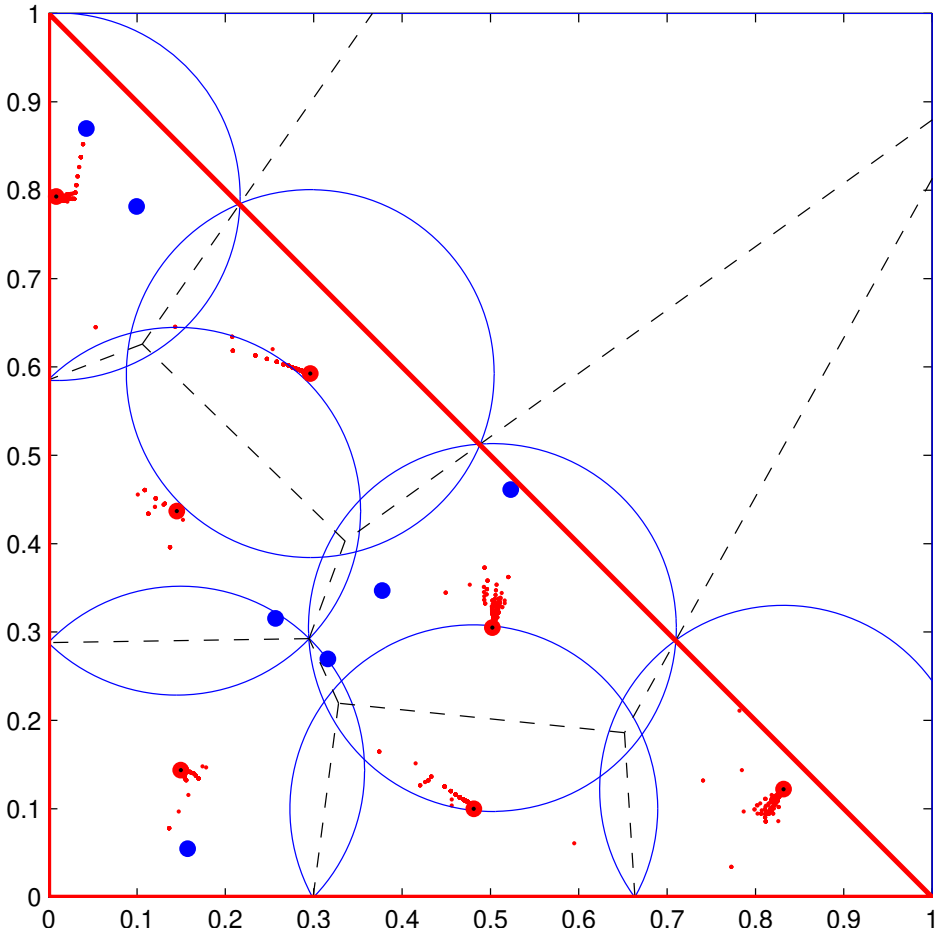
➠ one may also move each $\mathbf{x}_i$ towards the furthest point $\mathbf{x}^{*,i}$ in its Voronoï cell (Cortés and Bullo, 2005, 2009):

$$\mathbf{x}_i^{(k+1)} = \mathbf{x}_i^{(k)} - \gamma_{k,i}(\mathbf{x}_i^{(k)} - \mathbf{x}^{*,i})/\|\mathbf{x}_i^{(k)} - \mathbf{x}^{*,i}\|$$

Voronoï cells can be exact, or obtained by a discretization of $\mathscr{X}$ into a Q-point set $\mathscr{X}_Q$


x*
x_i
x_k
x_j

Ex: $\mathscr{X} =$ simplex $0 \leq x_1,\ 0 \leq x_2,\ x_1 + x_2 \leq 1,\ n = 7$ (radii $= \Phi_{mM}(\mathbf{X}_n)$)



B/ `k-means` and centroids

Minimize the L_2 energy functional

$$\mathcal{E}_2(\mathcal{T}_n, X_n) = \int_{\mathscr{X}} \left(\sum_{i=1}^{n} I_{\mathcal{C}_i}(\mathbf{x}) \, \|\mathbf{x} - \mathbf{x}_i\|^2 \right) \mathrm{d}\mathbf{x} = \sum_{i=1}^{n} \int_{\mathcal{C}_i} \|\mathbf{x} - \mathbf{x}_i\|^2 \, \mathrm{d}\mathbf{x}$$

where $\mathcal{T}_n = \{\mathcal{C}_i, \, i = 1, \ldots, n\}$ is a tessellation of $\mathscr{X}$

$I_{\mathcal{C}_i}$ = indicator function of $\mathcal{C}_i$

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where $\mathcal{T}_n = \{\mathcal{C}_i, \, i = 1, \ldots, n\}$ is a tessellation of $\mathscr{X}$
$I_{\mathcal{C}_i}$ = indicator function of $\mathcal{C}_i$

Then (Du et al., 1999):

- $\mathcal{C}_i = \mathcal{V}(\mathbf{x}_i)$ = Voronoï region for the site $\mathbf{x}_i$, for all i
  $(\Rightarrow \mathcal{E}_2(\mathcal{T}_n, X_n) = \int_{\mathscr{X}} d^2(\mathbf{x}, X_n) \, \mathrm{d}\mathbf{x})$
- simultaneously $\mathbf{x}_i$ = centroid of $\mathcal{C}_i$ (center of gravity) for all i:
  $\mathbf{x}_i = (\int_{\mathcal{C}_i} \mathbf{x} \, \mathrm{d}\mathbf{x})/\mathrm{vol}(\mathcal{C}_i)$

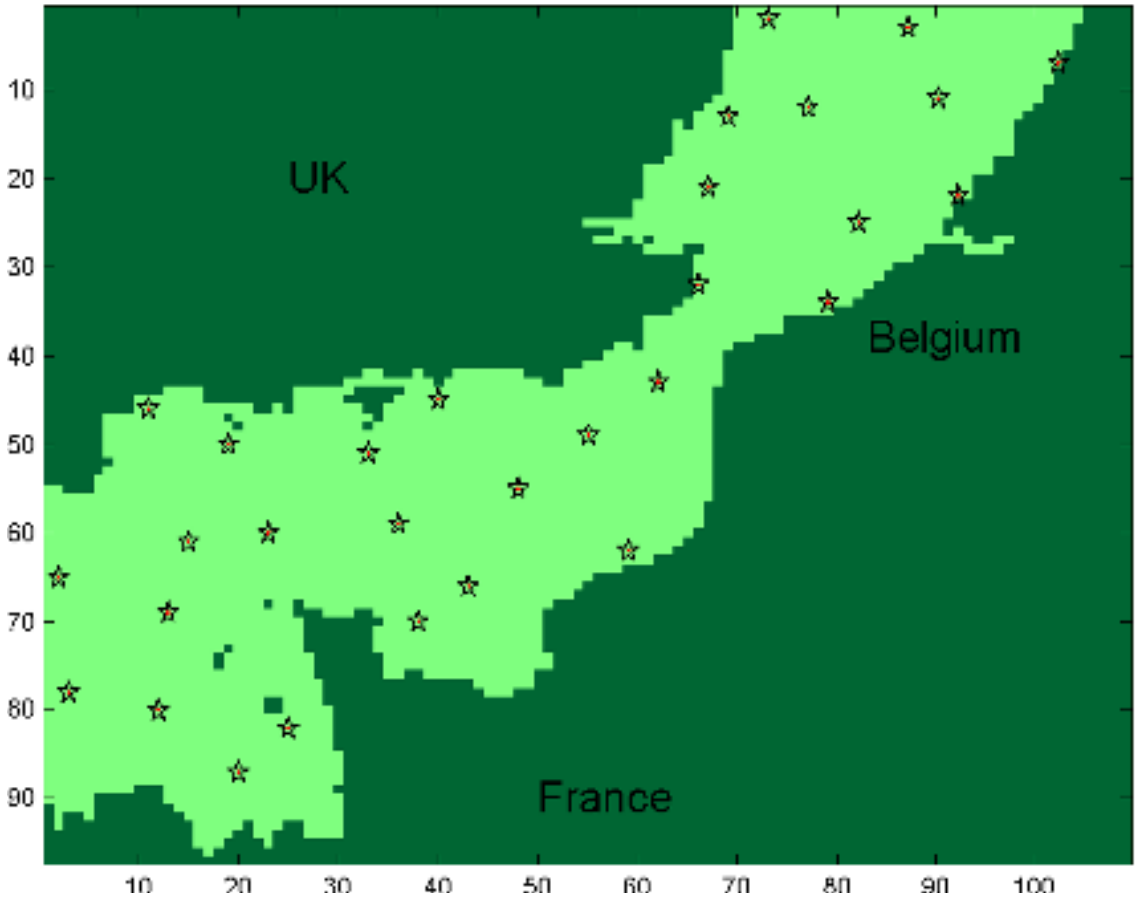
→ such a X_n should thus perform reasonably well in terms of space-filling (Lekivetz and Jones, 2015)

Lloyd's method (1982): (= fixed-point iterations)

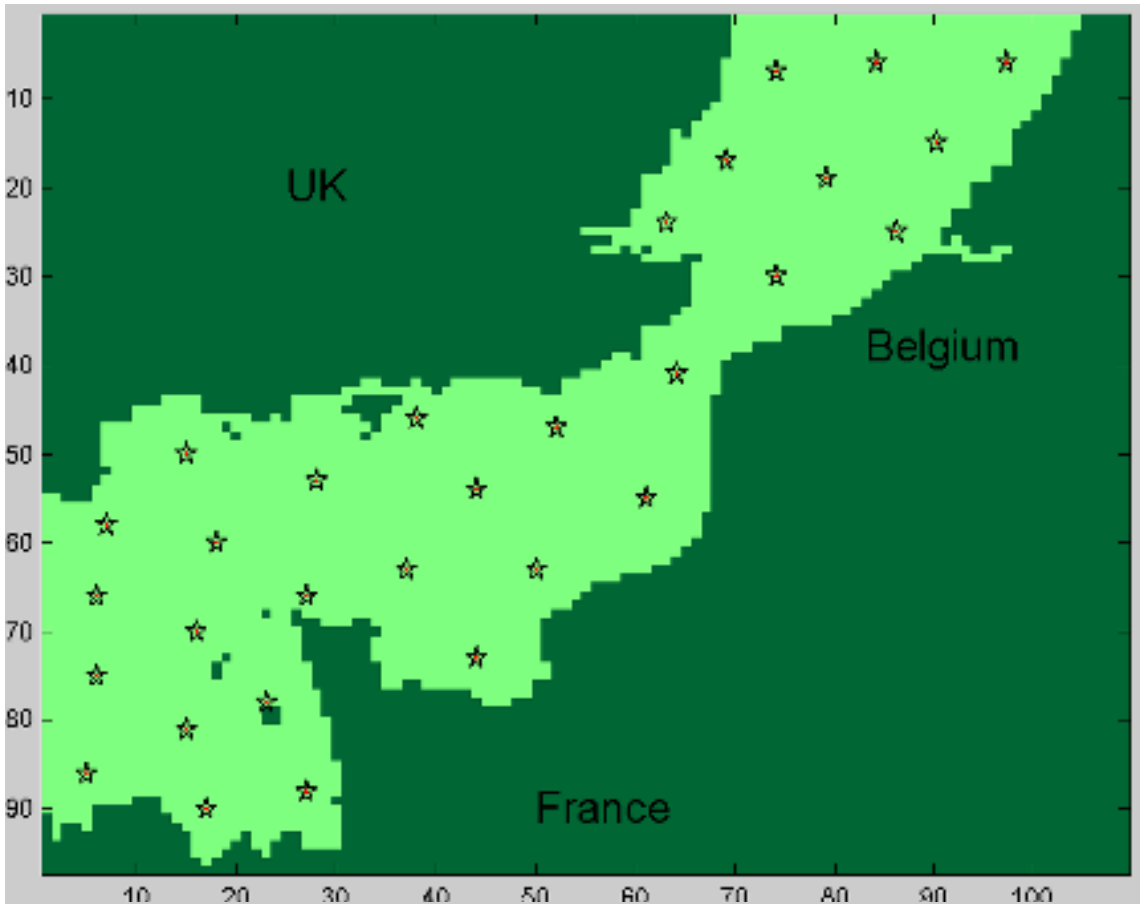
→ Move each $\mathbf{x}_i$ to the centroid of its own Voronoï cell, repeat ...

➠ Algorithmic geometry (Voronoï tessellation) if d very small,
use a finite set $\mathscr{X}_Q$ otherwise

30 points from Sobol' LDS



`k-means` clustering (30 clusters) of 1,000 point from Sobol' LDS



However... minimax-optimal design is related to the construction of a centroidal tessellation for

$$\mathcal{E}_q(\mathcal{T}_n, X_n) = \int_{\mathscr{X}} \left(\sum_{i=1}^{n} I_{\mathcal{C}_i}(\mathbf{x}) \, \|\mathbf{x} - \mathbf{x}_i\|^q \right) \mathrm{d}\mathbf{x} = \sum_{i=1}^{n} \int_{\mathcal{C}_i} \|\mathbf{x} - \mathbf{x}_i\|^q \, \mathrm{d}\mathbf{x}$$

for $q \to \infty$ (see (Mak and Joseph, 2016))

➠ use Chebyshev centers

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$$\mathcal{E}_q(\mathcal{T}_n, X_n) = \int_{\mathcal{X}} \left(\sum_{i=1}^{n} l_{\mathcal{C}_i}(\mathbf{x}) \, \|\mathbf{x} - \mathbf{x}_i\|^q \right) \mathrm{d}\mathbf{x} = \sum_{i=1}^{n} \int_{\mathcal{C}_i} \|\mathbf{x} - \mathbf{x}_i\|^q \, \mathrm{d}\mathbf{x}$$

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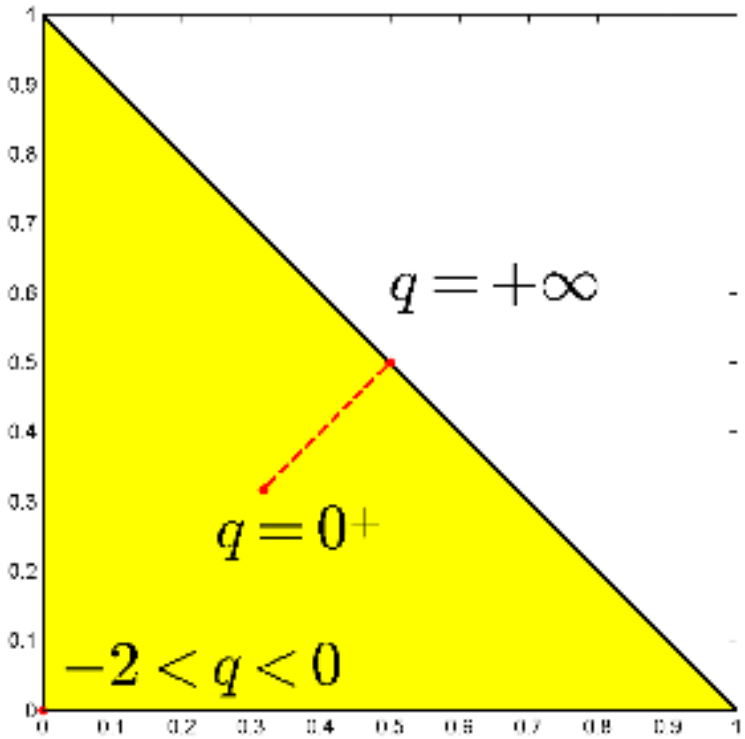
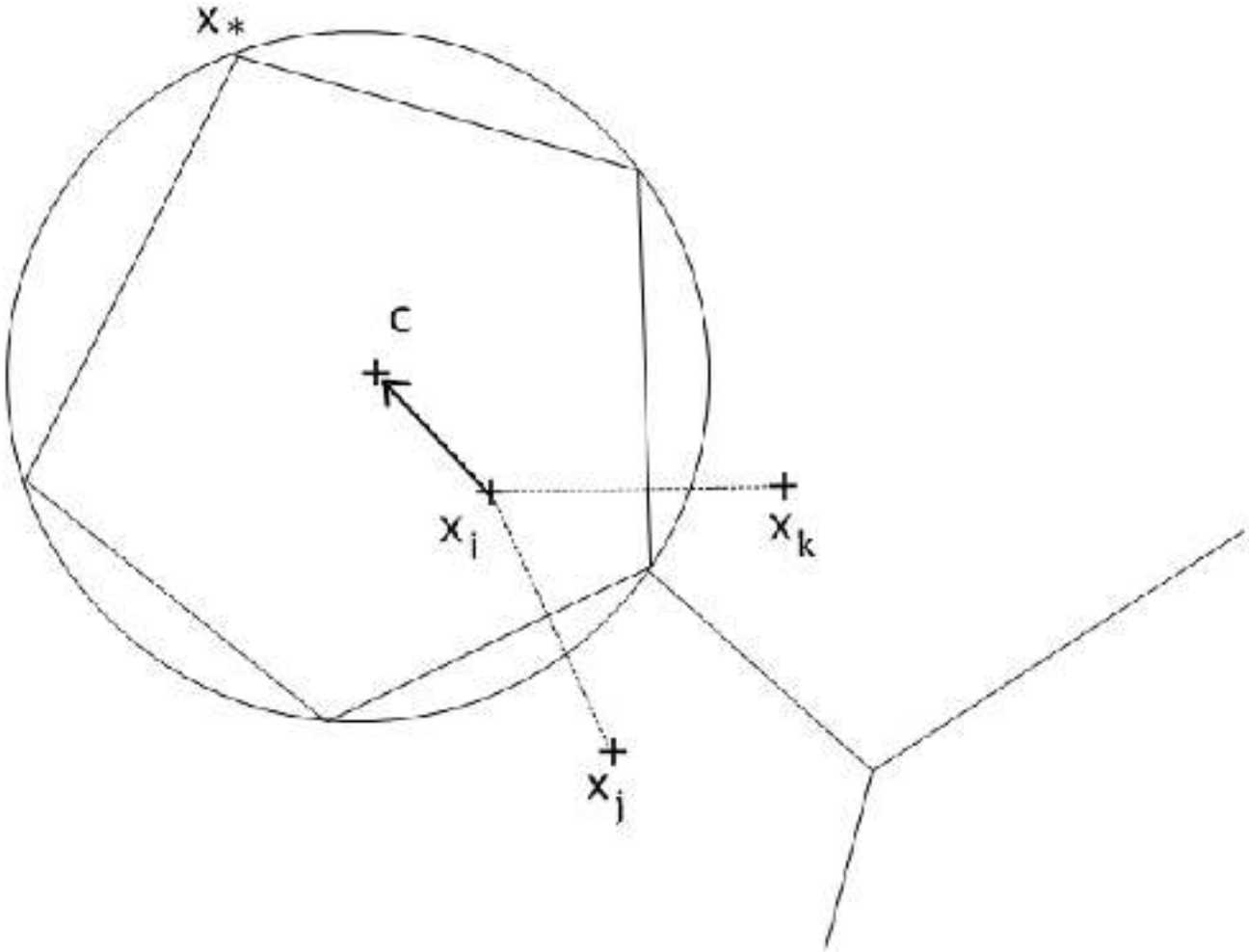


Variant of Lloyd's method:

0) Select $X_n^{(1)}$ and $\epsilon \ll 1$, set $k = 1$
1) Compute the Voronoï tessellation $\{\mathcal{V}_i,\ i = 1, \ldots, n\}$ of $\mathscr{X}$ (or $\mathscr{X}_Q$) based on $X_n^{(k)}$
2) For $i = 1, \ldots, n$
   ➤ determine the smallest ball $\mathscr{B}(\mathbf{c}_i, r_i)$ enclosing $\mathcal{V}_i$ (= convex QP problem)
   ➤ replace $\mathbf{x}_i$ by $\mathbf{c}_i$ in $X_n^{(k)}$ (Chebyshev center of $\mathcal{V}_i$)
3) if $\Phi_{mM}(\mathbf{X}_n^{(k)}) - \Phi_{mM}(\mathbf{X}_n^{(k+1)}) < \epsilon$, then stop; otherwise $k \leftarrow k + 1$, return to step 1

→ Move each $\mathbf{x}_i$ to the Chebyshev center of its own Voronoï cell, repeat ...

[$\Phi_{mM}(\mathbf{X}_n^{(k)})$ decreases monotonically, convergence to a local minimum (or a saddle point)]


x*
c
x_i
x_k
x_j

Determination of the smallest enclosing ball containing $\mathcal{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$
(vertices of a Voronoï cell, points of $\mathscr{X}_Q$ closest to $\mathbf{x}_i$):

$$\Leftrightarrow \text{ minimize } f(\mathbf{c}) = \max_{i=1,\ldots,N} \|\mathbf{z}_i - \mathbf{c}\|^2 \text{ with respect to } \mathbf{c} \in \mathbb{R}^d$$

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Direct problem = convex QP

Take any $\mathbf{c}_0 \in \mathbb{R}^d$, minimize $\|\mathbf{c} - \mathbf{c}_0\|^2 + t$

with respect to $(\mathbf{c}, t) \in \mathbb{R}^{d+1}$,

subject to $\|\mathbf{z}_i - \mathbf{c}_0\|^2 - 2(\mathbf{z}_i - \mathbf{c}_0)^\top(\mathbf{c} - \mathbf{c}_0) \leq t\,, \;\; i = 1, \ldots, N$

(N linear constraints)

Determination of the smallest enclosing ball containing $\mathcal{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$

Dual problem = similar to an optimal design problem:

maximize $\mathrm{trace}[\mathbf{V}(\xi)]$, with ξ a prob. measure on $\mathcal{Z}$,

$\mathbf{V}(\xi)$ = covariance matrix for ξ

center of the ball = $\mathbf{c}(\xi) = \int_{\mathcal{Z}} \mathbf{z}\, \xi(\mathrm{d}\mathbf{z})$

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→ Algorithms of the exchange-type (Yildirim, 2008)
(≈ Fedorov algorithm for D-optimal design: optimal step length is available)

→ One can remove inessential points from $\mathcal{Z}$: (P., 2017c)

➠ Combine this with the use of a standard QP solver for the direct problem

C/ Stochastic gradient (P., 2017)

d **is large**: Lloyd's algorithm cannot be used (computational geometry is too complicated, regular grids or LDS are not dense enough)

$$\text{minimize } \mathcal{E}_q{}^*(X_n) = \int_{\mathscr{X}} \left(\sum_{i=1}^{n} l_{\mathcal{V}_i}(\mathbf{x}) \, \|\mathbf{x} - \mathbf{x}_i\|^q \right) \mathrm{d}\mathbf{x}$$

with $\mathcal{V}_i$ = Voronoï region for the site $\mathbf{x}_i$

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with $\mathcal{V}_i$ = Voronoï region for the site $\mathbf{x}_i$

→ Stochastic gradient algorithm:
(MacQueen, 1967) for $q = 2$, (Cardot et al., 2012) for $q = 1$

0) $k = 1$, $X_n^{(1)}$, set $n_{i,0} = 0$ for all $i = 1, \ldots, n$

1) sample X uniformly distributed in $\mathscr{X}$

2) find $i^* = \arg\min_{i=1,\ldots,n} \|X - \mathbf{x}_i^{(k)}\|$, $n_{i^*,k} \leftarrow n_{i^*,k} + 1$ $\quad [\leftarrow X \in \text{cell } \mathcal{V}_i^*]$

3) $\mathbf{x}_{i^*}^{(k+1)} = \mathbf{x}_{i^*}^{(k)} - \gamma_{i^*,k} \underbrace{q\|X - \mathbf{x}_{i^*}^{(k)}\|^{q-2} (\mathbf{x}_{i^*}^{(k)} - X)}_{=\text{gradient}}$, $k \leftarrow k + 1$,

return to step 1, stop when $k = K$

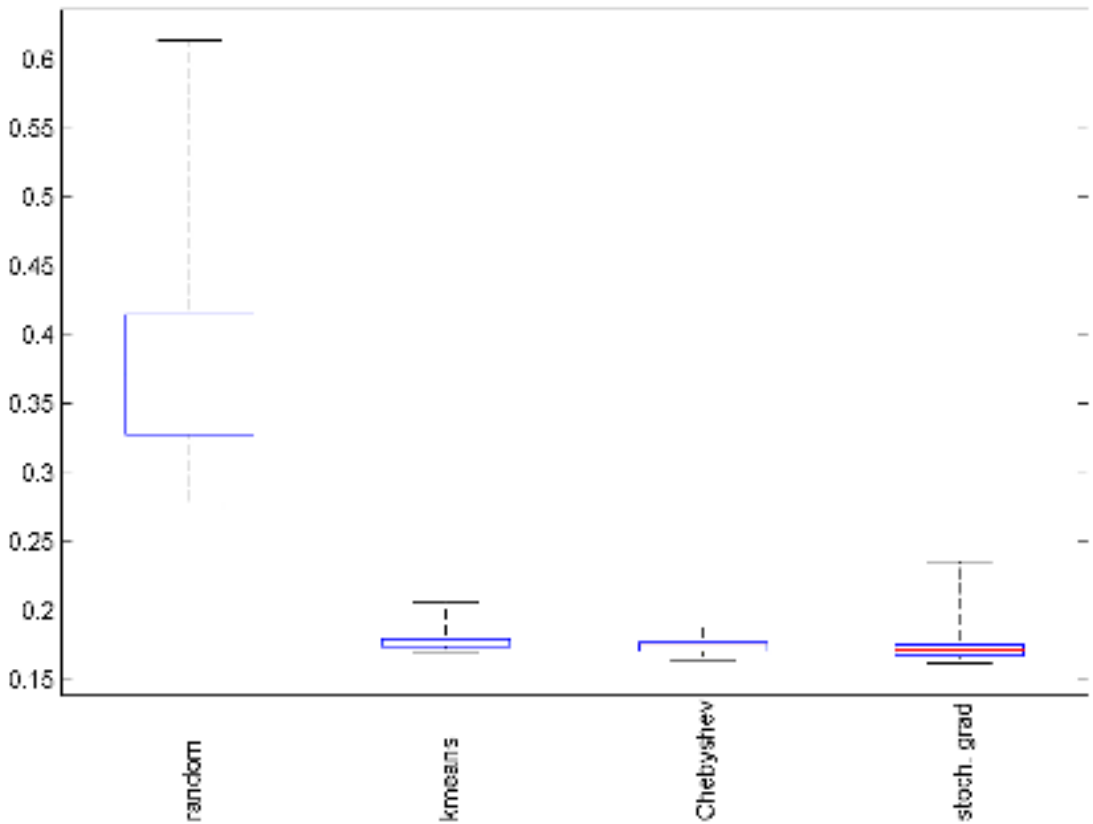
- Typical choice for $\gamma_{i^*,k} = c/n_{i^*,k}^{\alpha}$, with $\alpha \in (1/2, 1]$
  and consider $\widehat{X}_n = \frac{1}{K} \sum_{k=1}^{K} X_n^{(k)}$ when $\alpha < 1$
- Little information to store (no grid or other finite approximation of $\mathscr{X}$)
  $\rightarrow$ can also be used with large d

Example: $n = 10\,d$

all methods are initialized at the same random design, 100 repetitions

`k-means` and Lloyd's method with Chebyshev centers use 2^{d+8} points from a LDS (Sobol')

$$d = 2,\ n = 20$$



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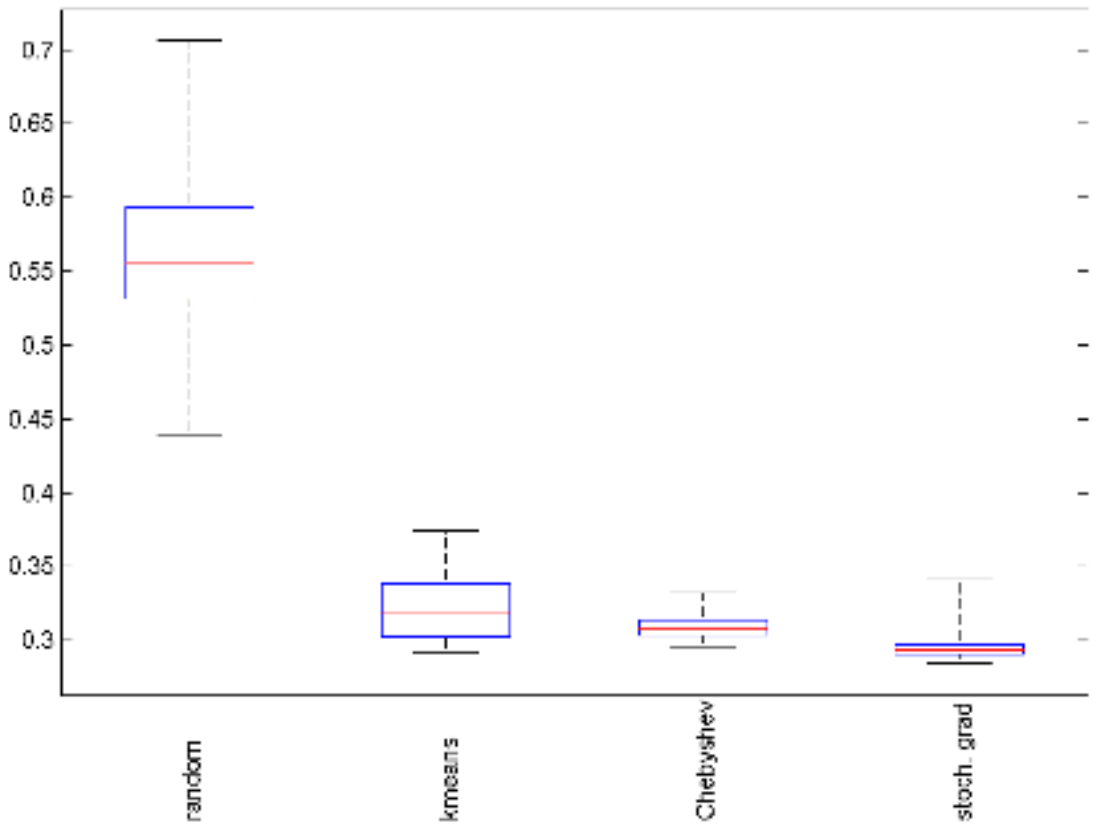
$$d = 3,\ n = 30$$



Example: $n = 10\,d$

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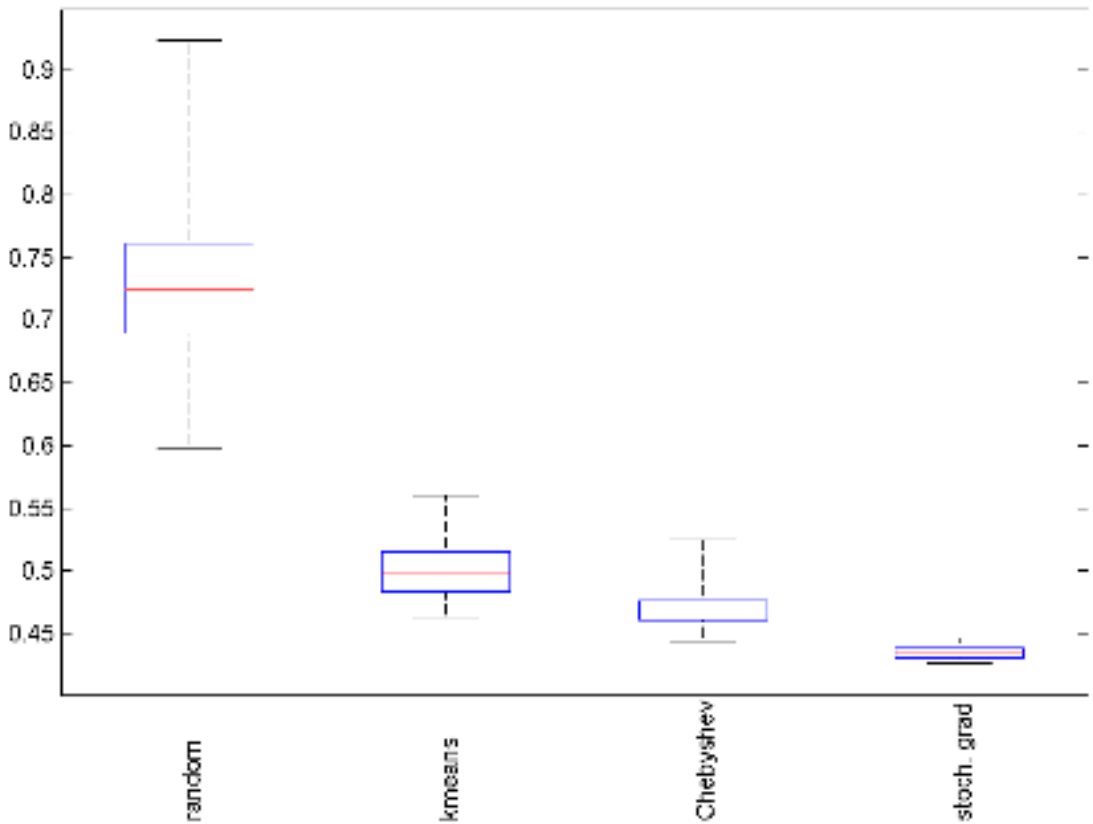
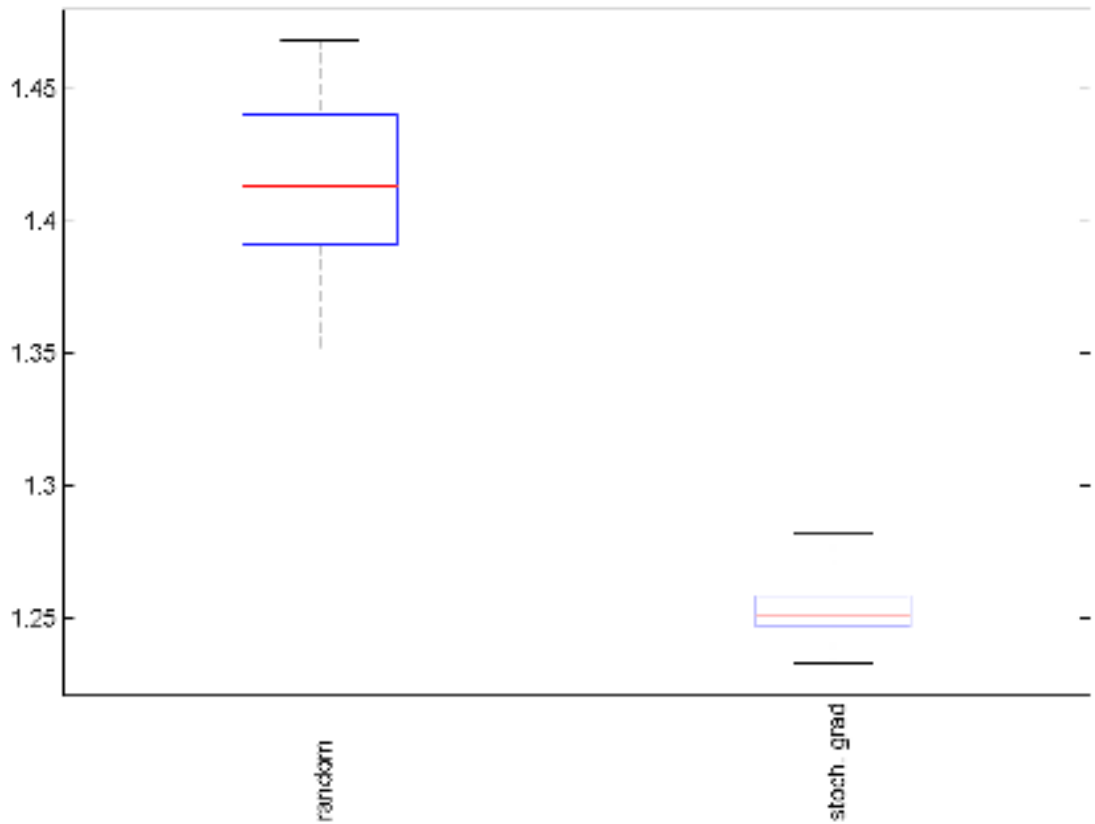
`k-means` and Lloyd's method with Chebyshev centers use 2^{d+8} points from a LDS (Sobol')

$$d = 4,\ n = 40$$



Example:

$$d = 10,\ n = 100$$



1.4 **Maximin criterion** $\Phi_{Mm}(\mathbf{X}_n) = \min_{i \neq j} d_{ij} = \min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\|$

Easy to compute (from distances d_{ij} between pairs of points)
$\Phi_{Mm}(\mathbf{X}_n)$ = minimum of convex functions $\Rightarrow$ not concave, non differentiable

- Use a global optimization method (e.g., simulated annealing)
- Local descent with some ad'hoc initialization
  (e.g., random multistart)

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Difficult problem, but:

$\Phi_{Mm}(\cdot)$ is global Lipschitz (with constant $\sqrt{2}$)
$\rightarrow$ $\Phi_{Mm}(\cdot)$ is differentiable almost everywhere (Cortés and Bullo, 2005, 2009)

Sub-differential $\partial\Phi_{Mm}(\mathbf{X}_n)$ easy to compute:

$$\partial\Phi_{Mm}(\mathbf{X}_n) = co\{\partial\Phi_{Mm\ ij}(\mathbf{X}_n) : \|\mathbf{x}_i - \mathbf{x}_j\| = \min_{k\neq\ell} \|\mathbf{x}_k - \mathbf{x}_\ell\|\}$$

with $\Phi_{Mm\ ij}(\mathbf{X}_n) = \|\mathbf{x}_i - \mathbf{x}_j\|$ and

$$\text{sub-gradient } \partial\Phi_{Mm\ ij}(\mathbf{X}_n) = (0,\ldots,0,\underbrace{\frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|}}_{i\text{th position}},0,\ldots,0,\underbrace{-\frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|}}_{j\text{th position}},0,\ldots,0)$$

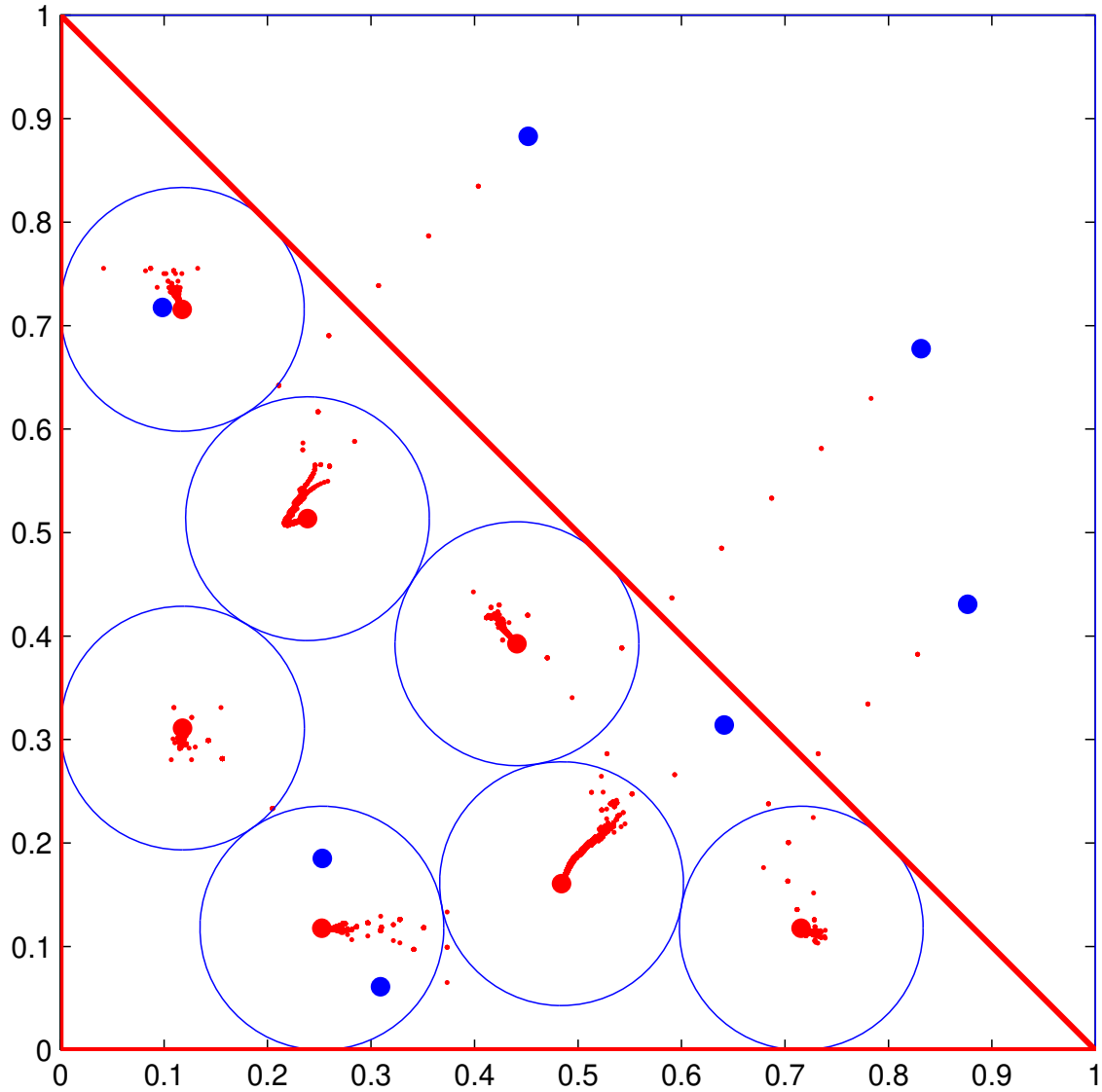
Sub-gradient algorithm to maximize $\Phi_{Mm}(\cdot)$:

$$\boxed{\mathbf{X}_n^{k+1} = \text{Proj}_{\mathscr{X}} \left[\mathbf{X}_n^k + \gamma_k \, \partial \Phi_{Mm \; ij}(\mathbf{X}_n^k) \right]}$$

for i, j such that $\|\mathbf{x}_i - \mathbf{x}_j\| = \Phi_{Mm}(\mathbf{X}_n^k)$
and $\gamma_k \searrow 0$, $\sum_k \gamma_k = \infty$

We can also force all points to remain far away from the boundary of $\mathscr{X}$:
$\Phi_{Mm \; B(\mathscr{X})}(\mathbf{X}_n) = \min\{\Phi_{Mm}(\mathbf{X}_n), 2 \min_i d[\mathbf{x}_i, \text{boundary}(\mathscr{X})]\}$

Ex: local maximization of $\Phi_{Mm\ B(\mathscr{X})}(\mathbf{X}_n)$, $n = 7$, $\mathscr{X}$ = simplex $0 \leq x_1$, $0 \leq x_2$, $x_1 + x_2 \leq 1$
(radius $= \frac{1}{2}\,\Phi_{Mm\ B(\mathscr{X})}(\mathbf{X}_n)$)



A few alternatives:

1) **Billiards** (Lubachevsky and Stillinger, 1990; Lubachevsky, 1991)

Principle :

$\mathbf{X}_n \to n$ balls in $\mathscr{X}$

random initial velocities

elastic collisions between balls and against boundaries

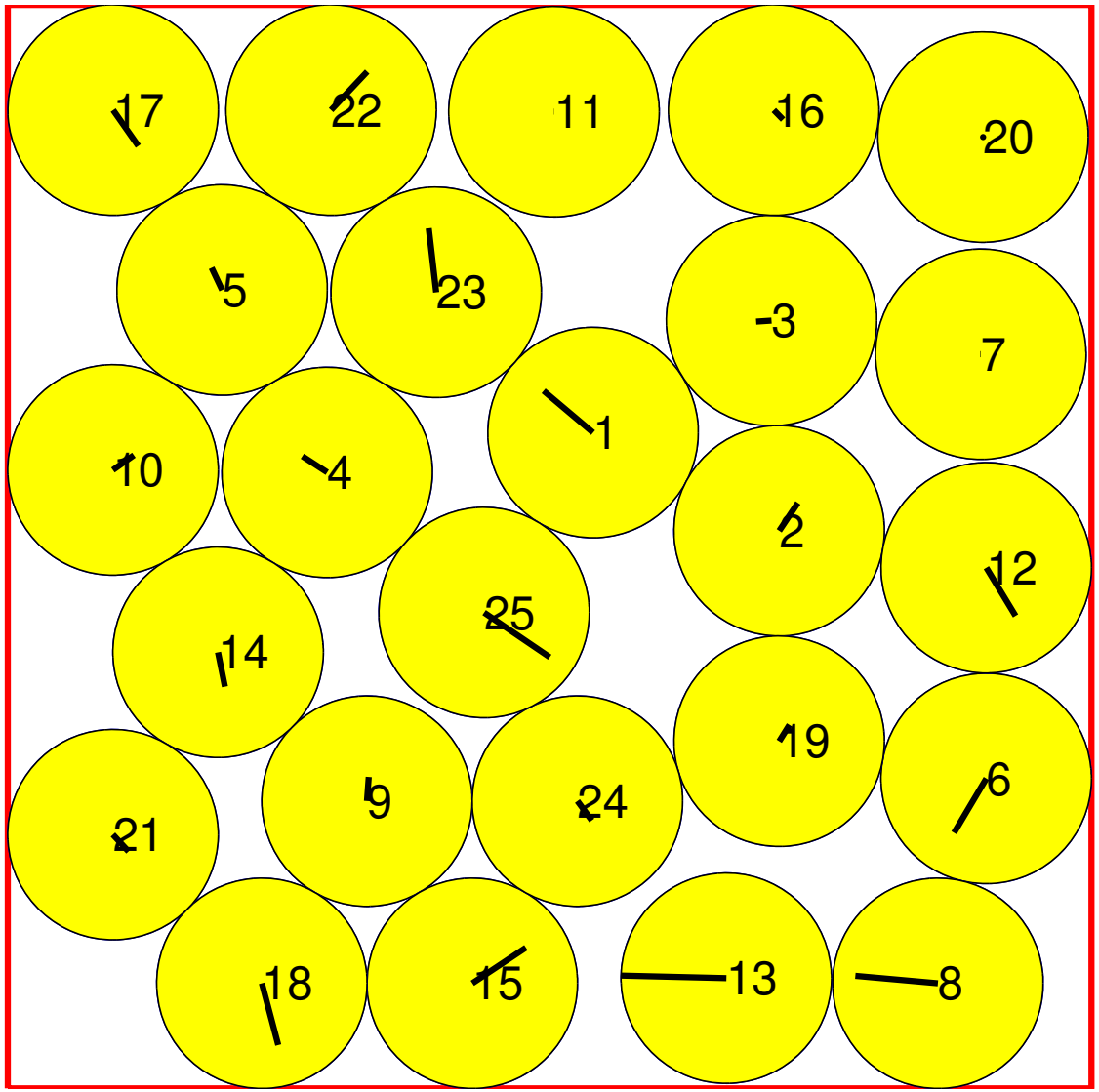
balls radius $R(t)$ linearly increasing with time t

➠ jamming occurs for a local max. of $\Phi_{Mm}(\cdot)$

Rather efficient for $d = 2$ (if $R(t)$ increases slowly enough...)

but not very efficient for $d > 2$

$n = 25$ ($R(t)$ increases too fast)



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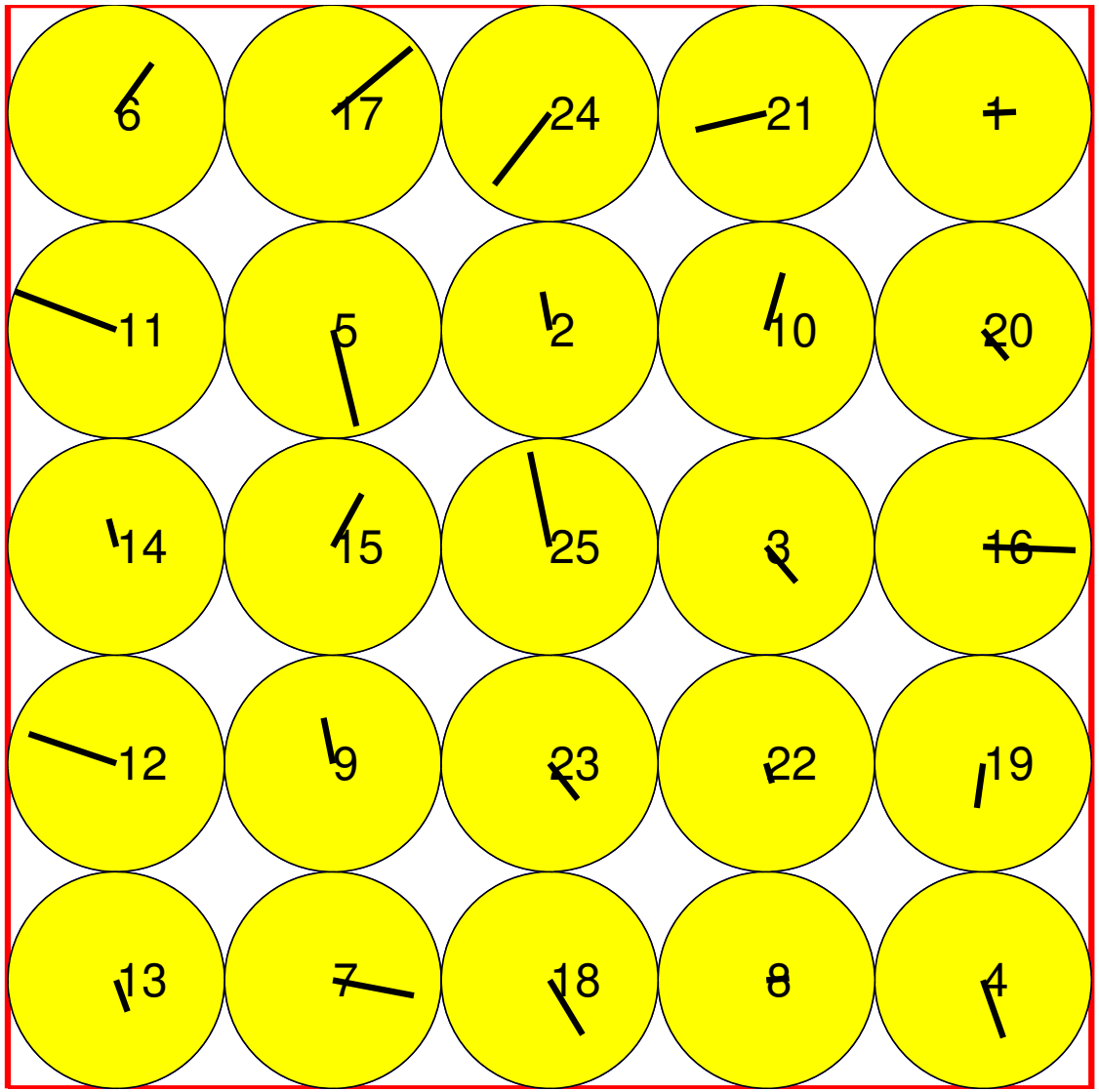
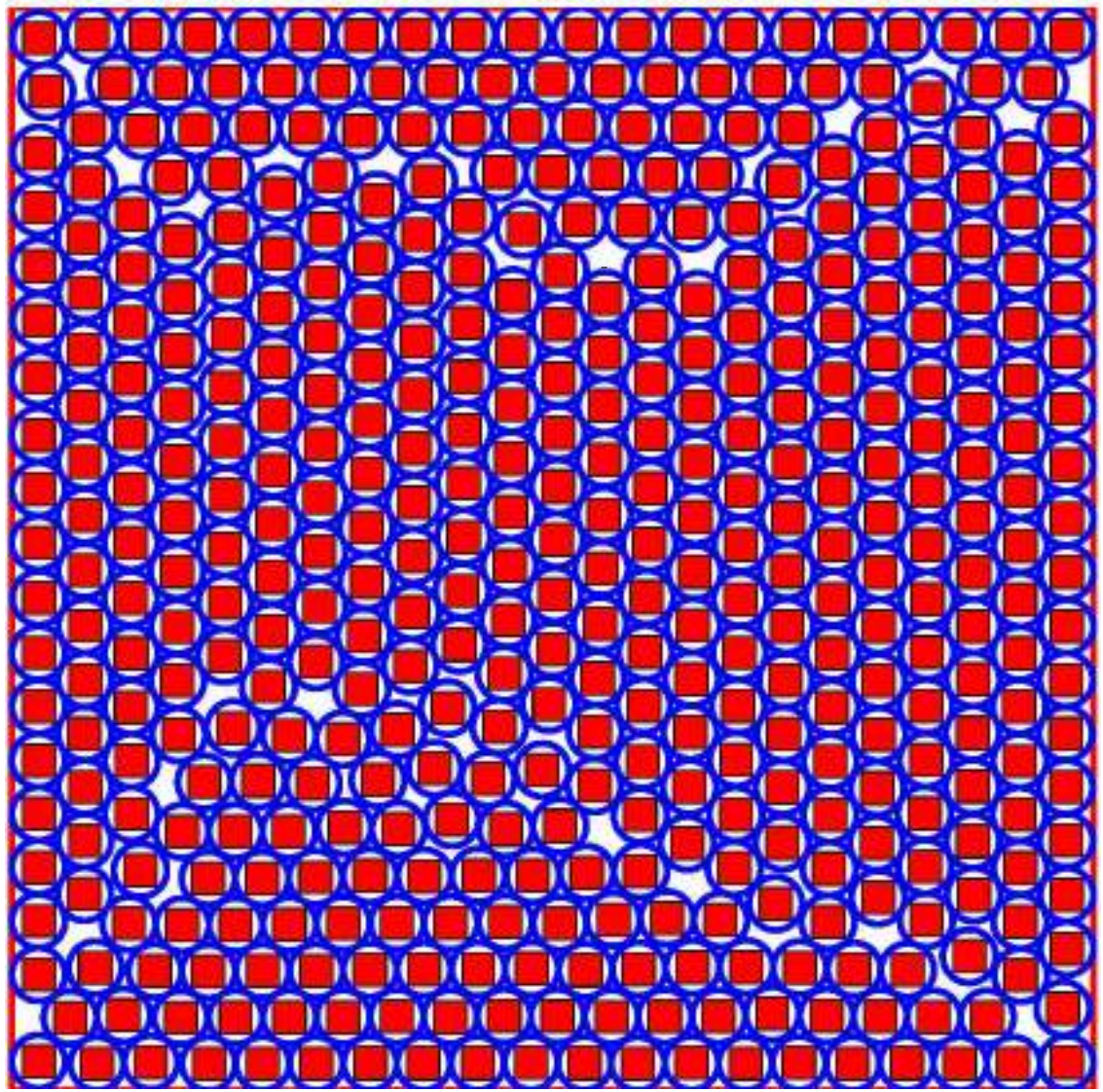


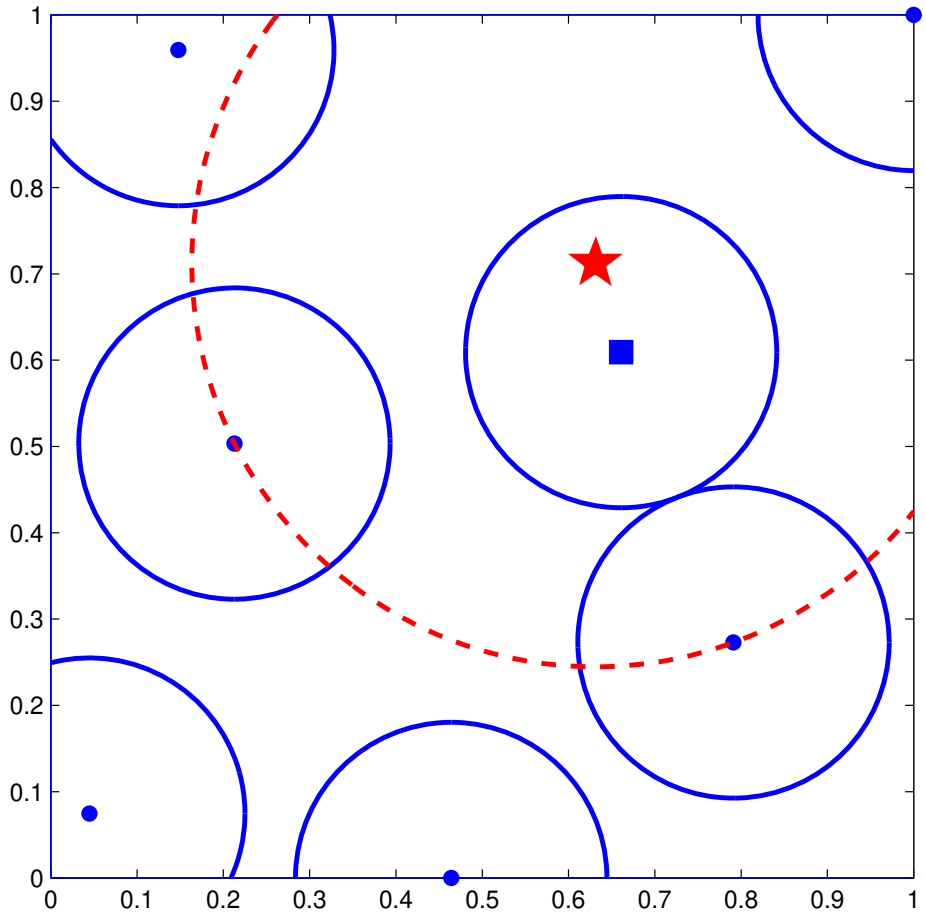
$n = 441$



2) **miniMax for Maximin**

Principle: repeat the following steps

a) Choose $\mathbf{x}_j$ from $\mathbf{X}_n$,
find $\mathbf{x}^*$ in $\mathscr{X}$ such that
$\min_{i \neq j} \|\mathbf{x}^* - \mathbf{x}_i\| =$
$\max_{\mathbf{x} \in \mathscr{X}} \min_{i \neq j} \|\mathbf{x} - \mathbf{x}_i\|$
(a byproduct of calculation of
$\Phi_{mM}(\mathbf{X}_{n \setminus j})$)



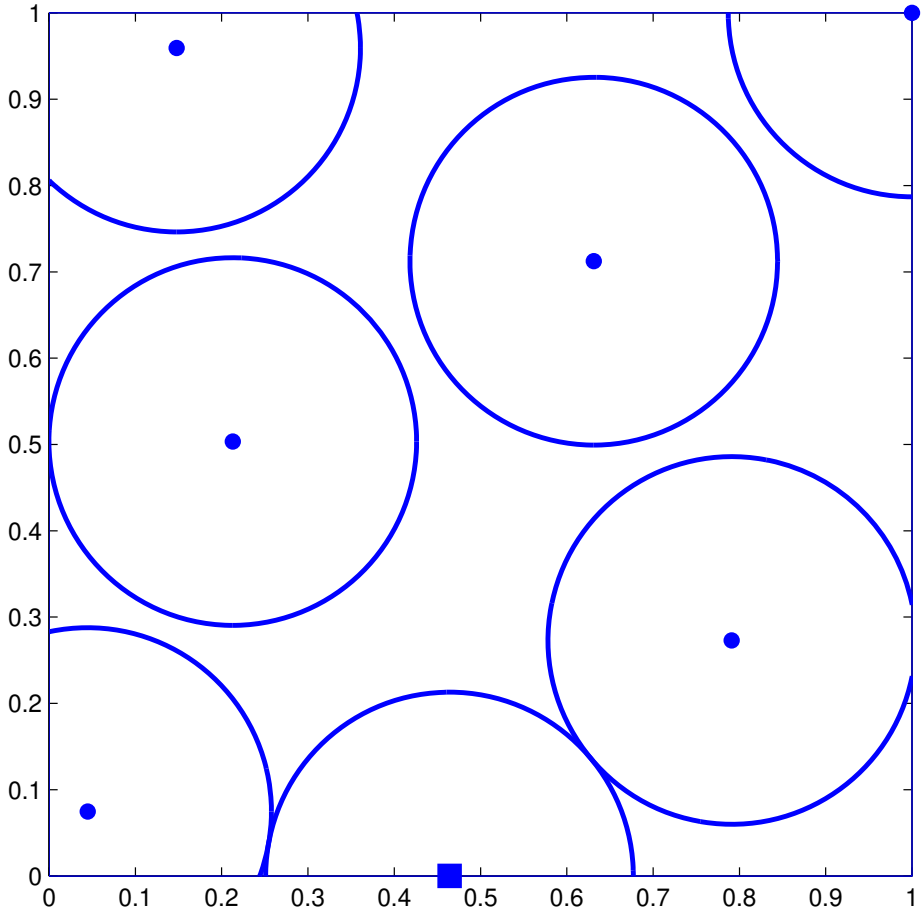
2) **miniMax for Maximin**

Principle: repeat the following steps

b) Replace $\mathbf{x}_j$ by $\mathbf{x}^*$

— which explains that

$$\Phi_{mM}(\mathbf{X}^*_{Mm,n}) \leq \Phi_{Mm}(\mathbf{X}^*_{Mm,n})$$



Related to "coffee-house design": start with $X_0 = \emptyset$, include points one by one $\mathbf{x}_1$ at the centre of $\mathscr{X}$, then $\mathbf{x}_{n+1}$ furthest point from X_n, $n \geq 1$
(called coffee-house design (Müller, 2007, Chap. 4))

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Guarantees $\boxed{\text{Eff}_{mM}(X_n) = \frac{\Phi^*_{mM,n}}{\Phi_{mM}(X_n)} \geq \frac{1}{2} \text{ and } \text{Eff}_{Mm}(X_n) = \frac{\Phi_{Mm}(X_n)}{\Phi^*_{Mm,n}} \geq \frac{1}{2} \text{ for all } n}$

with $\Phi_{Mm}(X_n) = \min_{i \neq j \in \{1,\ldots,n\}} \|\mathbf{x}_i - \mathbf{x}_j\|$ the maximin-distance criterion,
and $\Phi^*_{Mm,n}$ its optimal (maximum) value

Related to "coffee-house design": start with $X_0 = \emptyset$, include points one by one $\mathbf{x}_1$ at the centre of $\mathscr{X}$, then $\mathbf{x}_{n+1}$ furthest point from X_n, $n \geq 1$
(called coffee-house design (Müller, 2007, Chap. 4))

Guarantees $\boxed{\text{Eff}_{mM}(X_n) = \frac{\Phi^*_{mM,n}}{\Phi_{mM}(X_n)} \geq \frac{1}{2} \text{ and } \text{Eff}_{Mm}(X_n) = \frac{\Phi_{Mm}(X_n)}{\Phi^*_{Mm,n}} \geq \frac{1}{2} \text{ for all } n}$

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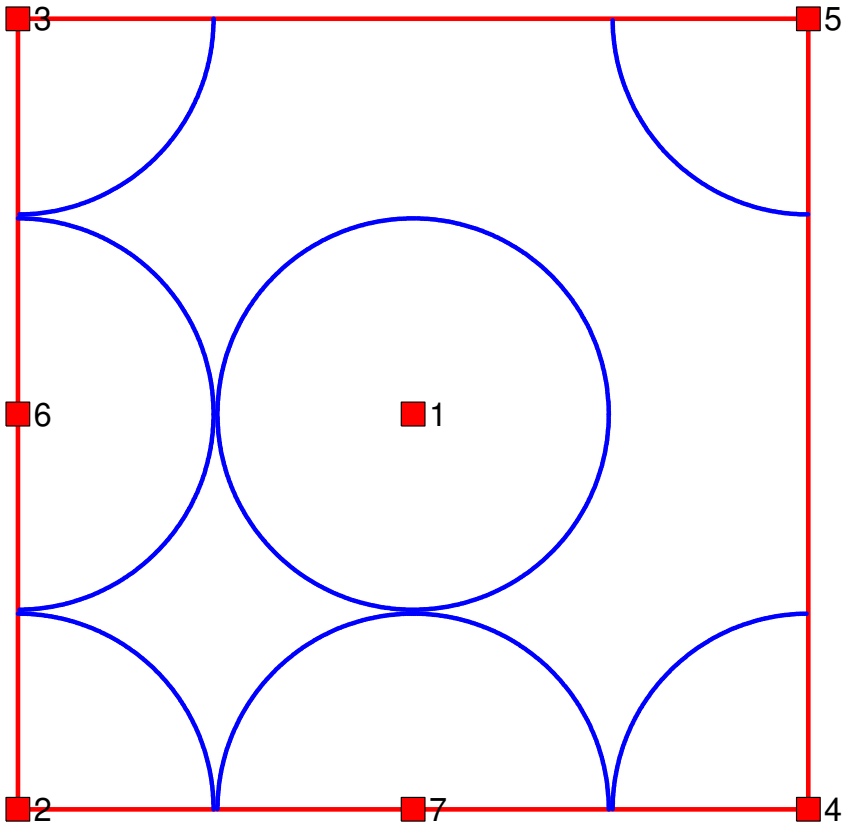
Proof. (Gonzalez, 1985) — repeated later

- by construction:
  $\Phi_{Mm}(X_{n+1}) \triangleq \min_{\mathbf{x}_i \neq \mathbf{x}_j \in X_{n+1}} \|\mathbf{x}_i - \mathbf{x}_j\| = d(\mathbf{x}_{n+1}, X_n) = \Phi_{mM}(X_n)$
- X^*_n a Φ_{mM}-optimal design: the n balls $\mathscr{B}(\mathbf{x}^*_i, \Phi_{mM}(X^*_n))$, $\mathbf{x}^*_i \in X^*_n$, cover $\mathscr{X}$
  $\Rightarrow$ one of them contains 2 points $\mathbf{x}_i$, $\mathbf{x}_j$ in X_{n+1} *for any* X_{n+1} *($n+1$ points)*
  $\Rightarrow \Phi_{Mm}(X_{n+1}) \leq \|\mathbf{x}_i - \mathbf{x}_j\| \leq 2\Phi_{mM}(X^*_n)$
  $\Rightarrow \Phi^*_{Mm,n+1} \leq 2\Phi_{mM}(X^*_n) \leq 2\Phi_{mM}(X_n) = \Phi_{Mm}(X_{n+1})$

$\mathscr{X} = [0,1]^2,\ n = 7$



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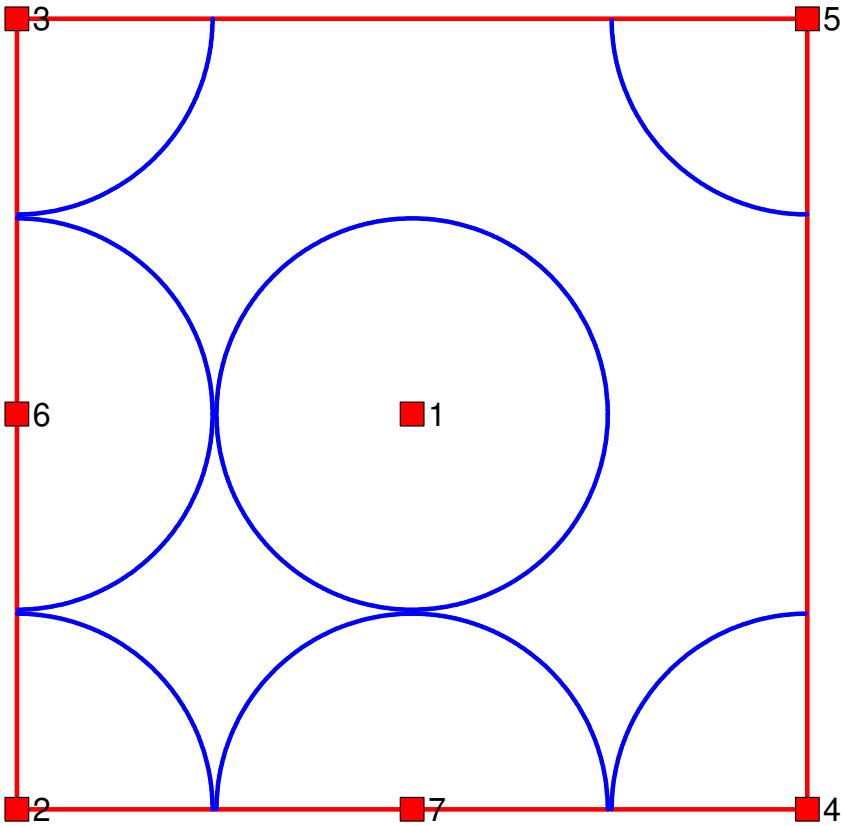
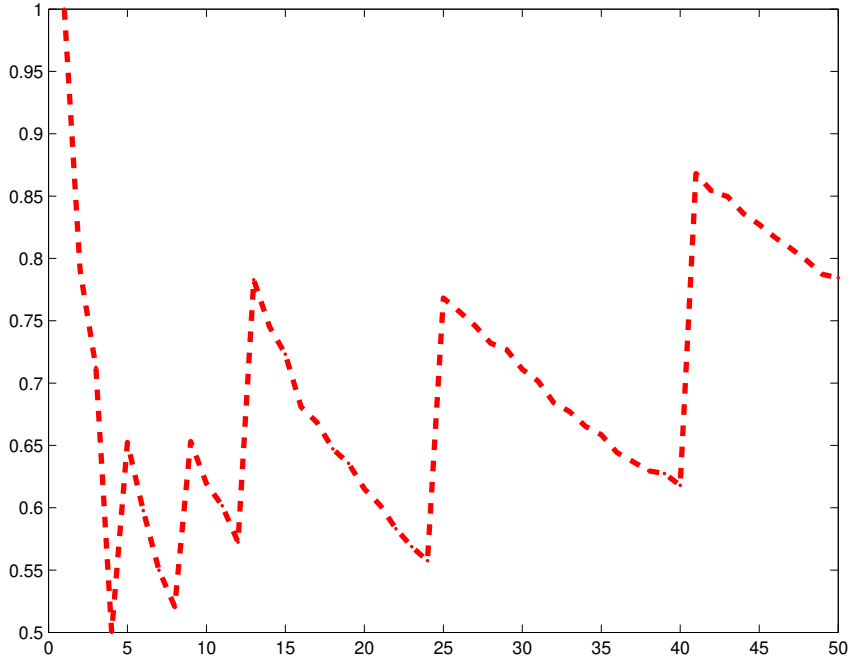


$\text{Eff}_{mM}(X_n)$, $n = 1 \ldots, 50$



Regular construction ➠ large fluctuations of $\text{Eff}_{mM}(X_n)$

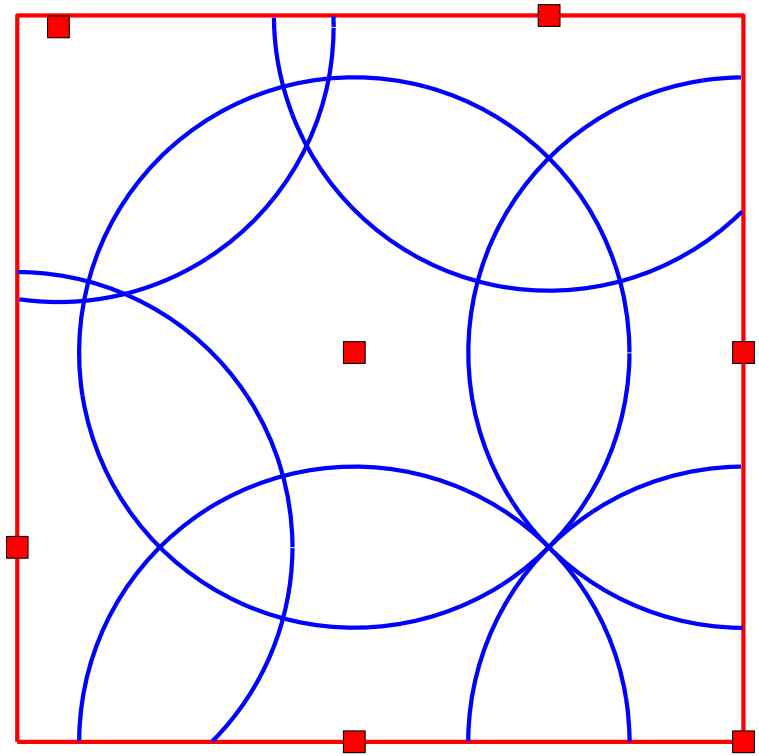
Remark: a Maximin distance design is useful for the miniMax criterion

Principle:

Points from a Maximin-optimal $\mathbf{X}^*_{Mm,n}$ tend to lie along the boundary of $\mathscr{X}$

➠ Apply an homothecy with center $\mathbf{c} \in \text{int}(\mathscr{X})$ and ratio $1/(1+\epsilon)$ to all points in $\mathbf{X}^*_{Mm,n}$ ($\mathscr{X} = [0,1]^d$, $\mathbf{c} = \frac{1}{2}\,\mathbf{1}$ ➠ $\mathbf{X}_n(\epsilon) = \mathbf{c} + \frac{1}{1+\epsilon}\,(\mathbf{X}^*_{Mm,n} - \mathbf{c})$)

$d = 2$, $n = 7$, $\mathbf{X}^*_{Mm,n}$ Maximin-optimal



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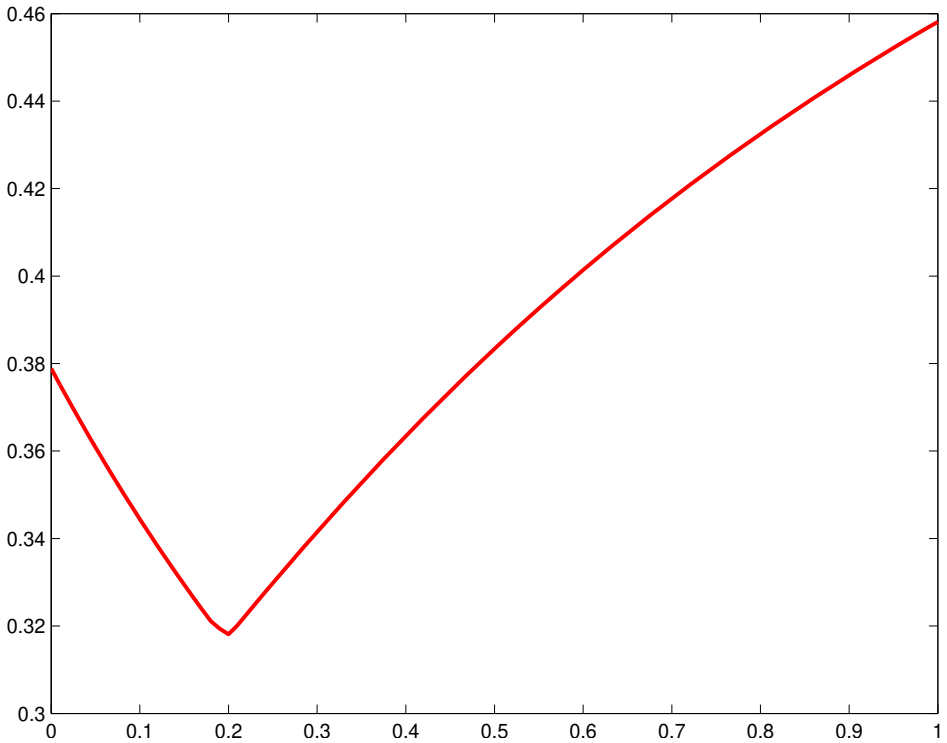
$\Phi_{mM}(\mathbf{X}_n(\epsilon))$, $0 \leq \epsilon \leq 1$ ➠ $\epsilon^* = 0.2$



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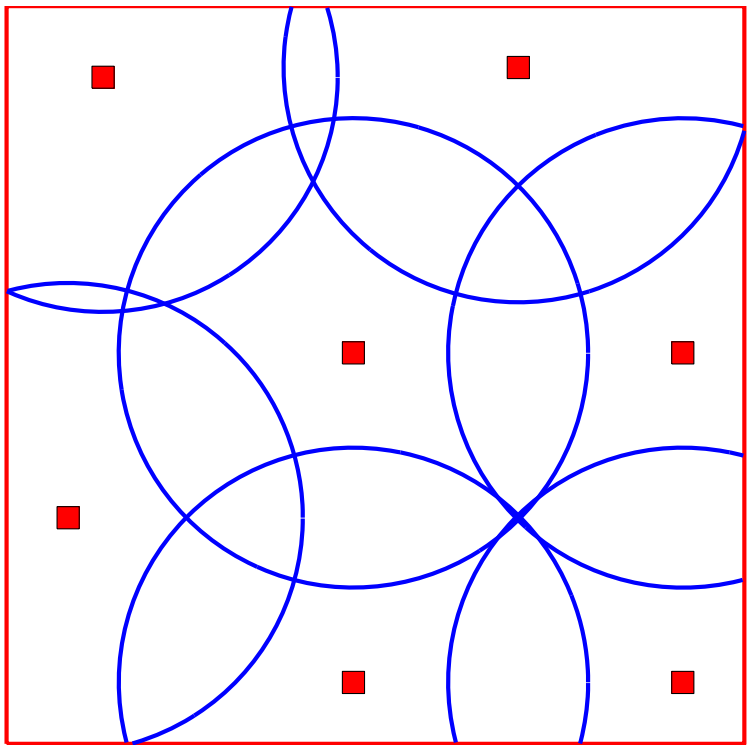
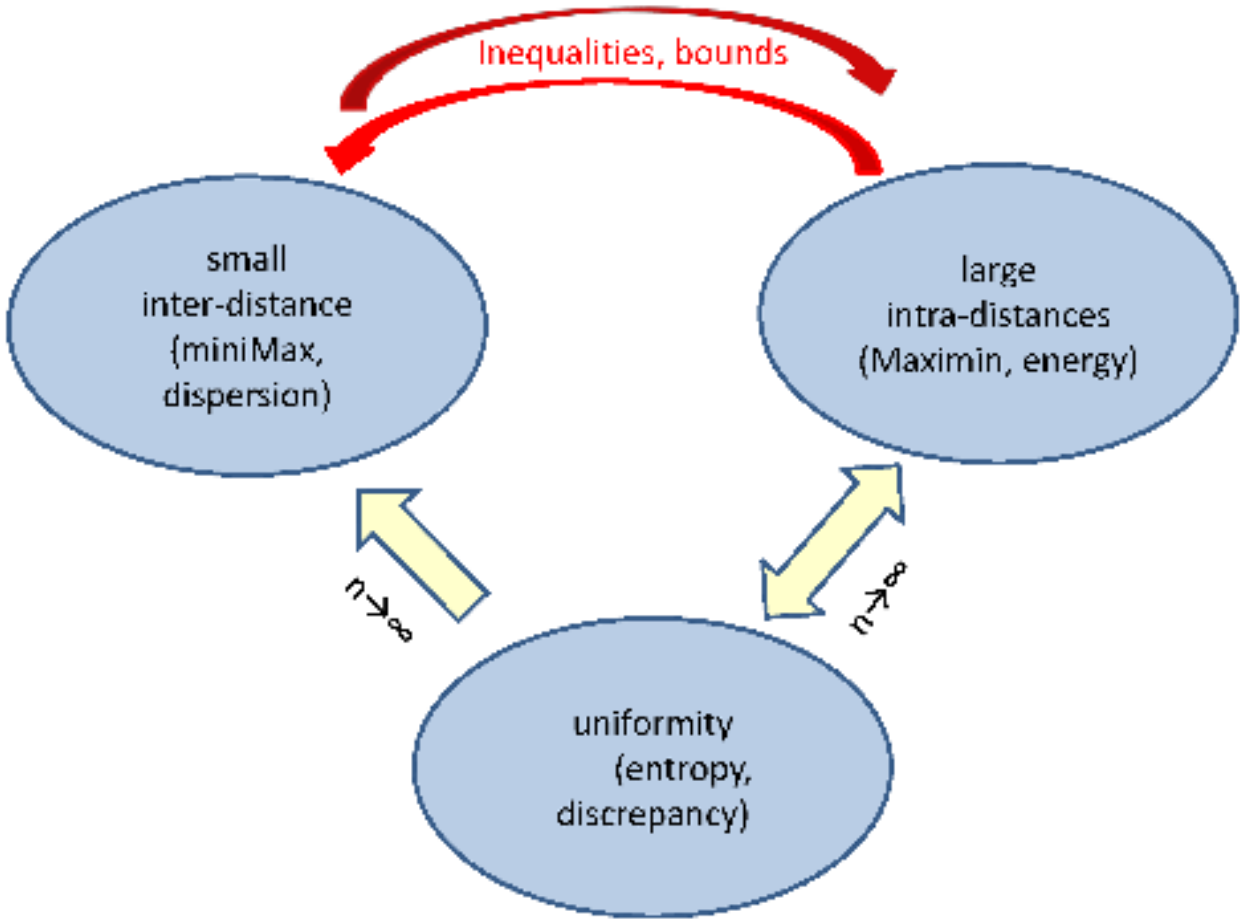
$\mathbf{X}_n(\epsilon^*)$ ➠ $\Phi_{mM}(\mathbf{X}_n(\epsilon^*)) = 0.3181$ (true miniMax optimum $= 0.2743$)



1.5 Relations between Φ_{Mm} and Φ_{mM} $(d \geq 2)$



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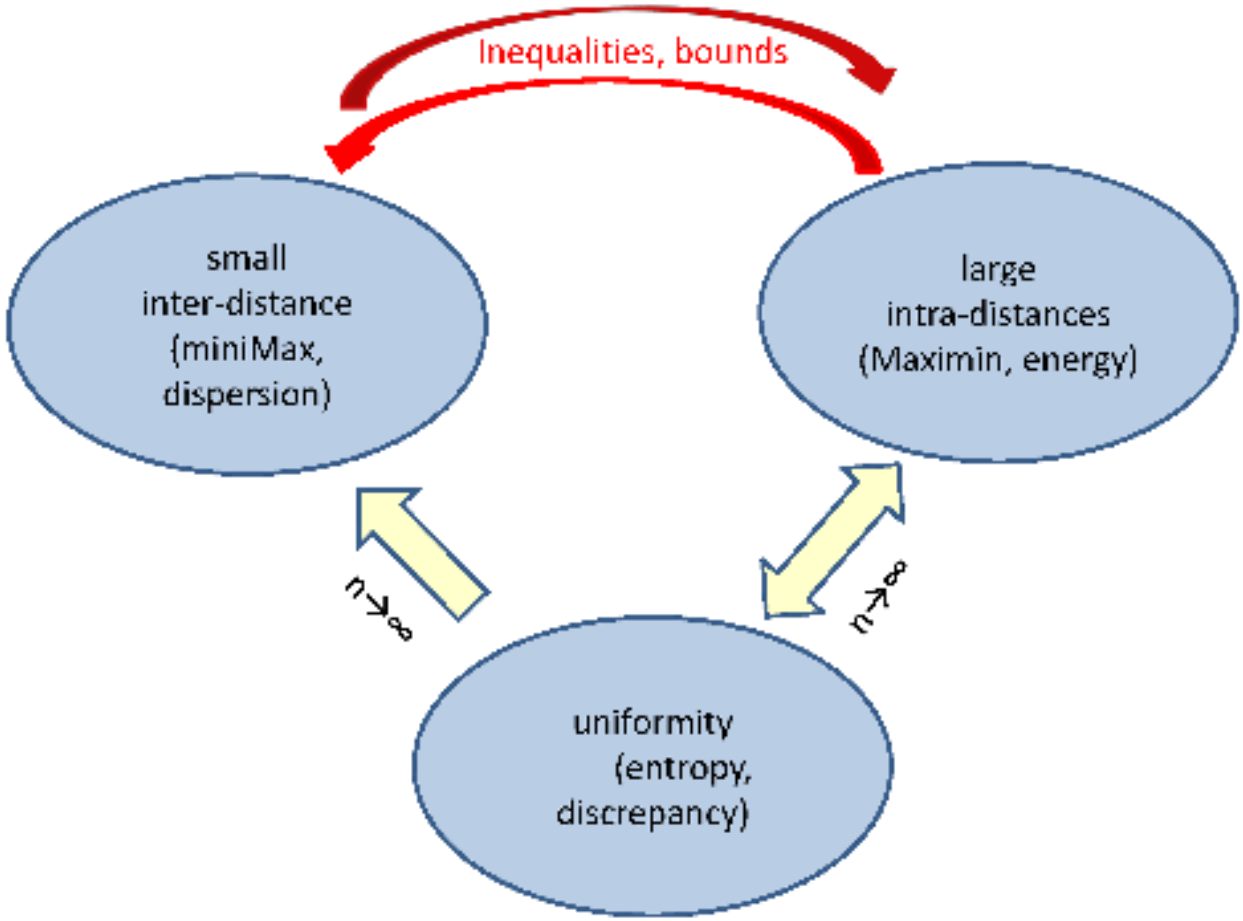

Regularized Maximin

Notation: $\mathscr{X} = [0,1]^d$, $V_d = \text{vol}[\mathscr{B}(\mathbf{0},1)] = \pi^{d/2}/\Gamma(d/2+1)$

$\triangleright$ $\Phi^*_{mM,n} \triangleq \min_{\mathbf{X}_n} \Phi_{mM}(\mathbf{X}_n)$, $\Phi^*_{Mm,n} \triangleq \max_{\mathbf{X}_n} \Phi_{Mm}(\mathbf{X}_n)$ $\triangleleft$

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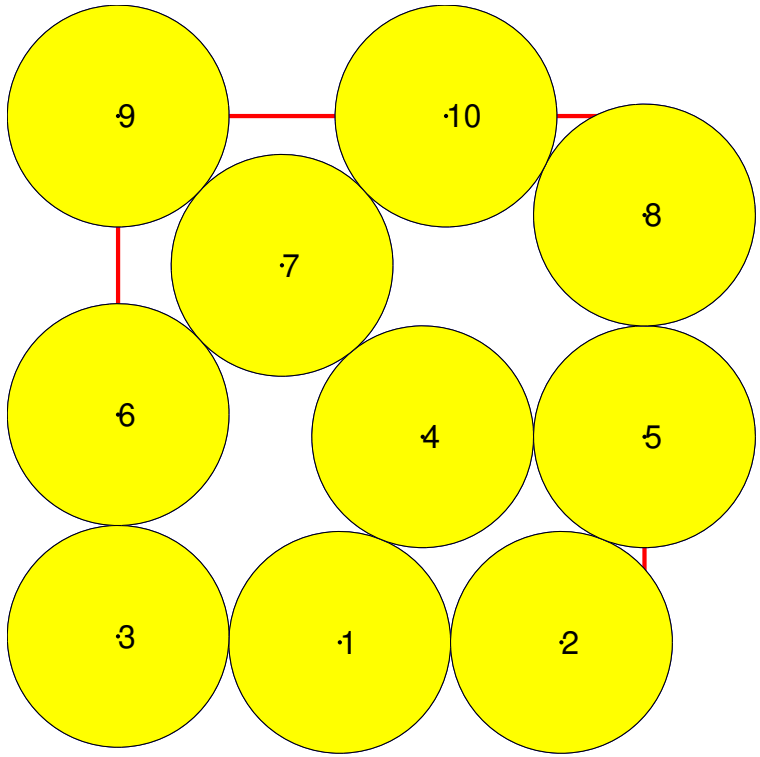
- $\boxed{\frac{1}{2}\Phi_{Mm}(\mathbf{X}_n) \leq \Phi_{mM}(\mathbf{X}_n), \text{ for all } \mathbf{X}_n \ (n \geq 2)}$

(the n balls $\mathscr{B}(\mathbf{x}_i, \frac{1}{2}\Phi_{Mm}(\mathbf{X}_n))$ do not cover $\mathscr{X}$)



- $\boxed{\frac{1}{2}\Phi_{Mm}(\mathbf{X}_{n+1}) \leq \Phi^*_{mM,n}, \text{ for all } \mathbf{X}_{n+1} \ (n \geq 1)}$

Proof: one of the n balls $\mathscr{B}(\mathbf{z}_i, \Phi^*_{mM,n})$, $\mathbf{z}_i \in \mathbf{X}^*_{mM,n}$, contains 2 points $\mathbf{x}_i$ and $\mathbf{x}_j$ from $\mathbf{X}_{n+1}$

$$\Longrightarrow \quad \Phi_{Mm}(\mathbf{X}_{n+1}) \leq \|\mathbf{x}_i - \mathbf{x}_j\| \leq 2\Phi^*_{mM,n}$$

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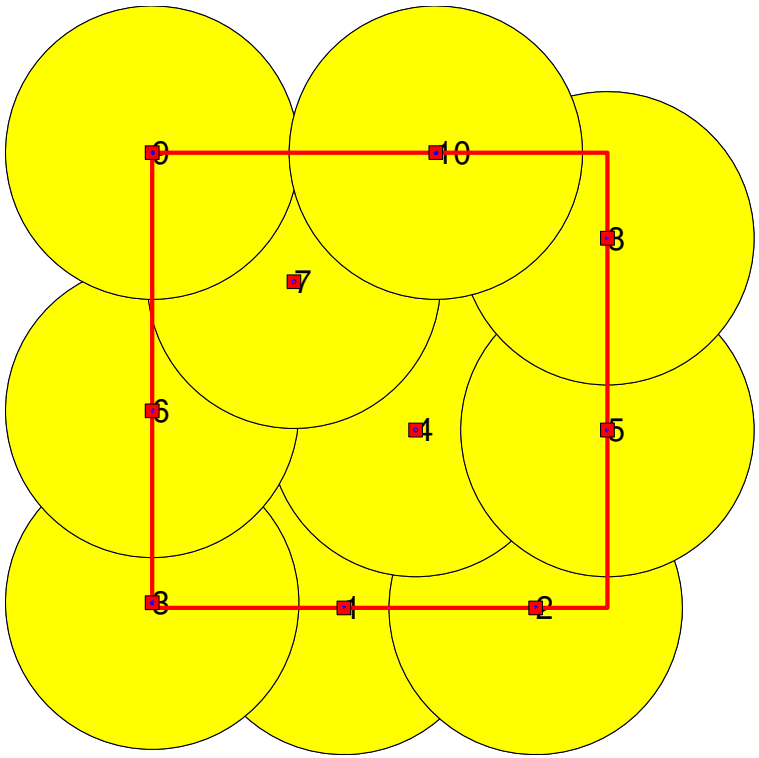
- The n balls $\mathscr{B}(\mathbf{x}_i, \Phi_{mM}(\mathbf{X}_n))$ cover $\mathscr{X}$, for all $\mathbf{X}_n$



- Sphere covering $\Rightarrow nV_d \left(\Phi^*_{mM,n}\right)^d > 1$

$$\boxed{R^*_n < \Phi^*_{mM,n}} \quad \text{with } R^*_n = (nV_d)^{-1/d}$$

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  (proof by contradiction)

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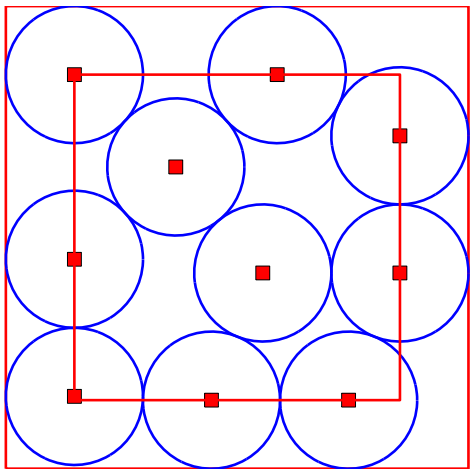
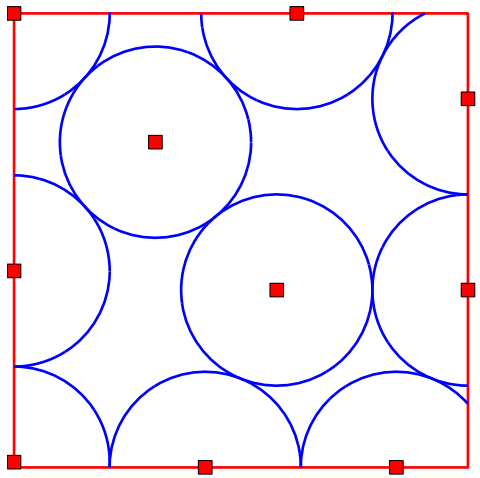
  (proof by contradiction)
- packing of n balls with radius R in $[0,1]^d$

  $\Rightarrow nV_d\,R^d < 1$, i.e., $\boxed{R < R^*_n}$

  (and $R^*_n < \frac{1}{2}$ for $n > \lceil 2^d/V_d \rceil$)





$$\boxed{R^*_n < \Phi^*_{mM,n} \leq \Phi^*_{Mm,n} < \frac{2R^*_n}{1-2R^*_n}} \quad \text{with } R^*_n = (nV_d)^{-1/d}$$

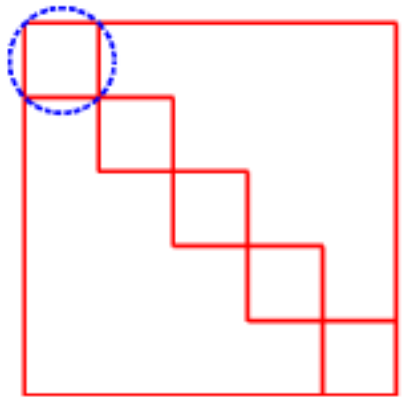
(these bounds are rather loose — factor $\frac{2}{1-2R^*_n} > 2$)

Other upper bounds on $\Phi^*_{mM,n} = \Phi_{mM}(X^*_n)$ when $\mathscr{X} = [0,1]^d$

Upper bound: use any design!

m^d-point regular grid in $\mathscr{X}$:

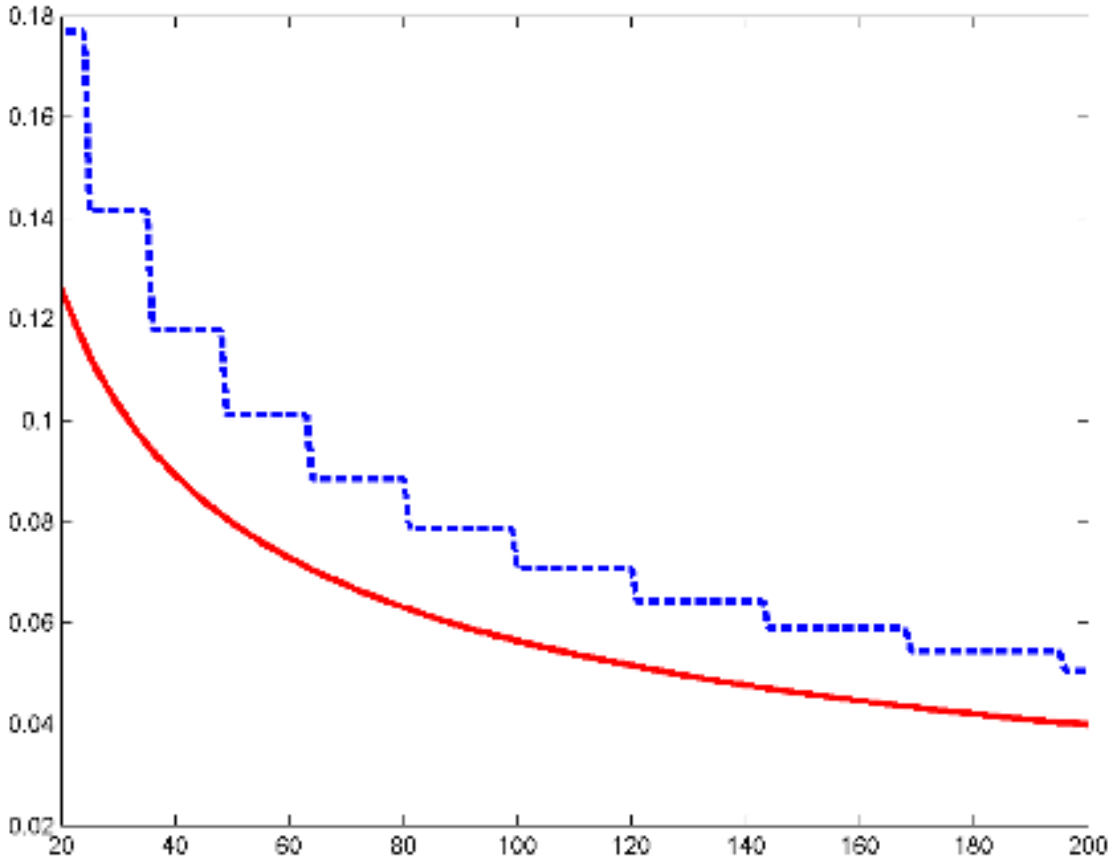
$$\Phi^*_{mM,m^d} \leq \frac{\sqrt{d}}{2m}:$$



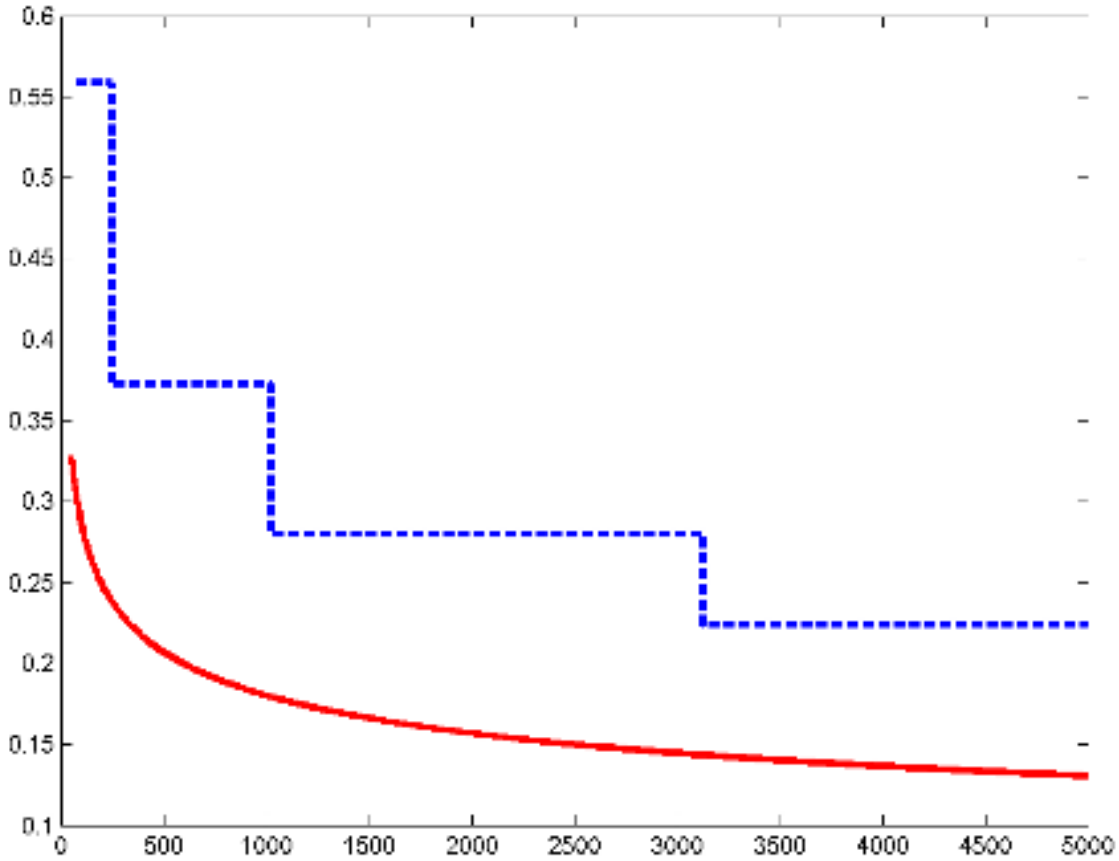
Take $m = \lfloor n^{1/d} \rfloor$, so that $m^d \leq n$ and $\Phi^*_{mM,n} \leq \Phi^*_{mM,m^d}$, therefore

$$\boxed{\Phi^*_{mM,n} \leq \overline{R}^*_n = \frac{\sqrt{d}}{2\lfloor n^{1/d} \rfloor}}$$

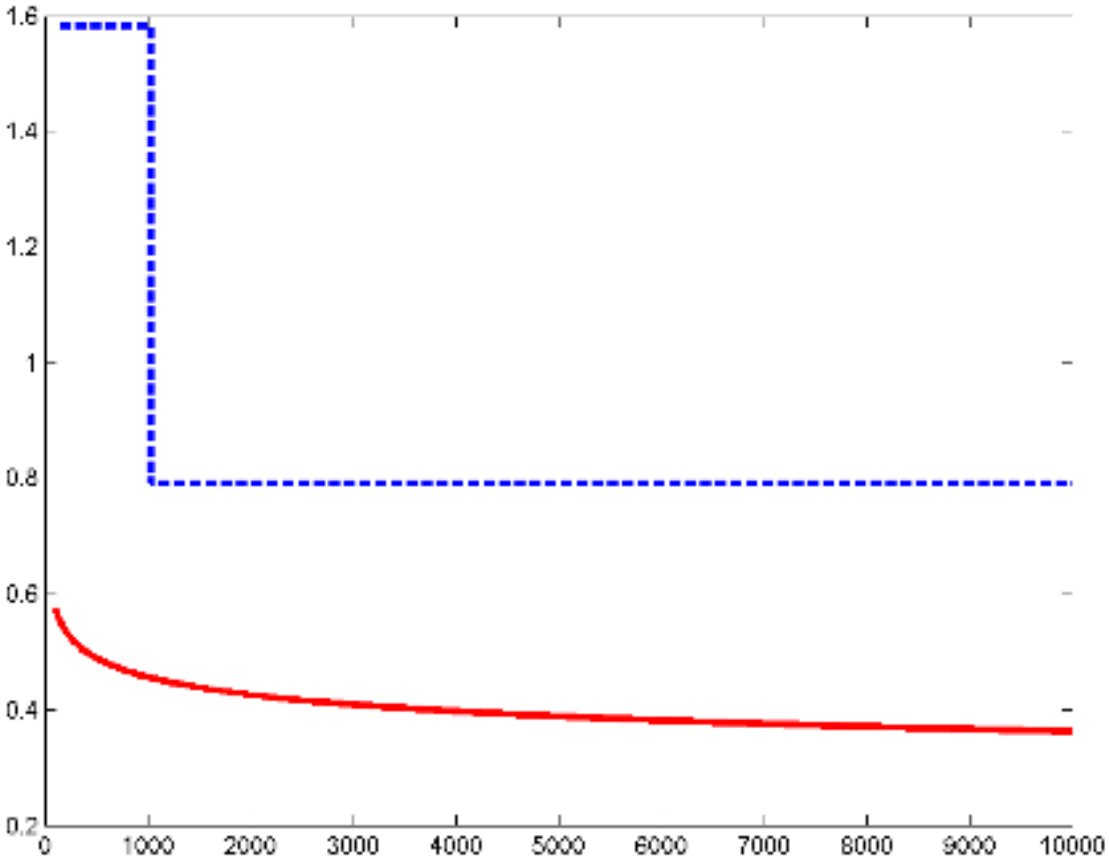
$$d = 2,\ R_n^* \leq \Phi_{mM,n}^* \leq \overline{R}_n^*$$



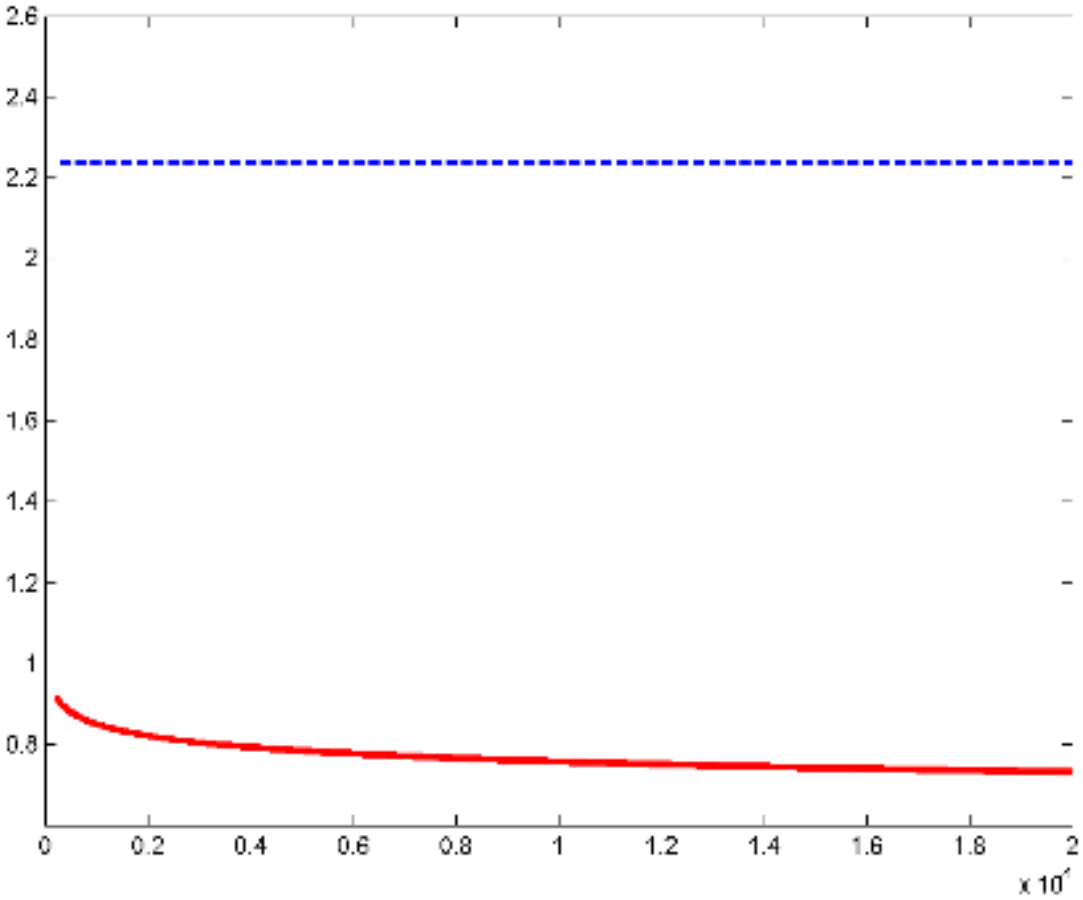
$$d = 5,\ R_n^* \leq \Phi_{mM,n}^* \leq \overline{R}_n^*$$



$$d = 10,\ R_n^* \leq \Phi_{mM,n}^* \leq \overline{R}_n^*$$



$$d = 20,\ R_n^* \leq \Phi_{mM,n}^* \leq \overline{R}_n^*$$



Why are such bounds useful?

- They give an idea of the suboptimality of a given design (for small d)

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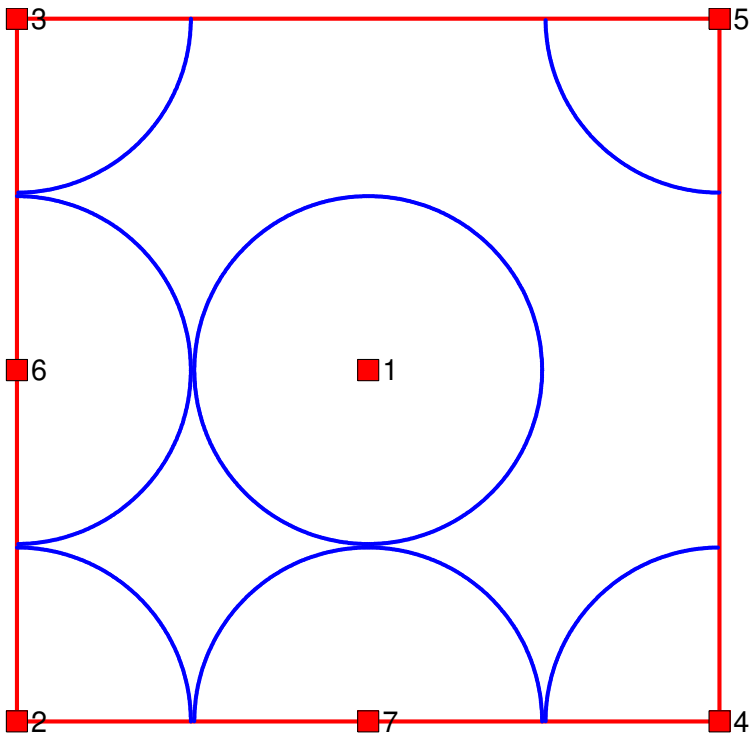
- They give an idea of the suboptimality of a given design (for small d)
- They help understand algorithms:
  - 1/ Method "miniMax for Maximin"

    uses $\boxed{\Phi_{mM}(\mathbf{X}^*_{Mm,n}) \leq \Phi_{Mm}(\mathbf{X}^*_{Mm,n})}$
  - 2/ **Greedy algorithm of "coffee-house design"**
    0) Choose $\mathbf{x}_1 \in \mathscr{X}$, set $\mathbf{X}_1 = \{\mathbf{x}_1\}$
    1) For $k = 1, 2, \ldots$, find $\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathscr{X}} d(\mathbf{x}, \mathbf{X}_k)$, set $\mathbf{X}_{k+1} = \mathbf{X}_k \cup \{\mathbf{x}^*\}$



A bit primitive . . . but (Gonzalez, 1985) :

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$\boxed{\frac{1}{2}\Phi_{Mm}(\mathbf{X}_{k+1}) \leq \Phi^*_{mM,k}, \text{ for all } \mathbf{X}_{k+1} \ (k \geq 1)}$ implies

a) $\Phi^*_{mM,k} \geq (1/2)\,\Phi_{mM}(X_k)$ and
b) $\Phi^*_{Mm,k+1} \leq 2\Phi^*_{mM,k} \leq 2\,\Phi_{mM}(X_k) = 2\,\Phi_{Mm}(X_{k+1})$

⏩ Regularized Maximin

Remark:

- There exist better bounds $d = 2, 3$: packing n balls with radius R in $[0, 1]^d$ $\Rightarrow nV_d R^d < \delta_d =$ *packing density*, with
  - $\delta_2 = \pi\sqrt{3}/6 \simeq 0.9069$
    [Lagrange, 1773 for lattices, Tóth 1940 for general packings]
  - $\delta_3 = \pi\sqrt{2}/6 \simeq 0.7405$
    [Kepler conjecture 1611, Gauss 1831 for lattices, Hales-Ferguson 2006 for general packings]
- Little is known for $d > 3$: best (densest) lattice packing known for $d \leq 8$, best general packings are known for $d = 8$ (Viazovska, 2016) and $d = 24$ (Cohn et al., 2017)

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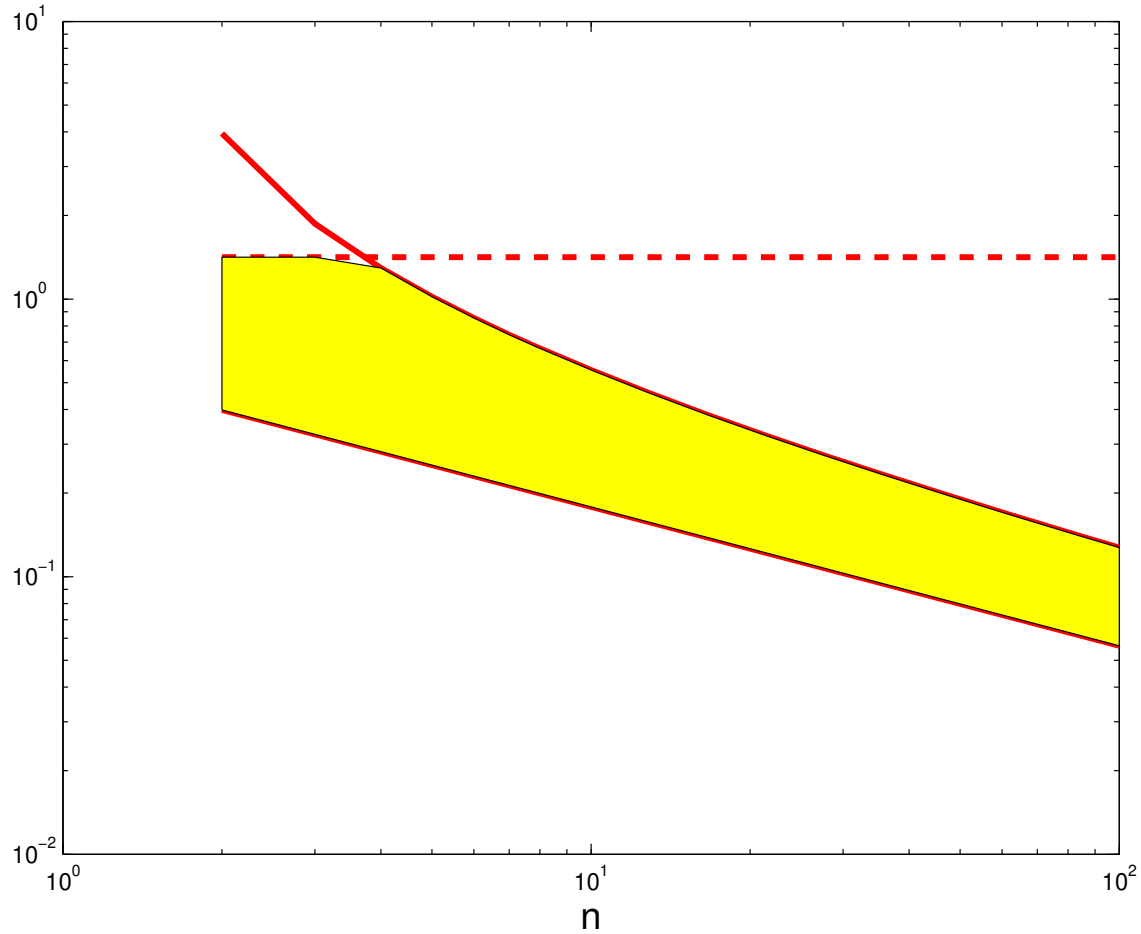
⏩ Regularized Maximin

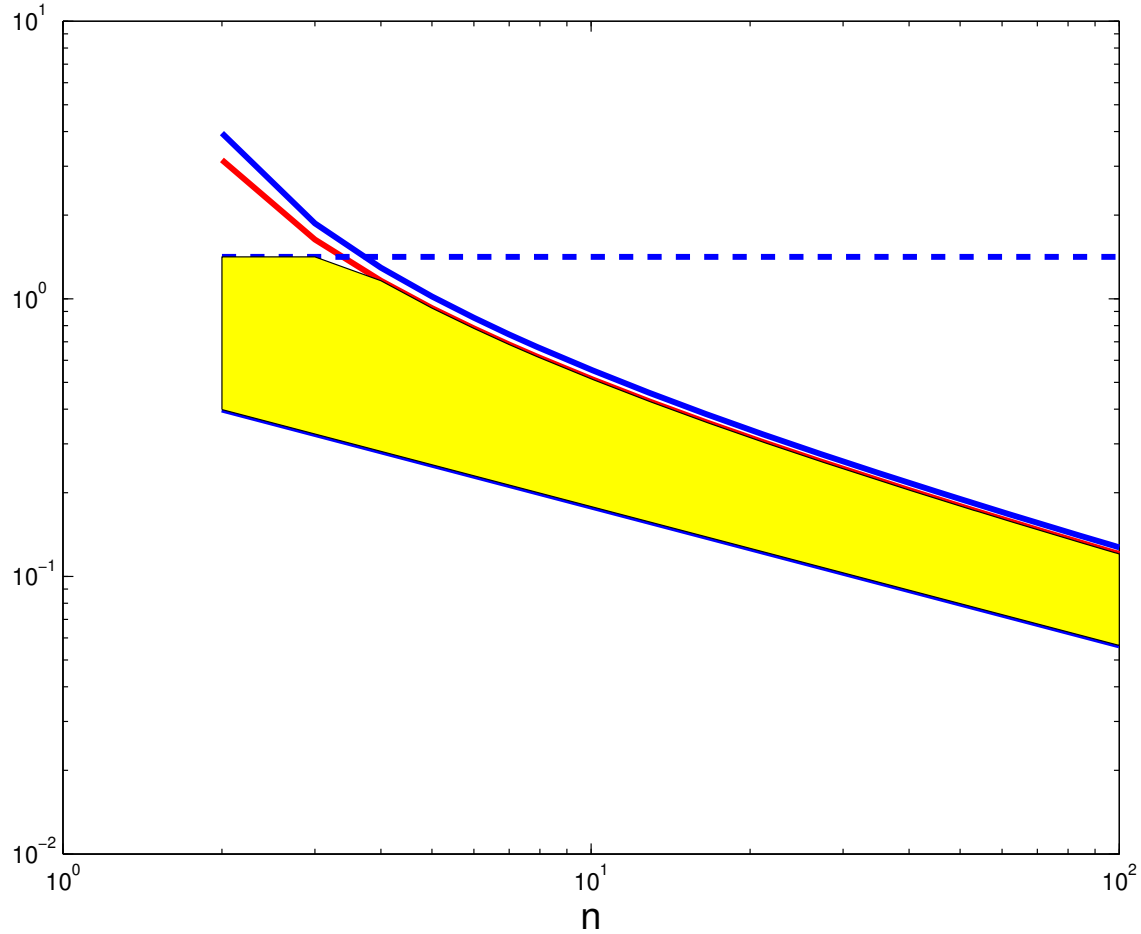
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$ using $\boxed{R^*_n < \Phi^*_{mM,n} \leq \Phi^*_{Mm,n} < \min\{\frac{2R^*_n}{1-2R^*_n}, \sqrt{d}\}}$



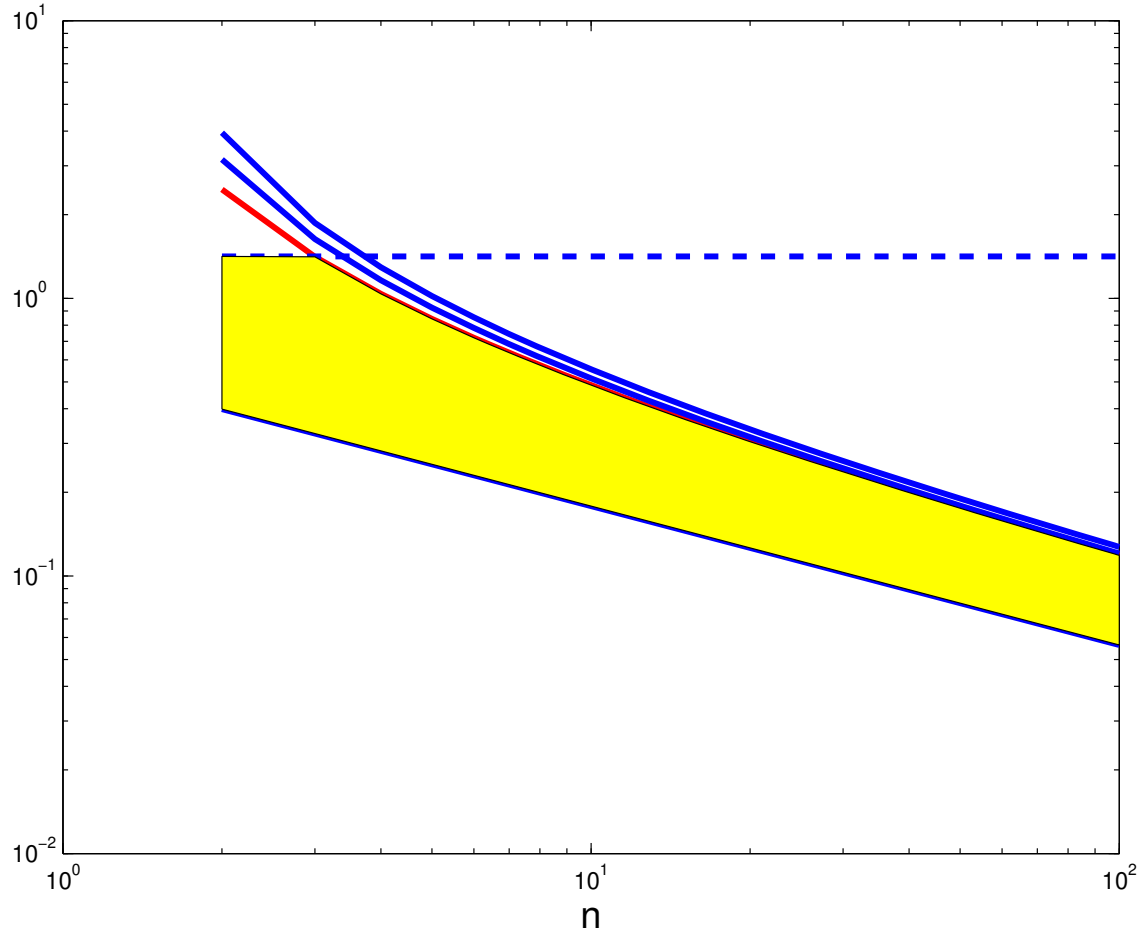
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$ with moreover $\boxed{\Phi^*_{Mm,n} < \frac{1}{3^{1/4}\sqrt{n/2-1}}}$ (*packing density*)



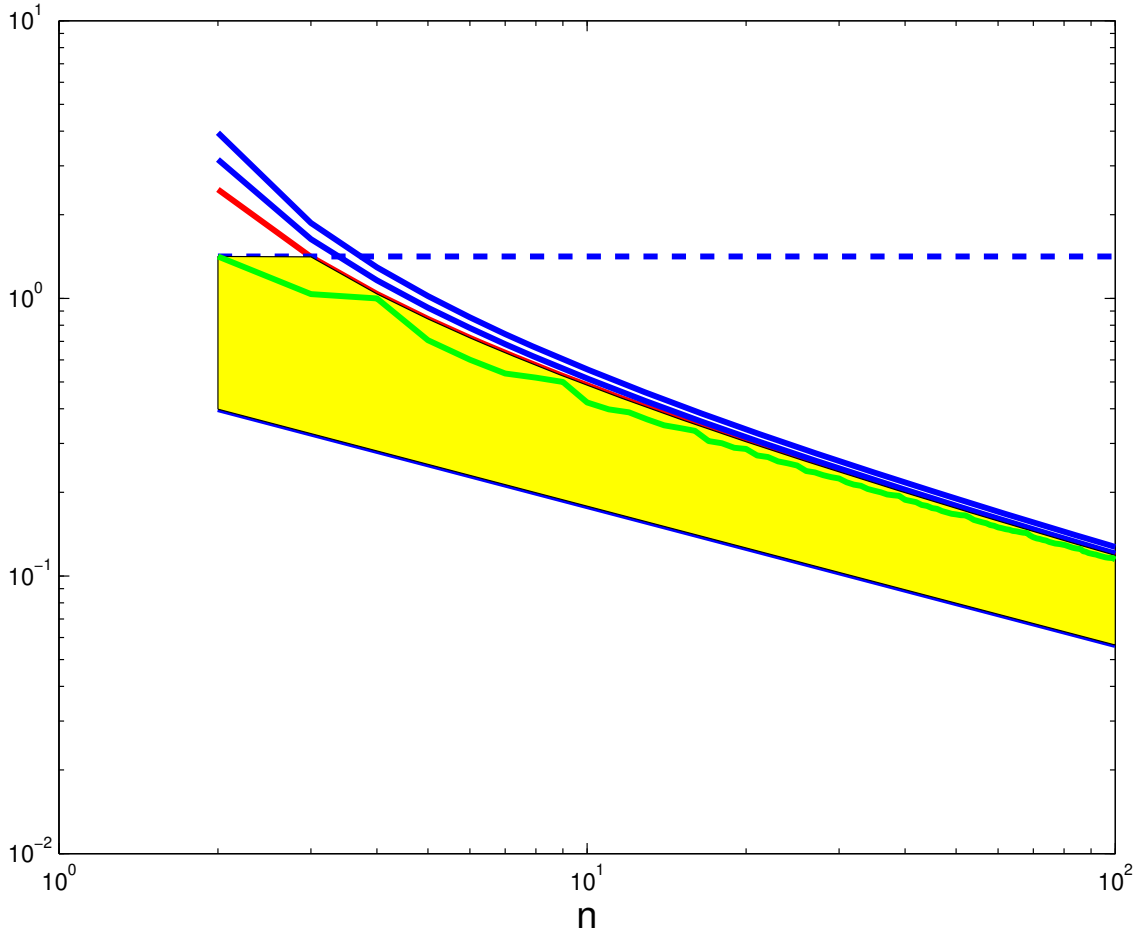
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$ with moreover $\boxed{\Phi^*_{Mm,n} < \frac{1+\sqrt{1+2\,(n-1)\,/\sqrt{3}}}{n-1}}$ (Oler, 1961)



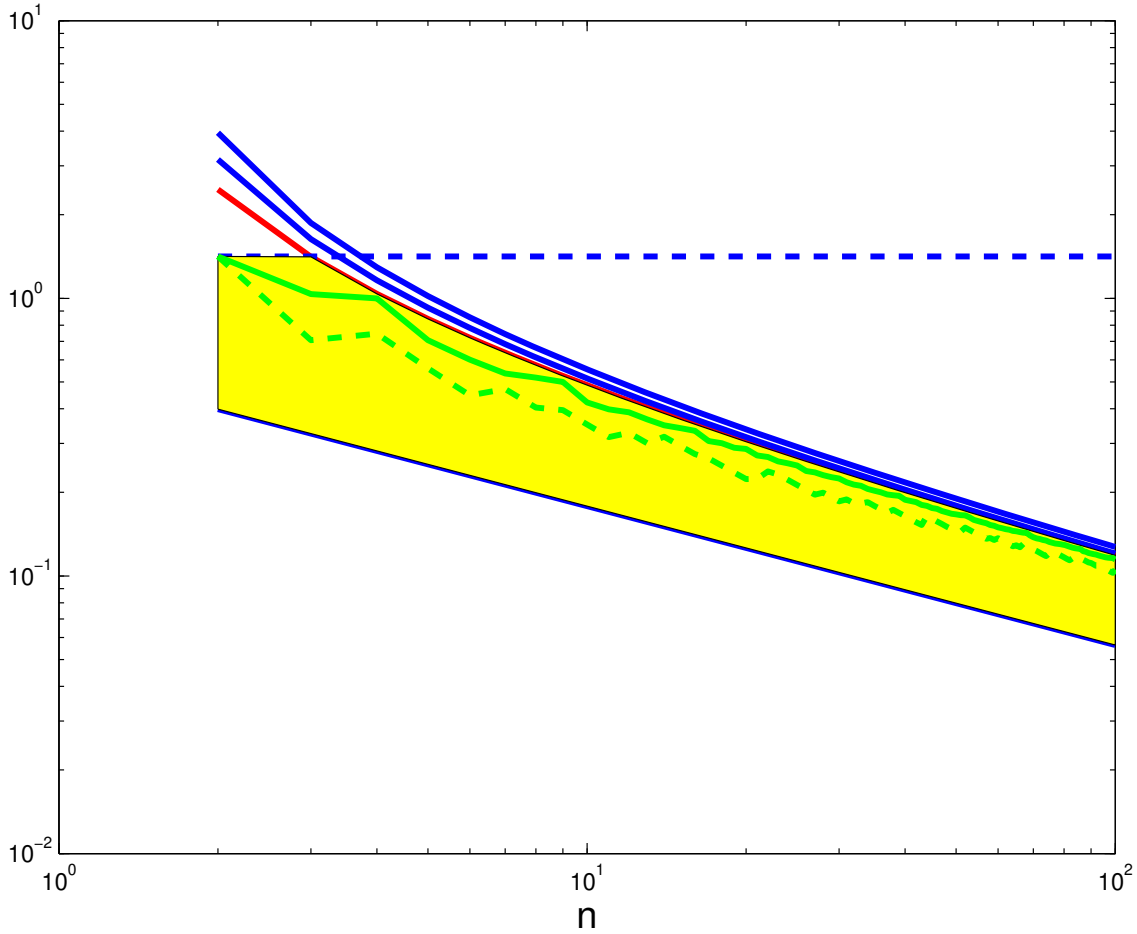
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$, including $\Phi^*_{Mm,n}$ (proved up to $n = 30$ `http://www.packomania.com/`)



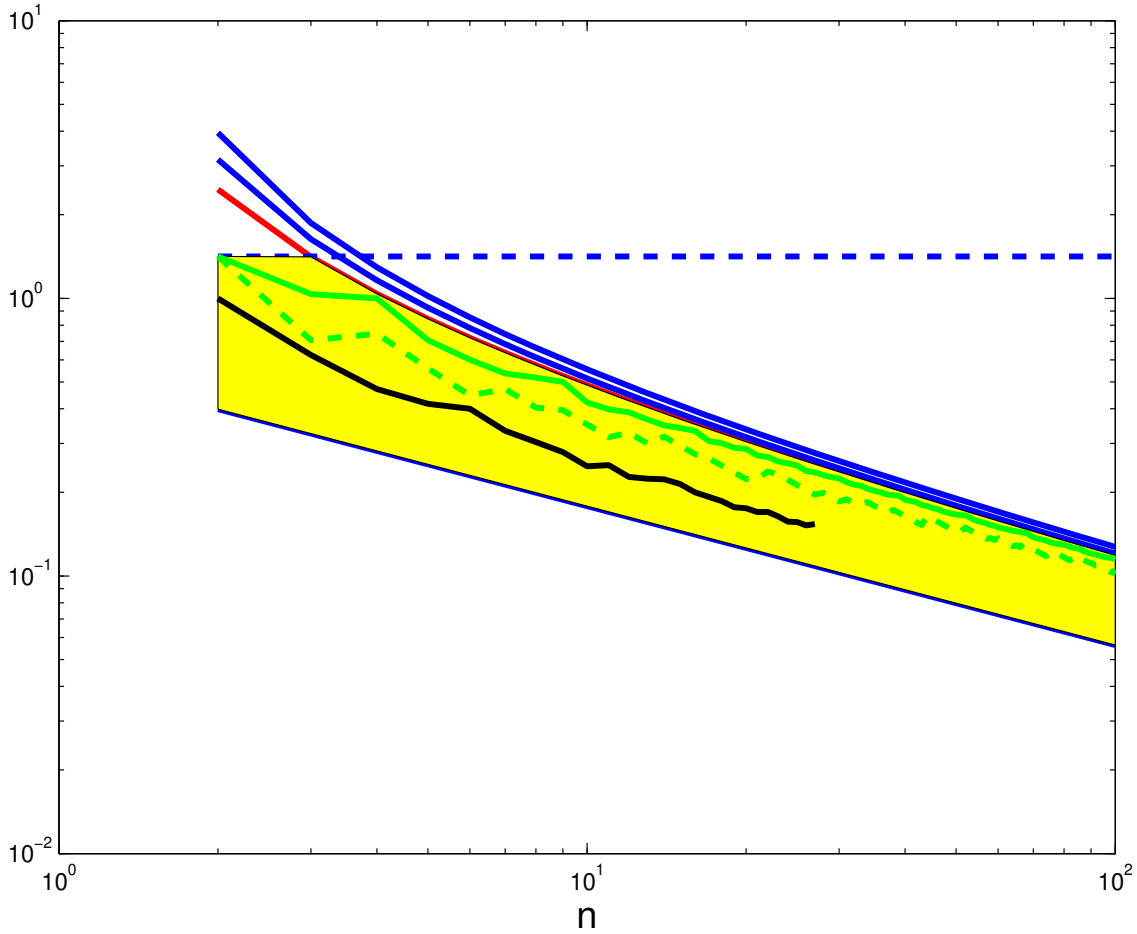
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$, including $\Phi^*_{Mm-Lh,n}$ (proved up to $n = 70$ van Dam et al. (2007), `http://www.spacefillingdesigns.nl/`)



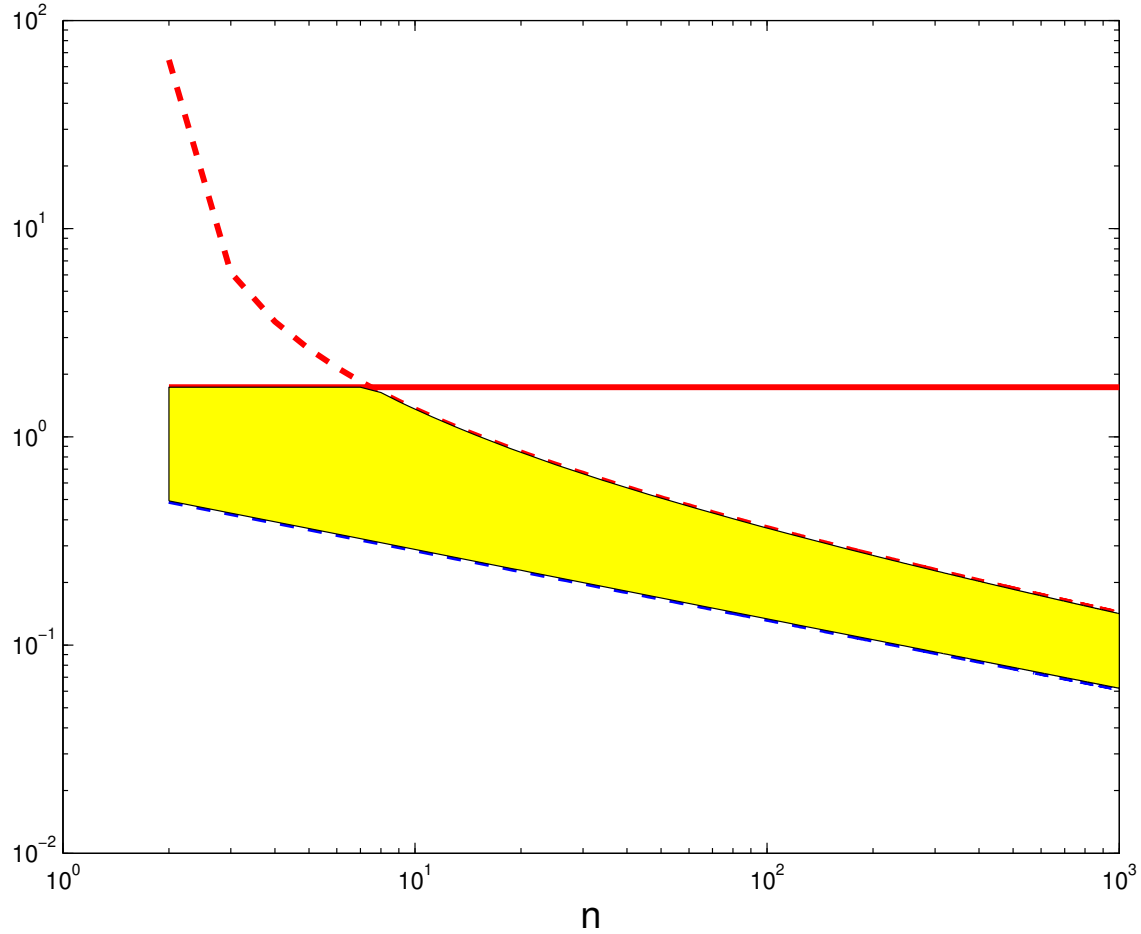
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 2$

$d = 2$, including $\Phi^*_{mM-Lh,n}$ (proved up to $n = 27$ (van Dam, 2008))



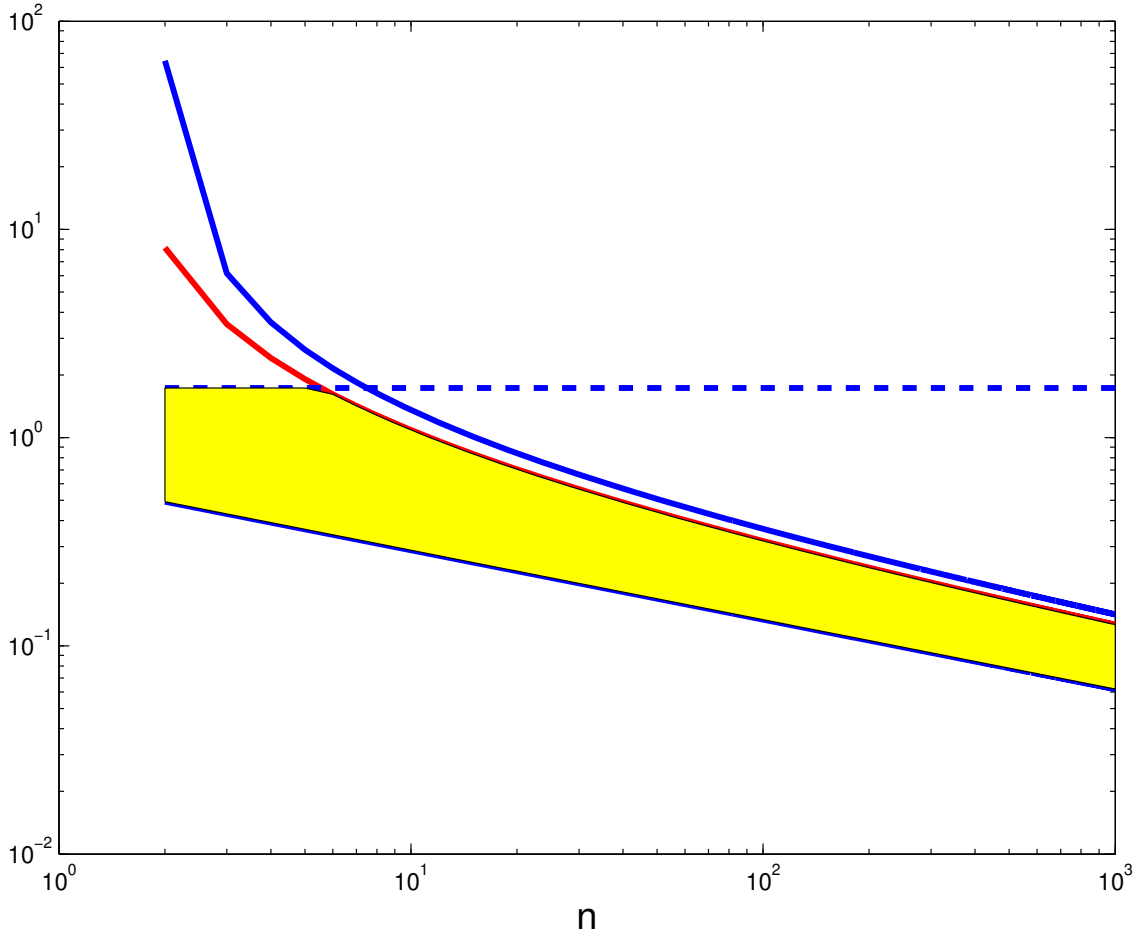
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 3$

$d = 3$ using $\boxed{R^*_n < \Phi^*_{mM,n} \leq \Phi^*_{Mm,n} < \min\{\frac{2R^*_n}{1-2R^*_n}, \sqrt{d}\}}$



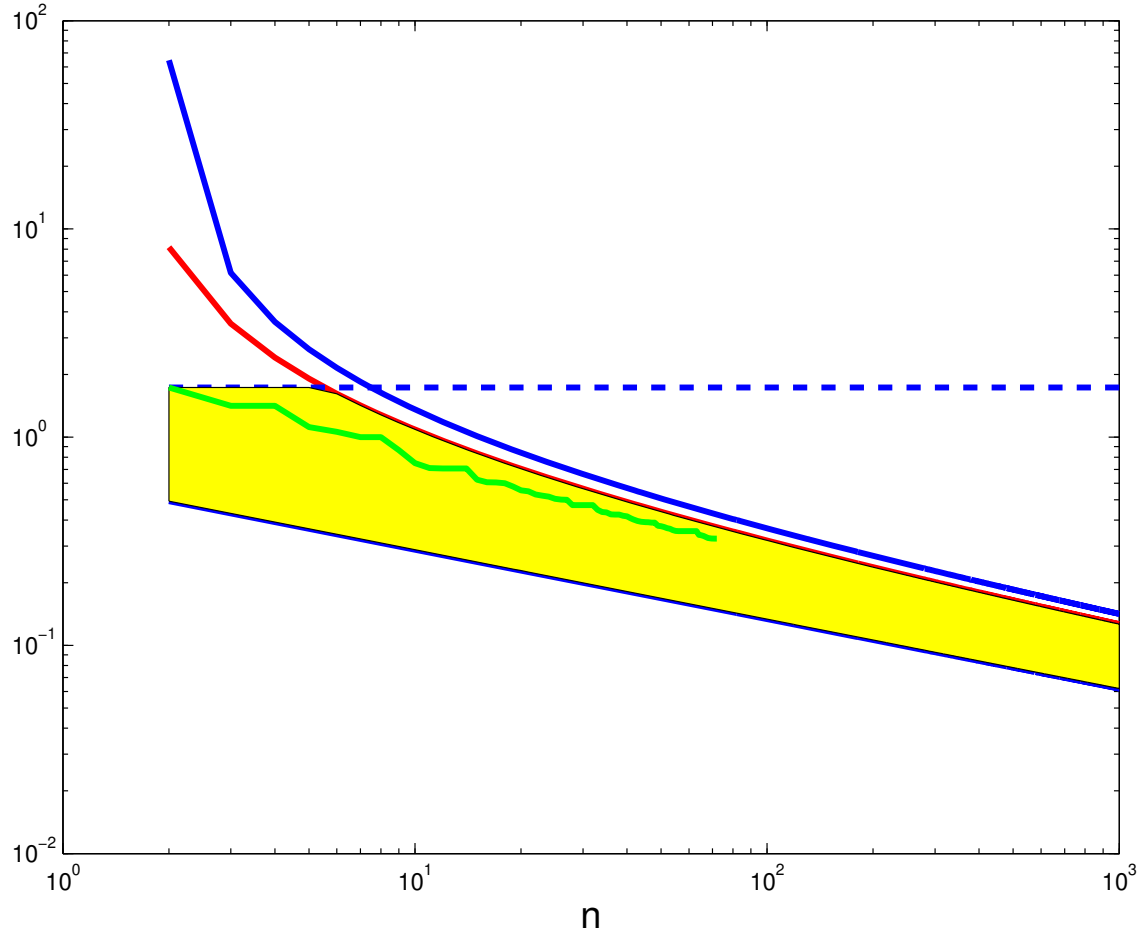
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 3$

$d = 3$ with moreover $\boxed{\Phi^*_{Mm,n} < \frac{1}{(n/\sqrt{2})^{1/3}-1}}$ (*packing density*)



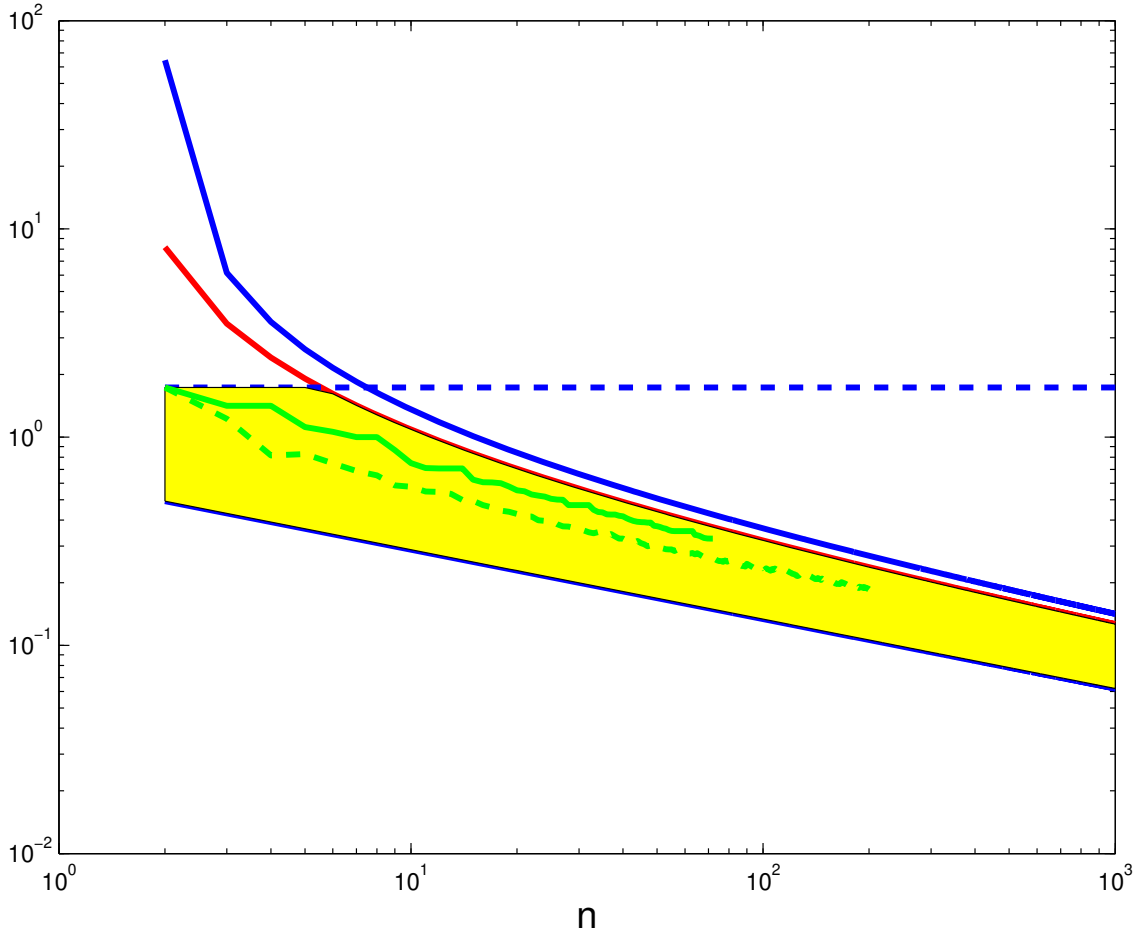
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 3$

$d = 3$, including $\Phi^*_{Mm,n}$ (`http://www.randomwalk.de/sphere/incube/`)



Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 3$

$d = 3$, including $\Phi^*_{Mm-Lh,n}$ (proved up to $n = 15$ `http://www.spacefillingdesigns.nl/`)



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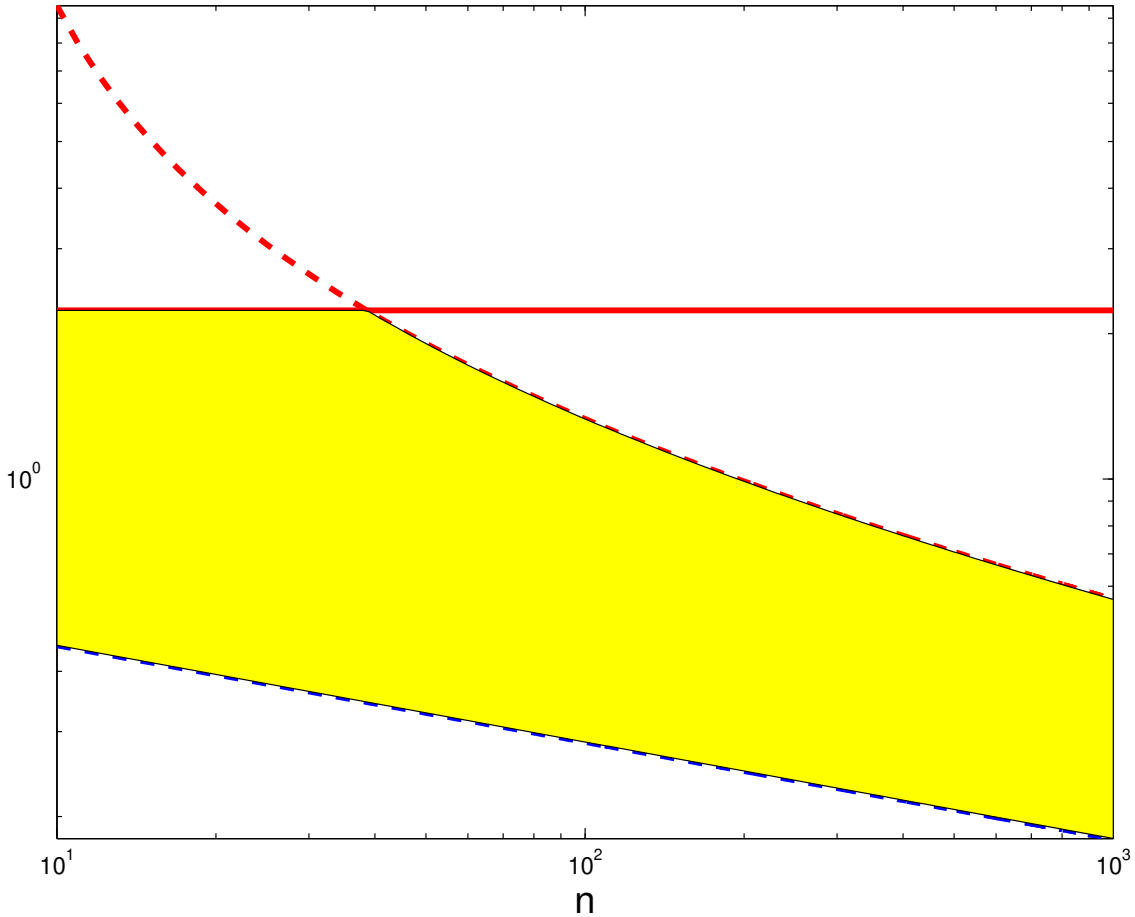
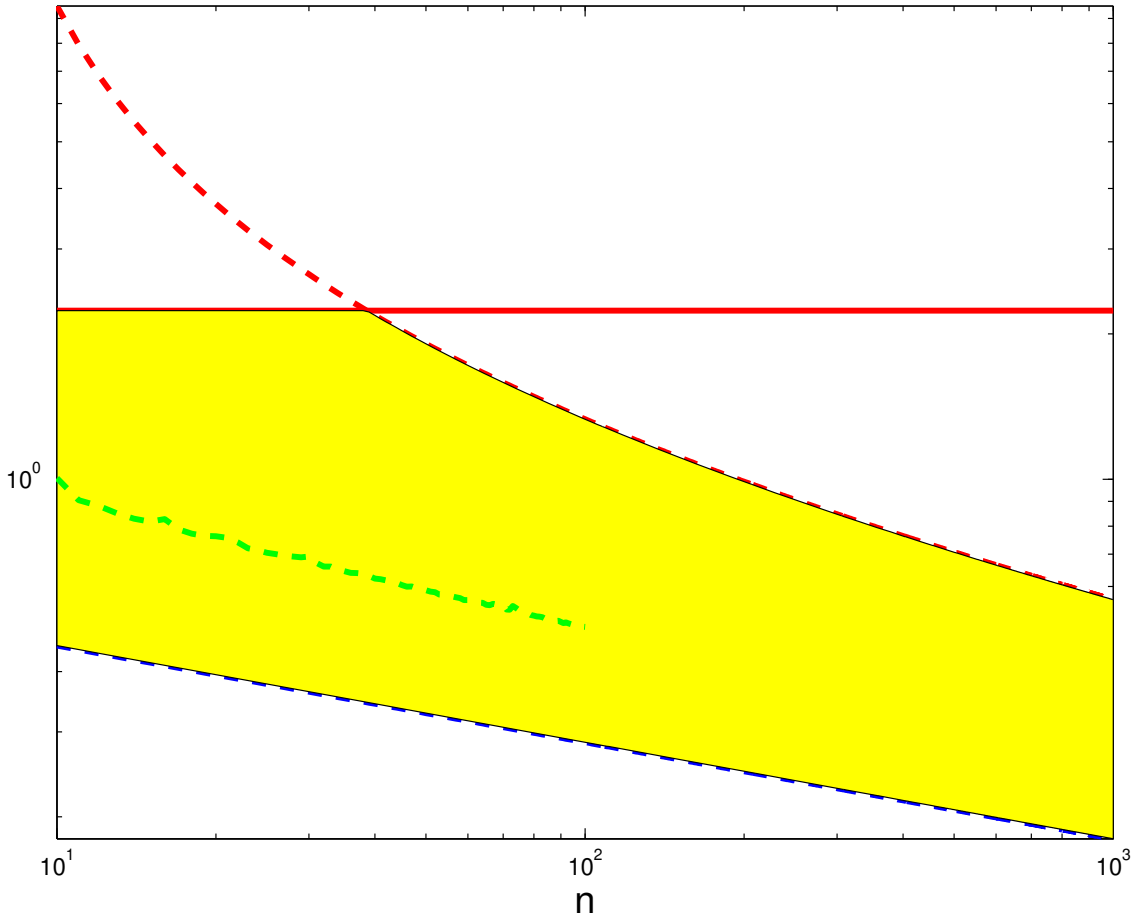


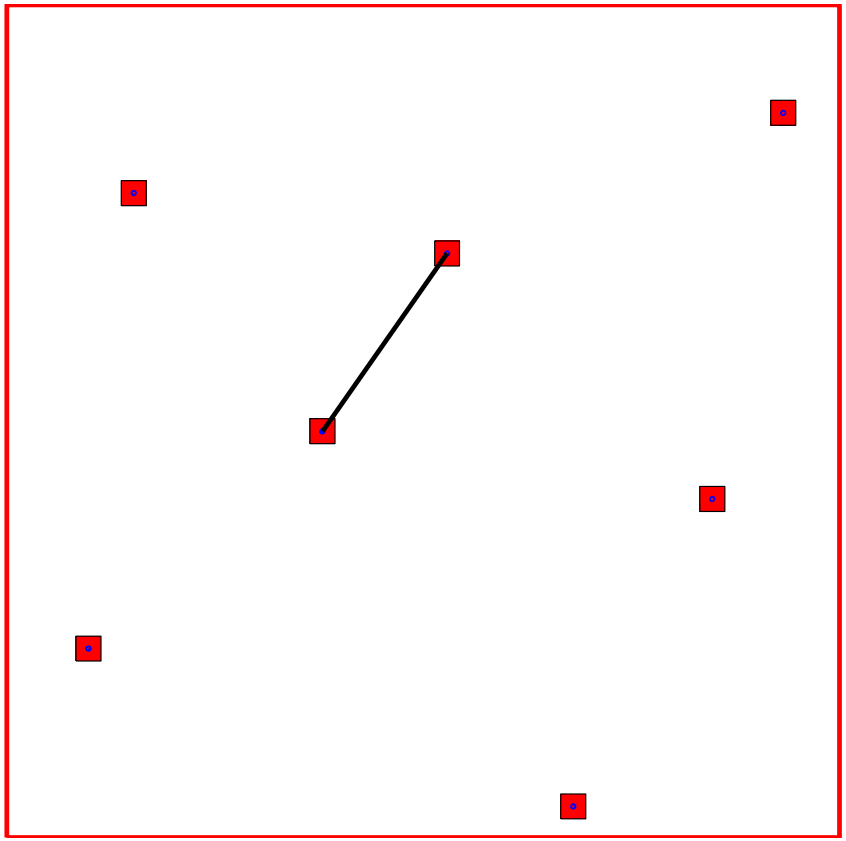
Bounds on $\Phi^*_{Mm,n}$ and $\Phi^*_{mM,n}$: $d = 5$

$d = 5$, including $\Phi^*_{Mm-Lh,n}$ (proved up to $n = 6$ http://www.spacefillingdesigns.nl/)



1.6 Regularized Maximin, energy

Maximin



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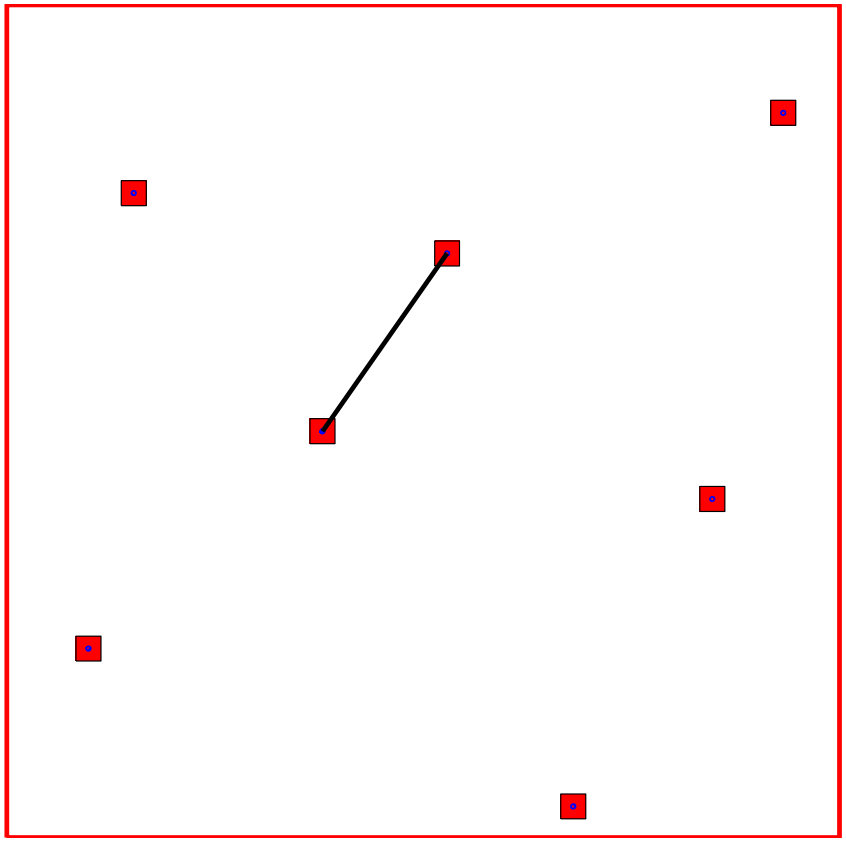
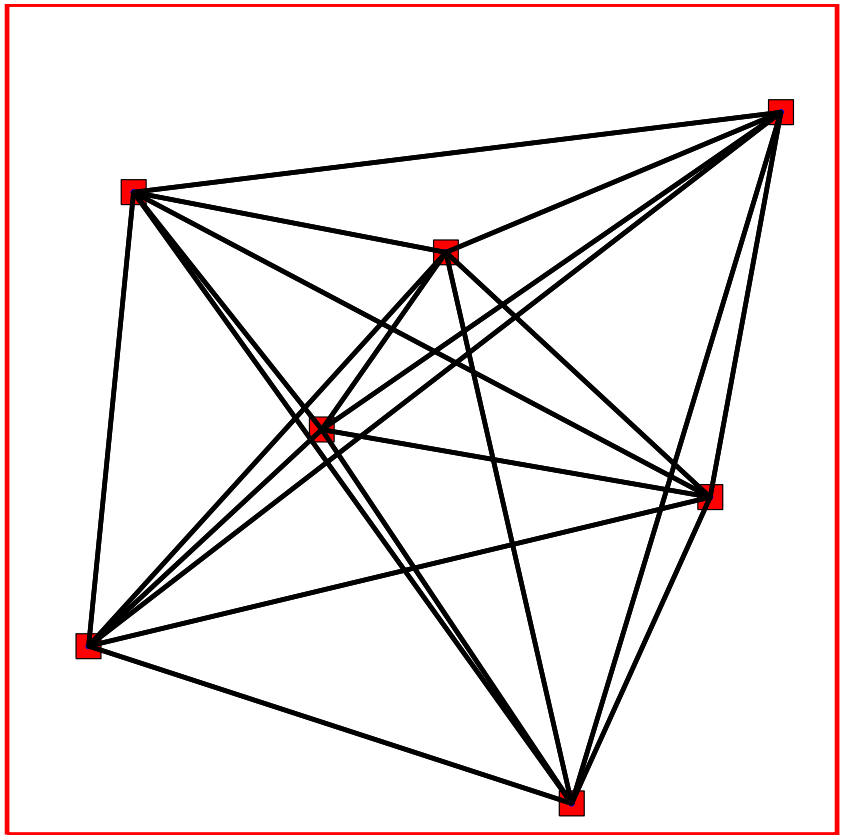


Regularization: we account for distances between all pairs of points



Denote $d_{ij} \triangleq \|\mathbf{x}_i - \mathbf{x}_j\|$ ➠ $\Phi_{Mm}(\mathbf{X}_n) = \min_{i \neq j} d_{ij}$

$$\underline{\Phi}_{[q]}(\mathbf{X}_n) \triangleq \left[\sum_{i<j} d_{ij}^{-q} \right]^{-1/q} \quad \text{and} \quad \overline{\Phi}_{[q]}(\mathbf{X}_n) \triangleq \left[\frac{1}{N} \sum_{i<j} d_{ij}^{-q} \right]^{-1/q}$$

with $N = \binom{n}{2} = n(n-1)/2$

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Then, $\boxed{\underline{\Phi}_{[q]}(\mathbf{X}_n) \leq \Phi_{Mm}(\mathbf{X}_n) \leq \overline{\Phi}_{[q]}(\mathbf{X}_n) \leq N^{1/q}\,\underline{\Phi}_{[q]}(\mathbf{X}_n)}$, $q > 0$,
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(monotonic convergence to $\Phi_{Mm}(\mathbf{X}_n)$ on both sides when $q \to \infty$)

By continuity, $\overline{\Phi}_{[0]}(\mathbf{X}_n) = \exp\left[\frac{1}{N}\sum_{i<j}\log(d_{ij})\right]$

Let $\underline{\mathbf{X}}^*_{n[q]}$ be optimal for $\underline{\Phi}_{[q]}$:

$$\frac{\Phi_{Mm}(\underline{\mathbf{X}}^*_{n[q]})}{\Phi^*_{Mm,n}} \geq N^{-1/q}\,, \text{ tends to 1 as } q \to \infty$$

(Maximin efficiency $> 1 - \epsilon$ for $q > \frac{2\log(n)}{\epsilon}$)

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➤ Maximize $\underline{\Phi}_{[q]}$ is equivalent to minimizing the energy
$E_q(\mathbf{X}_n) = \frac{2}{n(n-1)} \sum_{i,j=1,\, i\neq j}^{n} \|\mathbf{x}_i - \mathbf{x}_j\|^{-q}$

Audze and Eglais (1977) have proposed $q = 2$; when $q \lesssim 5$ optimization of Lh designs is easier than for Φ_{Mm} (Morris and Mitchell, 1995)

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Regularized version $\underline{\Phi}_{[q]}(\mathbf{X}_n)$: non-concave but differentiable
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but q should be large enough to get a good approximation of $\Phi_{Mm}(\mathbf{X}_n)$

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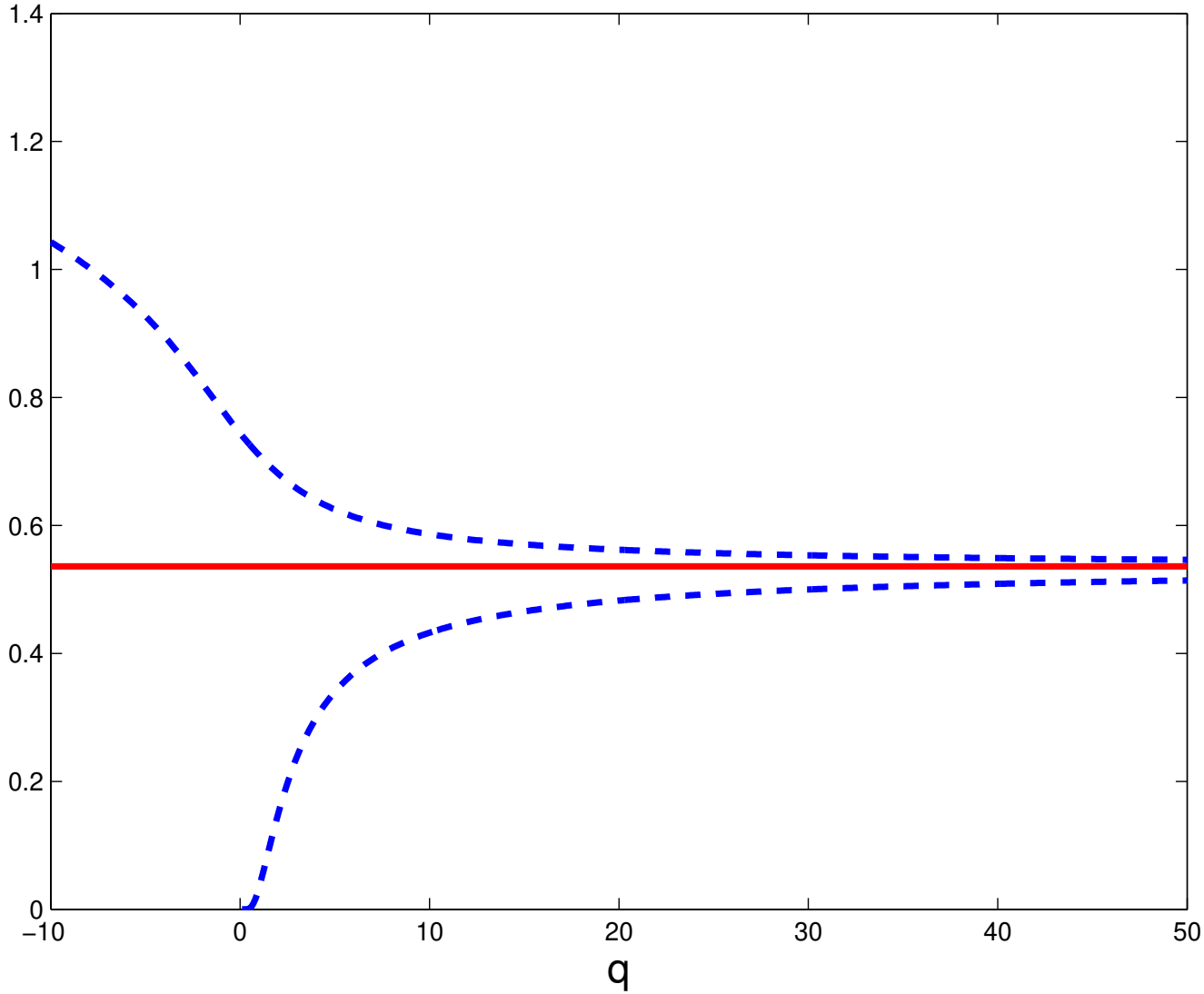
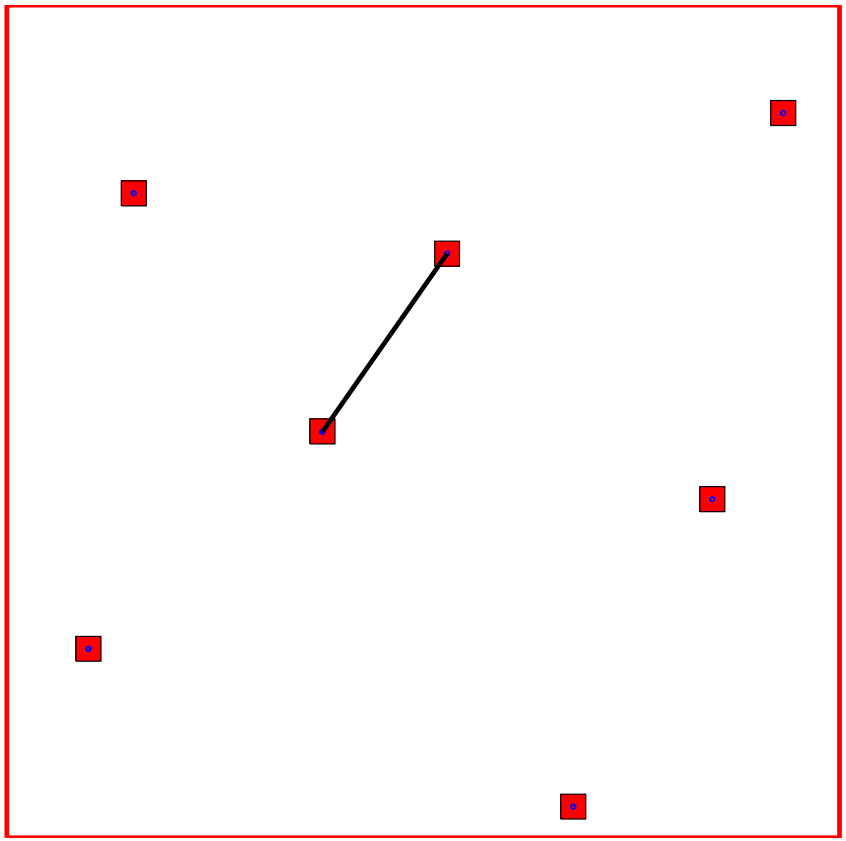
Relation with potential theory Landkof (1972); Saff (2010), P., Wynn and Zhigljavsky (2016): $\underline{\mathbf{X}}^*_{n[q]}$ = Fekete points, asymptotically distributed ($n \to \infty$) uniformly in $\mathscr{X}$ if $\boxed{q \geq d}$

$\mathbf{X}_n$ Maximin-optimal, $n = 7$, $d = 2$: Φ_{Mm} and bounds $\underline{\Phi}_{[q]}$ and $\overline{\Phi}_{[q]}$



6) Regularized Maximin with Nearest Neighbors (NN)

Maximin



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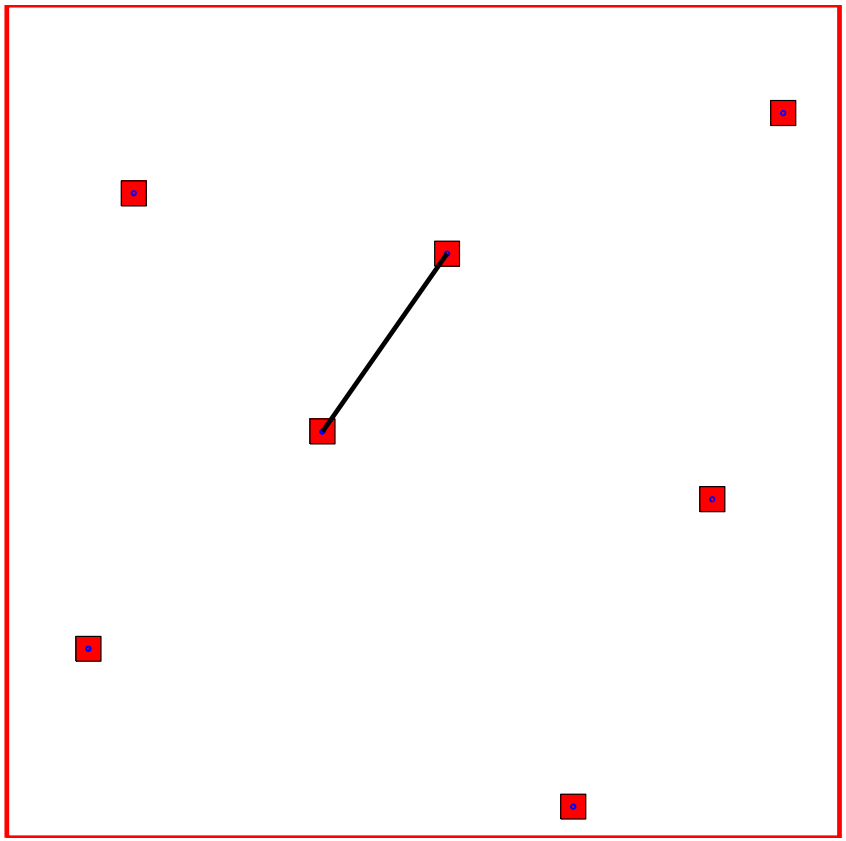
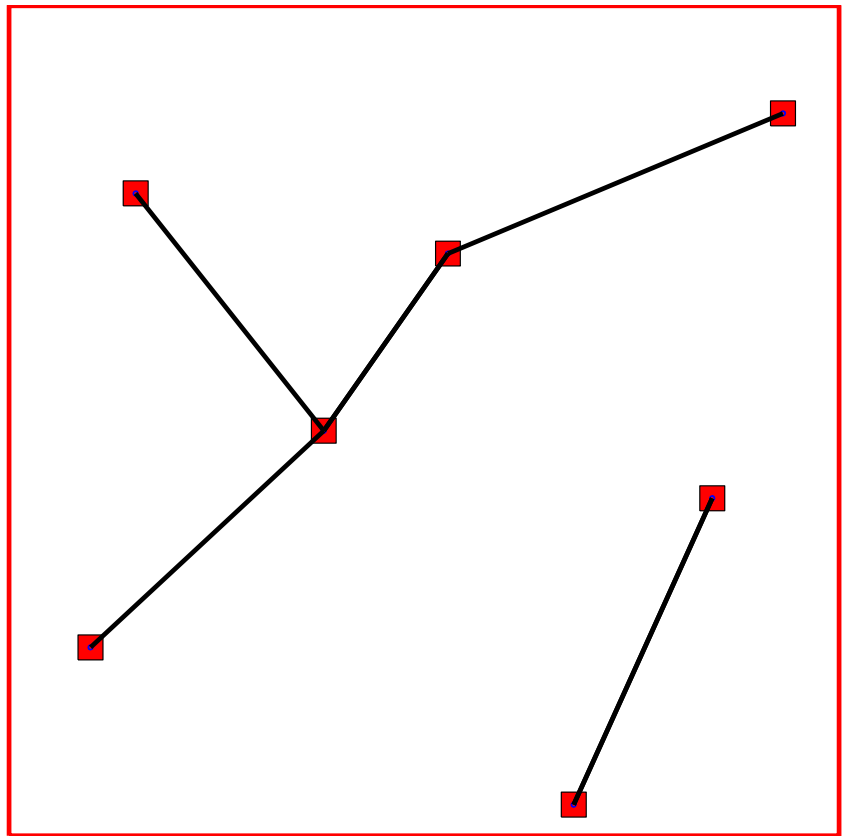


Regularization: we account for the distance between each point and its NN



We can write $\Phi_{Mm}(\mathbf{X}_n) = \min_i d_i^*$, with $d_i^* \triangleq \min_{j \neq i} \|\mathbf{x}_i - \mathbf{x}_j\|$
$=$ distance to NN of X_i

Define

$$\underline{\Phi}_{[NN,q]}(\mathbf{X}_n) = \left[\sum_{i=1}^{n} (d_i^*)^{-q}\right]^{-1/q} \quad , \quad \overline{\Phi}_{[NN,q]}(\mathbf{X}_n) = \left[\sum_{i=1}^{n} \frac{(d_i^*)^{-q}}{n}\right]^{-1/q}$$

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Then, $\boxed{\underline{\Phi}_{[NN,q]}(\mathbf{X}_n) \leq \Phi_{Mm}(\mathbf{X}_n) \leq n^{1/q}\, \underline{\Phi}_{[NN,q]}(\mathbf{X}_n)}$, $q > 0$

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By continuity: $\overline{\Phi}_{[NN,0]}(\mathbf{X}_n) = \exp\left[\sum_{i=1}^{n} \frac{\log(d_i^*)}{n}\right]$

Maximin efficiency:

$$\frac{\Phi_{Mm}(\underline{\mathbf{X}}^*_{n[NN,q]})}{\Phi^*_{Mm,n}} \geq n^{-1/q},$$

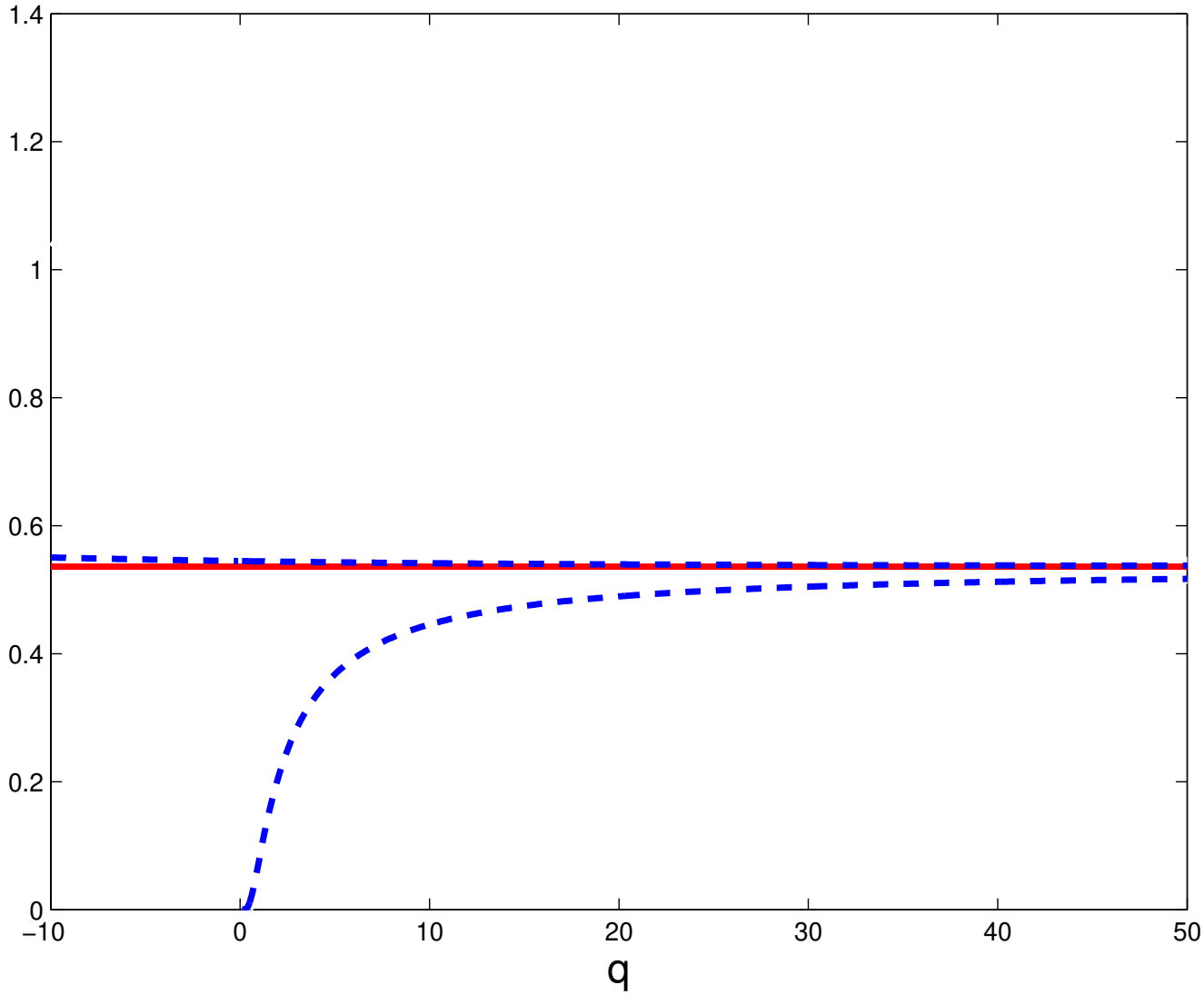
with $\underline{\mathbf{X}}^*_{n[NN,q]}$ optimal for $\underline{\Phi}_{[NN,q]}$

Maximin efficiency $> 1-\epsilon$ for $q > \frac{\log(n)}{\epsilon}$

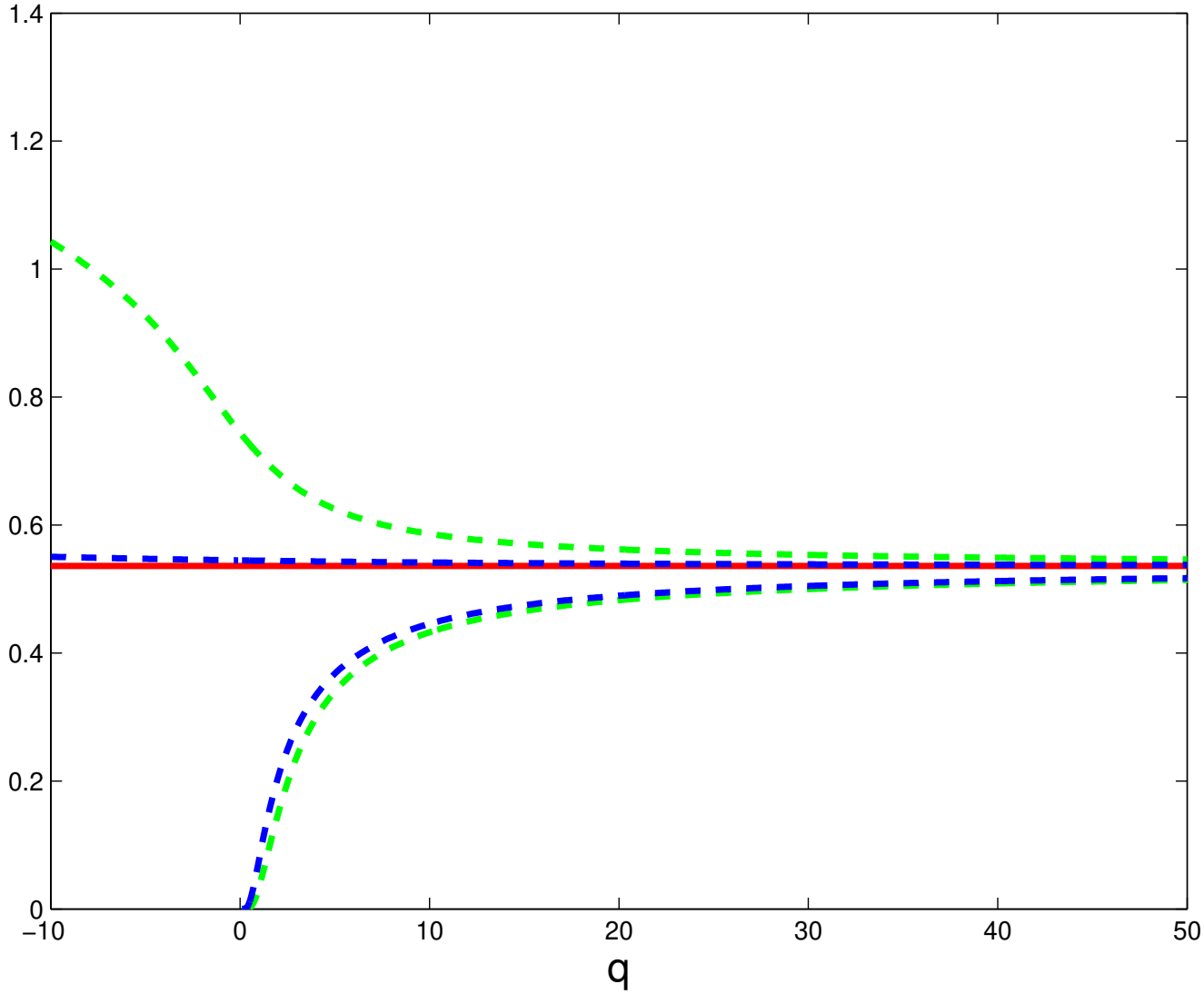
$\rightarrow$ we gain a factor 2 comparatively to $\underline{\Phi}_{[q]}(\mathbf{X}_n)$

(we only regularized $\min_i$)

$\mathbf{X}_n$ Maximin-optimal, $n = 7$, $d = 2$: Φ_{Mm} and regularization with $\underline{\Phi}_{[NN,q]}$



$\mathbf{X}_n$ Maximin-optimal, $n = 7$, $d = 2$: Φ_{Mm} and regularization with $\underline{\Phi}_{[NN,q]}$ and $\underline{\Phi}_{[q]}$



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➠ modification of regularized Maximin that produces designs with good space-filling properties in all lower dimensional subspaces

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$(\underline{\Phi}_{[q]}(\mathbf{X}_n) \to \Phi_{Mm}(\mathbf{X}_n) = \min_{i \neq j} d_{ij}$ as $q \to \infty)$

Replace ℓ_2 distance d_{ij} by weighted-ℓ_2 distance (measure of importance on factors)

$$d_{ij,\mathbf{w}} = \left[\sum_{k=1}^{d} w_k (\{\mathbf{x}_i\}_k - \{\mathbf{x}_j\}_k)^2\right]^{1/2}$$

➞ minimize $\sum_{i<j} d_{ij,\mathbf{w}}^{-q}$ for a large q, but which $\mathbf{w}$?

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➞ minimize $\sum_{i<j} d_{ij,\mathbf{w}}^{-q}$ for a large q, but which $\mathbf{w}$?

Take $\mathbf{w} \in \mathcal{P}_d = \{\mathbf{w} : w_k \geq 0,\ \sum_{k=1}^{d} w_k = 1\}$

Put a uniform prior π on $(w_1, \ldots, w_{d-1})$

For $q = 2d$, $\boxed{\mathrm{E}_{\mathbf{w}}\left\{\sum_{i<j} d_{ij,\mathbf{w}}^{-q}\right\} = \frac{1}{[(d-1)!]^2} \sum_{i<j} \frac{1}{\prod_{k=1}^{d} (\{\mathbf{x}_i\}_k - \{\mathbf{x}_j\}_k)^2}}$ Very promising!

Remark: measures of regularity (and not of space fillingness!)

$$R_1(\mathbf{X}_n) \triangleq \frac{\text{var}^{1/2}(d_i^*)}{\text{E}(d_i^*)} = \frac{\left[\frac{1}{n}\sum_{i=1}^{n}(d_i^* - \bar{d})^2\right]^{1/2}}{\bar{d}}, \text{ with } \bar{d} \triangleq \text{E}(d_i^*) = \frac{1}{n}\sum_{i=1}^{n} d_i^*$$

$= 0$ for a regular grid

▲ invariant by scale transformation ▲

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$R_2(\mathbf{X}_n) \triangleq \frac{\max_{1\leq i\leq n} d_i^*}{\min_{1\leq i\leq n} d_i^*}$ (≥ 1, $= 1$ for a regular grid)

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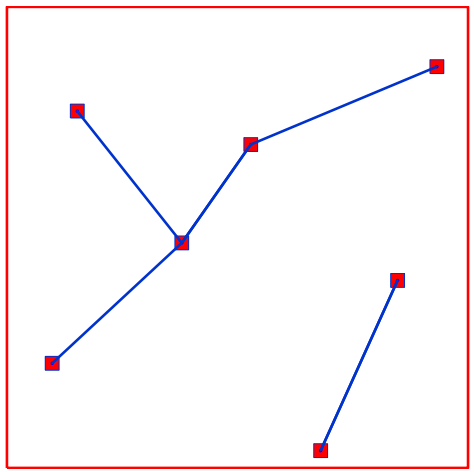
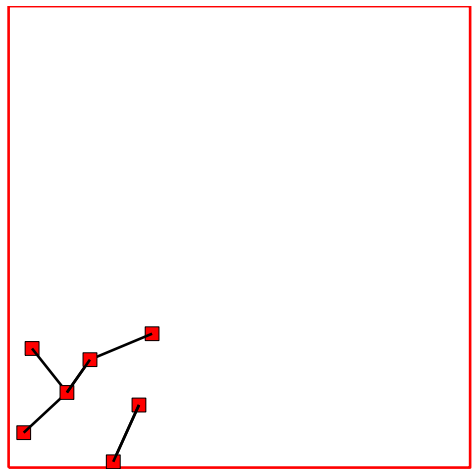
▲ invariant by scale transformation ▲

These two designs have the same R_1 and R_2 values





2 Uniformity: quasi Monte-Carlo, discrepancy

2.1 Entropy, optimal graphs

Consider $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ as a sample of size n of variables $\mathbf{x}_i$ i.i.d. in $\mathscr{X}$ with p.d.f. $\varphi(\cdot)$

Rényi entropy of $\varphi(\cdot)$ of order α :

$$H_\alpha{}^*(\varphi) \triangleq \frac{1}{1-\alpha} \log \int \varphi^\alpha(\mathbf{x})\,\mathrm{d}\mathbf{x} \ (\alpha \neq 1)$$

Tsallis entropy of $\varphi(\cdot)$ of order α :

$$H_\alpha(\varphi) \triangleq \frac{1}{\alpha-1}\left[1 - \int \varphi^\alpha(\mathbf{x})\,\mathrm{d}\mathbf{x}\right] \ (\alpha \neq 1)$$

which tend to

$$H_1(\varphi) \triangleq -\log \int \varphi(\mathbf{x}) \log[\varphi(\mathbf{x})]\,\mathrm{d}\mathbf{x} \text{ (Shannon entropy) as } \alpha \to 1$$

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which tend to

$$H_1(\varphi) \triangleq -\log \int \varphi(\mathbf{x}) \log[\varphi(\mathbf{x})]\, \mathrm{d}\mathbf{x} \text{ (Shannon entropy) as } \alpha \to 1$$

➤ For $\alpha > 0$, $H_\alpha{}^*(\varphi)$, $H_\alpha(\varphi)$ maximum for φ uniform over $\mathscr{X}$

2 Uniformity: quasi Monte-Carlo, discrepancy

2.1 Entropy, optimal graphs

Consider $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ as a sample of size n of variables $\mathbf{x}_i$ i.i.d. in $\mathscr{X}$ with p.d.f. $\varphi(\cdot)$

Rényi entropy of $\varphi(\cdot)$ of order α :

$$H_\alpha{}^*(\varphi) \triangleq \frac{1}{1-\alpha} \log \int \varphi^\alpha(\mathbf{x})\, \mathrm{d}\mathbf{x} \ (\alpha \neq 1)$$

Tsallis entropy of $\varphi(\cdot)$ of order α :

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➤ For $\alpha > 0$, $H_\alpha{}^*(\varphi)$, $H_\alpha(\varphi)$ maximum for φ uniform over $\mathscr{X}$

➠ Construct an estimate $\hat{H}_{n\alpha}$ of $H_\alpha^*(\varphi)$ from $\mathbf{X}_n$, use $\hat{H}_{n\alpha}$ as design criterion, to be maximized w.r.t. $\mathbf{X}_n$

▲ Entropie of "distribution of $\mathbf{x}_i$" $\neq$ entropy criterion for Gaussian Random Fields, see § II-1.3 (although relations exist)

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1) A rather natural idea: plug-in

- Construct a kernel estimator $\hat{\varphi}_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} K_{\sigma^2}(\mathbf{x} - \mathbf{x}_i)$, $K_{\sigma^2}(\cdot)$ = p.d.f. with mean $\mathbf{0}$ and variance $\sigma^2\mathbf{I}_d$ (small enough)
- Use $H_\alpha(\hat{\varphi}_n)$, $\alpha > 0$, as design criterion

Jourdan and Franco (2010) use $H_1(\varphi)$, computationally costly for large d

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A peculiarity of H_2: if $K_{\sigma^2}(\cdot)$ corresponds to $\mathcal{N}(0,\sigma^2)$, then

$$\int_{\mathbb{R}^d} \hat{\varphi}_n^2(\mathbf{x})\,\mathrm{d}\mathbf{x} = \frac{1}{n^2}\sum_{i,j=1}^n K_{2\sigma^2}(\mathbf{x}_i-\mathbf{x}_j)$$

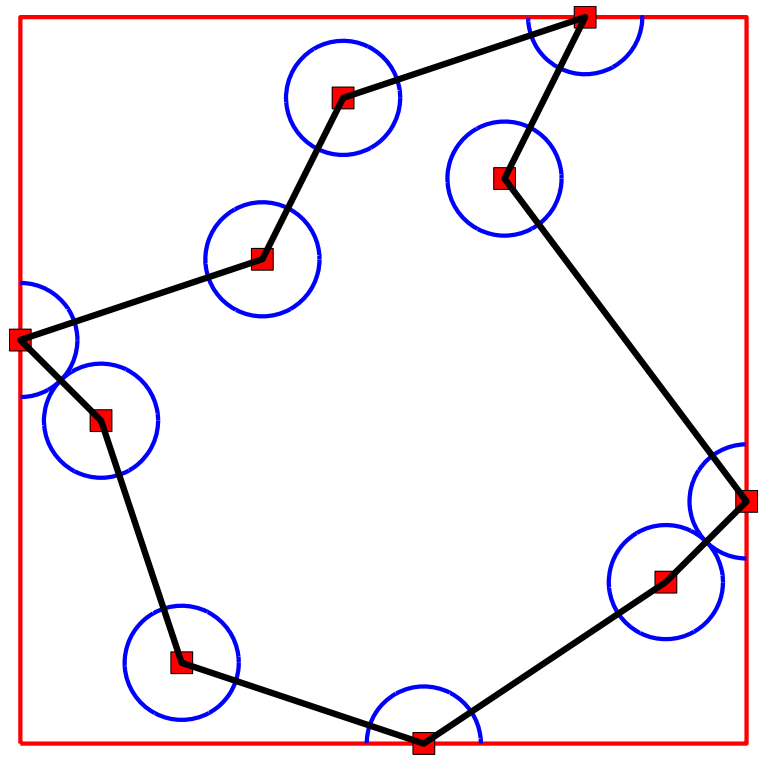
$$\Rightarrow \boxed{H_2(\hat{\varphi}_n) = 1 - \frac{1}{n^2}\sum_{i,j=1}^n K_{2\sigma^2}(\mathbf{x}_i-\mathbf{x}_j)}$$

= intra-distances criterion

2) Optimal graphs:

n points $\mathbf{X}_n$
(here, a Lh with $n = 10$, $d = 2$)

Traveling Salesman (TS) graph $\mathcal{G}_{TS}(\mathbf{X}_n)$



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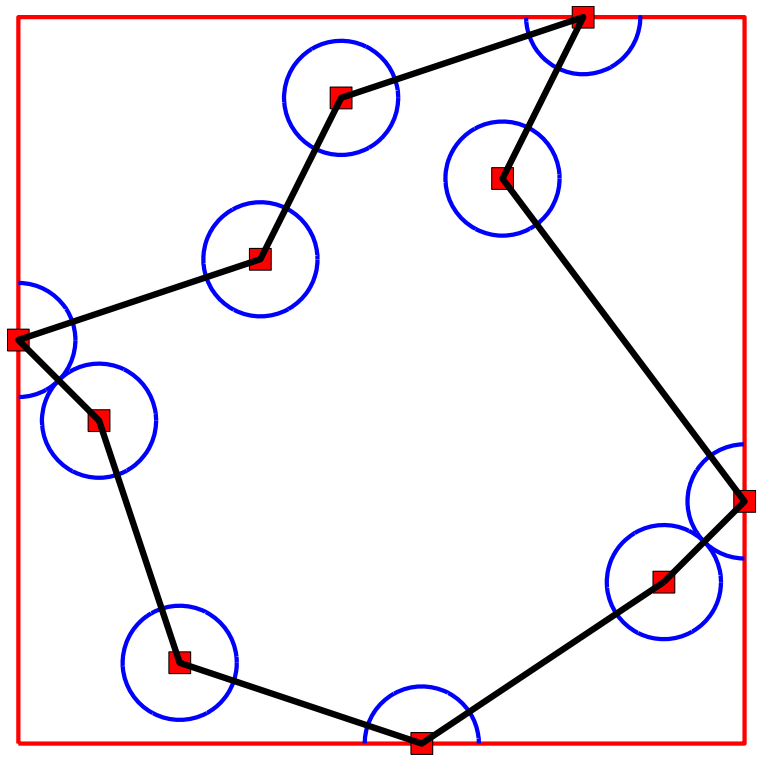

(Beardwood et al., 1959): $\mathbf{x}_i$ i.i.d. with p.d.f. φ, the edges e_i of $\mathcal{G}_{TS}(\mathbf{X}_n)$ satisfy:

$$\frac{\sum_{e_i \in \mathcal{G}_{TS}(\mathbf{X}_n)} |e_i|}{n^{(d-1)/d}} \to C(d) \int \varphi^{(d-1)/d}(\mathbf{x})\, \mathrm{d}\mathbf{x} \text{ a.s.}, \quad n \to \infty$$

Later (Steele, 1981) considered other Euclidean functionals on $\mathbf{X}_n$, (Redmond and Yukich, 1994) used the notion of quasi-additivity

Many results... (Redmond and Yukich, 1996; Yukich, 1998; Penrose and Yukich, 2003; Wade, 2007; Penrose and Yukich, 2011)...

$$\frac{\sum_{e_i \in \mathcal{G}(\mathbf{X}_n)} |e_i|^\beta}{n^{1-\beta/d}} \to C(\beta, d) \int \varphi^{1-\beta/d}(\mathbf{x})\, \mathrm{d}\mathbf{x}\,, \quad n \to \infty$$

with $\mathcal{G}(\mathbf{X}_n)$ Minimum Spanning Tree (MST), NN, TS, Voronoï, Delaunay, Sphere of Influence, Gabriel... (different types of convergence (L_p), different conditions on φ and β...)

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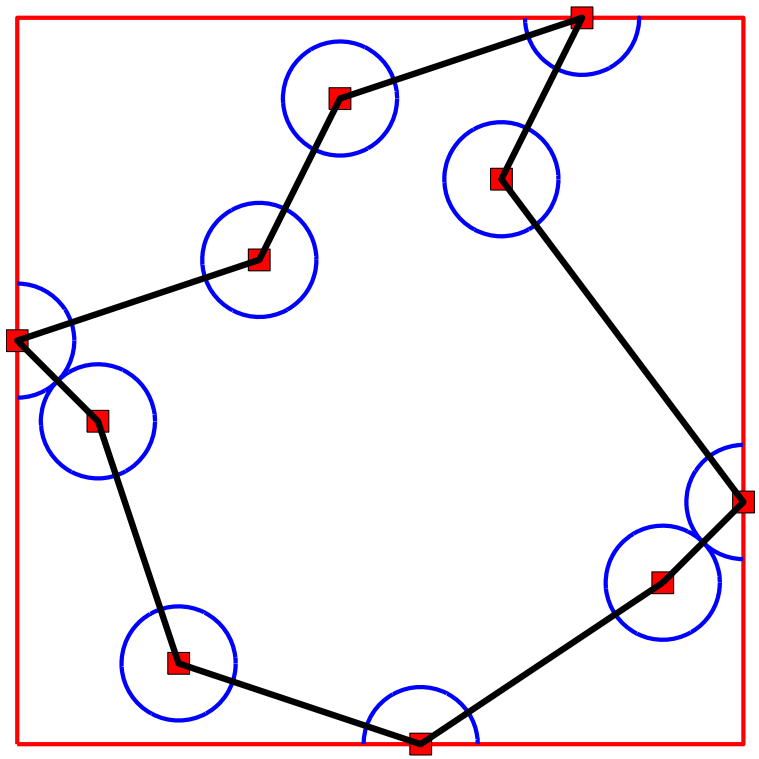

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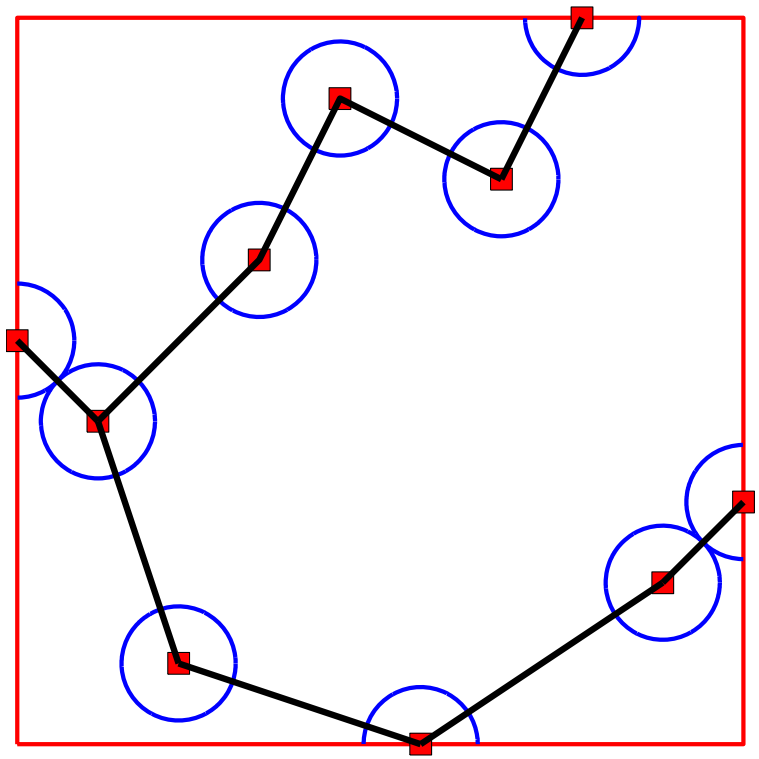
$\mathbf{X}_n$ a Lh with $n = 10$, $d = 2$: $\mathcal{G}_{MST}(\mathbf{X}_n)$



Many results... (Redmond and Yukich, 1996; Yukich, 1998; Penrose and Yukich, 2003; Wade, 2007; Penrose and Yukich, 2011)...

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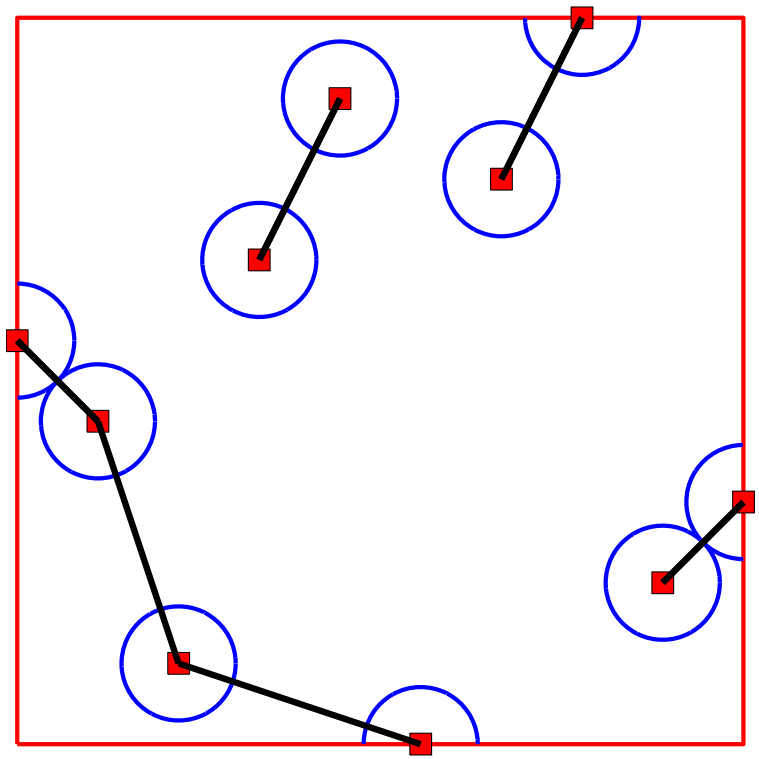
$\mathbf{X}_n$ a Lh with $n = 10$, $d = 2$: $\mathcal{G}_{NN}(\mathbf{X}_n)$



To summarize: we construct such a graph $\mathcal{G}$ on $\mathbf{X}_n$, then

$$\Phi_{\mathcal{G},\beta}(\mathbf{X}_n) = \frac{\sum_{e_i \in \mathcal{G}(\mathbf{X}_n)} |e_i|^\beta}{n^{1-\beta/d}} \quad \to \quad C(\beta, d) \int \varphi^{1-\beta/d}(\mathbf{x})\, \mathrm{d}\mathbf{x}\,, \;\; n \to \infty$$

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- Choice of $\mathbf{X}_n$? maximize H_α with $\alpha > 0$

  if $\alpha > 1$ $(-d < \beta < 0)$ ⇛ minimize $\int \varphi^\alpha(\mathbf{x})\,\mathrm{d}\mathbf{x}$

  ⇛ minimize $\Phi_{\mathcal{G},\beta}(\mathbf{X}_n)$

  For $\mathcal{G}_{NN}$ ⇛ maximize $\overline{\Phi}_{[NN,q]}(\mathbf{X}_n)$ with $0 < q = -\beta < d$

= maximize an intra-distances criterion

▲ Maximizing $\overline{\Phi}_{[NN,q]}(\mathbf{X}_n)$ with $q < 0$ is not always convenient ▲
(= maximize $\Phi_{\mathcal{G}_{NN},\beta}(\mathbf{X}_n)$ with $\beta > 0$)

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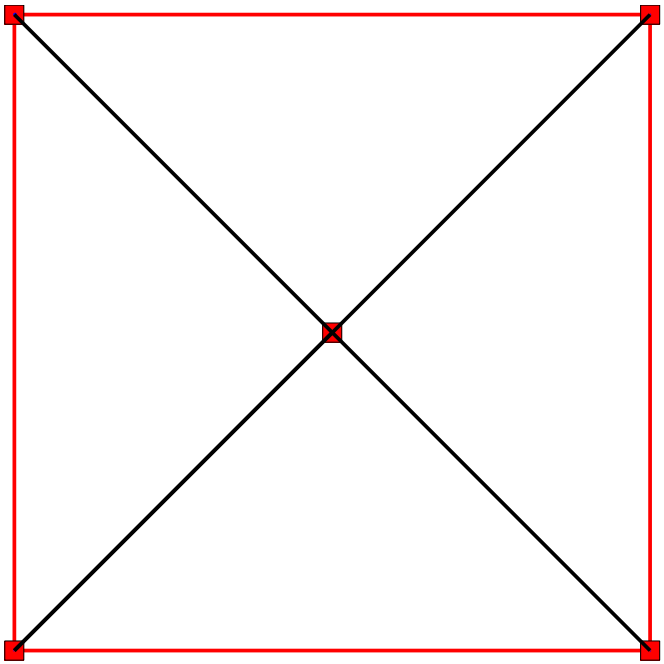
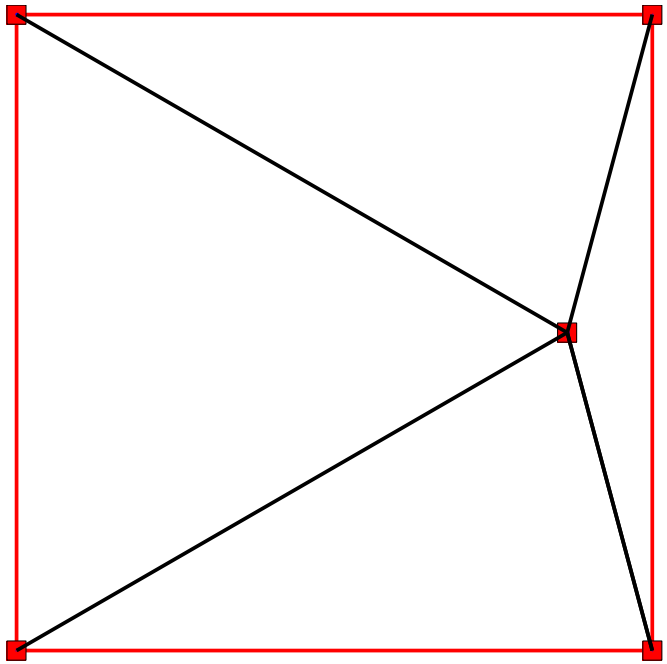
Ex: $\mathscr{X} = [0,1]^2$, comparaison between 2 designs $\mathbf{X}_n^a$ and $\mathbf{X}_n^b$ for $\overline{\Phi}_{[NN,q]}$ with $q = -1$ ($\beta = 1$)

$\mathbf{X}_n^a$

$(1/n)\sum_{e_i \in \mathcal{G}_{NN}(\mathbf{X}_n^a)} |e_i| = \frac{\sqrt{2}}{2} \simeq 0.70711$



$\mathbf{X}_n^b$
central point at $(\sqrt{3}/2, 1/2)$
$(1/n)\sum_{e_i \in \mathcal{G}_{NN}(\mathbf{X}_n^b)} |e_i| \simeq 0.71058$



. . . but the $|e_i|$ have a larger variance for $\mathbf{X}_n^b$ than for $\mathbf{X}_n^a$

MST Graph: Franco (2008); Franco et al. (2009) use a representation in the plane defined by

the mean $E_n = (1/n) \sum_{e_i \in \mathcal{G}_{MST}(\mathbf{X})} |e_i|$ and

the standard deviation $S_n = \left(\text{var}_{\mathcal{G}_{MST}(\mathbf{X})} \{|e_i|\} \right)^{1/2}$

to classify different sorts of space-filling designs $\mathbf{X}_n$

$\rightarrow$ we wish to have a large E_n and a small S_n

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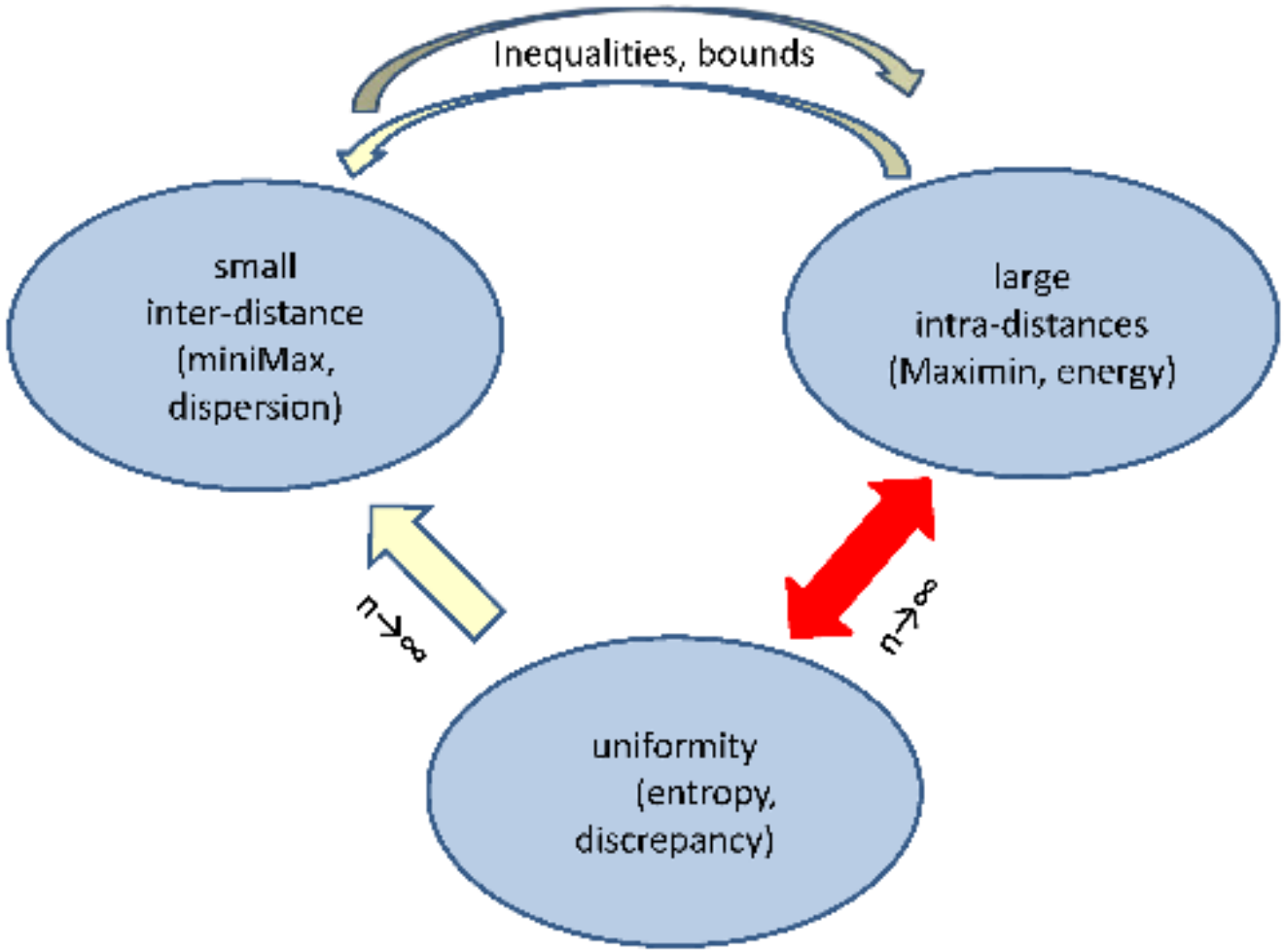
➠ For $\Phi_{Mm}(\cdot)$, or $\overline{\Phi}_{[q]}(\cdot)$ with $q > d$, or $\overline{\Phi}_{[NN,q]}(\cdot)$ with $q > 0$,
the distribution of an optimum design should be close to uniformity


Inequalities, bounds
small
inter-distance
(miniMax,
dispersion)
large
intra-distances
(Maximin, energy)
uniformity
(entropy,
discrepancy)
$n \to \infty$
$n \to \infty$

2.2 **Discrepancy: motivation** (see (Niederreiter, 1992, Chap. 1,2) — true monument with 371 references)

Integration with Monte Carlo (MC) method

$\mathscr{X}$ compact $\subset \mathbb{R}^d$,

$$\int_{\mathscr{X}} f(\mathbf{u})\,\mathrm{d}\mathbf{u} \quad \simeq \quad \mathrm{vol}(\mathscr{X})\frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

for x_i i.i.d. $\sim \mu$ uniform over $\mathscr{X}$ ➠ error $\simeq \mathcal{O}(n^{-1/2})$

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Trapezoidal rule in dimension d ➠ error $\simeq \mathcal{O}(n^{-2/d})$

➠ MC better than trapezoidal rule for $d \geq 5$ (without any regularity assumption on f)

We can do better: quasi-Monte Carlo (QMC) method

➠ discrepancy

Quasi-Monte Carlo (QMC) method

Evaluate f at deterministic $\mathbf{x}_i$ in $\mathscr{X} = \mathbb{I}_d \triangleq [0,1]^d$:

$$\widehat{I}_n \triangleq \frac{1}{n}\sum_{i=1}^n f(\mathbf{x}_i) \to I(f) = \int_{\mathbb{I}_d} f(\mathbf{u})\,\mathrm{d}(\mathbf{u}),\ n \to \infty,$$

for all Riemann integrable f if the $\mathbf{x}_1, \mathbf{x}_2, \ldots$ are uniformly distributed in $\mathbb{I}_d$

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➠ requires $\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^n \mathcal{I}_{\mathbb{B}}(\mathbf{x}) = \mathrm{vol}(\mathbb{B})$ for all $\mathbb{B} \subset \mathbb{I}_d$

Speed of convergence of $\widehat{I}_n \to I(f)$?

The distribution of $\mathbf{x}_i$ must be close to uniform:

discrepancy measures distance to uniformity

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Discrepancy

$$\triangleright \quad D_n(\mathscr{B}, \mathbf{X}_n) \triangleq \sup_{\mathbb{B}\in\mathscr{B}} \left| \frac{\text{nb. of } \mathbf{x}_i \text{ in } \mathbb{B}}{n} - \mathrm{vol}(\mathbb{B}) \right| \quad \triangleleft$$

with $\mathscr{B}$ a family of subsets of $\mathbb{I}_d$ ($\Rightarrow 0 \leq D_n(\mathscr{B}, \mathbf{X}_n) \leq 1$)

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with $\mathscr{B}$ a family of subsets of $\mathbb{I}_d$ ($\Rightarrow 0 \leq D_n(\mathscr{B}, \mathbf{X}_n) \leq 1$)

We shall consider particular families $\mathscr{B}$ ...

Two important special cases:

- Star-discrepancy $D_n^*(\mathbf{X}_n) = D_n(\mathscr{B}, \mathbf{X}_n)$ when
  $\mathscr{B}$ contains all subsets defined by $\prod_{\ell=1}^d [0, u_\ell)$
  $\boxed{D_n^*(\mathbf{X}_n) = \sup_{\mathbf{u}\in[0,1]^d} |\mathrm{F}_n(\mathbf{u}) - \mathrm{F}_U(\mathbf{u})|}$
  ($\mathrm{F}_n(\cdot) \triangleq$ empirical d.d.f., $\mathrm{F}_U(\mathbf{u}) \triangleq \prod_{\ell=1}^d \{\mathbf{u}\}_\ell =$ c.d.f. of uniform)
- Extreme discrepancy $D_n(\mathbf{X}_n) = D_n(\mathscr{B}, \mathbf{X}_n)$ when
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For any $\mathbf{X}_n \subset \mathbb{I}_d^n$, we have $D_n^*(\mathbf{X}_n) \leq D_n(\mathbf{X}_n) \leq 2^d D_n^*(\mathbf{X}_n)$

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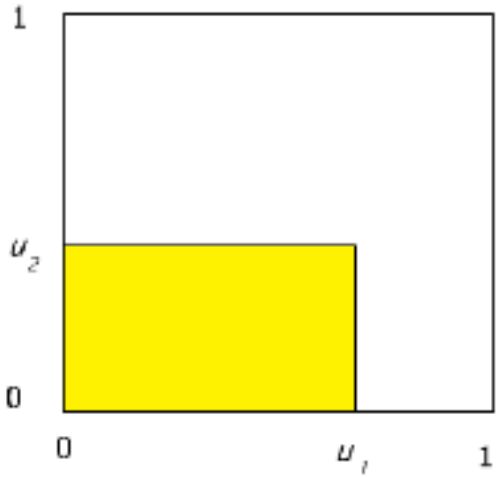
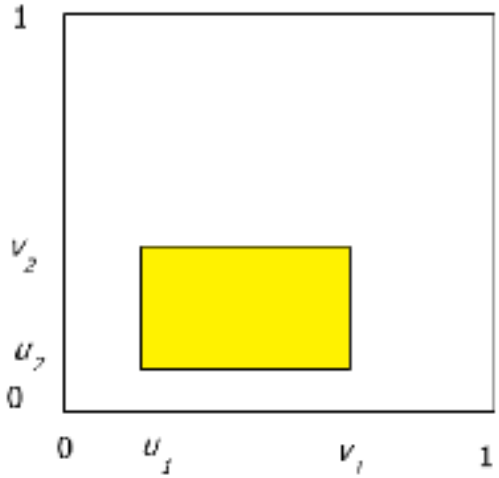


$D_n^*(\mathbf{X}_n)$: $\mathbb{B} = \prod_{\ell=1}^d [0, u_\ell)$



$D_n(\mathbf{X}_n)$: $\mathbb{B} = \prod_{\ell=1}^d [u_\ell, v_\ell)$

In dimension $d = 1$, with $0 \leq x_1 \leq x_2 \leq \cdots \leq x_n \leq 1$:

$$D_n^*(\mathbf{X}_n) = \frac{1}{2n} + \max_{1 \leq i \leq n} \left| x_i - \frac{2i-1}{2n} \right|$$

(➠ Kolmogorov-Smirnov test for uniformity)

$$D_n(\mathbf{X}_n) = \frac{1}{n} + \max_{1 \leq i \leq n} \left(\frac{i}{n} - x_i \right) - \min_{1 \leq i \leq n} \left(\frac{i}{n} - x_i \right)$$

and $D_n^*(\mathbf{X}_n) \geq \frac{1}{2n}$, $D_n(\mathbf{X}_n) \geq \frac{1}{n}$, with equality for $\mathbf{X}_{mM,n}^* : x_i = \frac{2i-1}{2n} \ \forall i$

In dimension $d = 1$, with $0 \leq x_1 \leq x_2 \leq \cdots \leq x_n \leq 1$:

$$D_n^*(\mathbf{X}_n) = \frac{1}{2n} + \max_{1 \leq i \leq n} \left| x_i - \frac{2i-1}{2n} \right|$$

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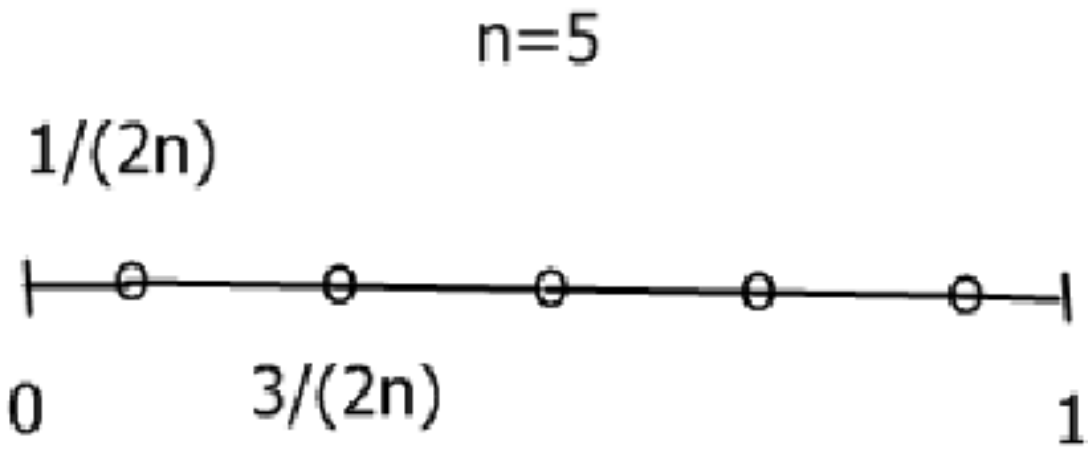
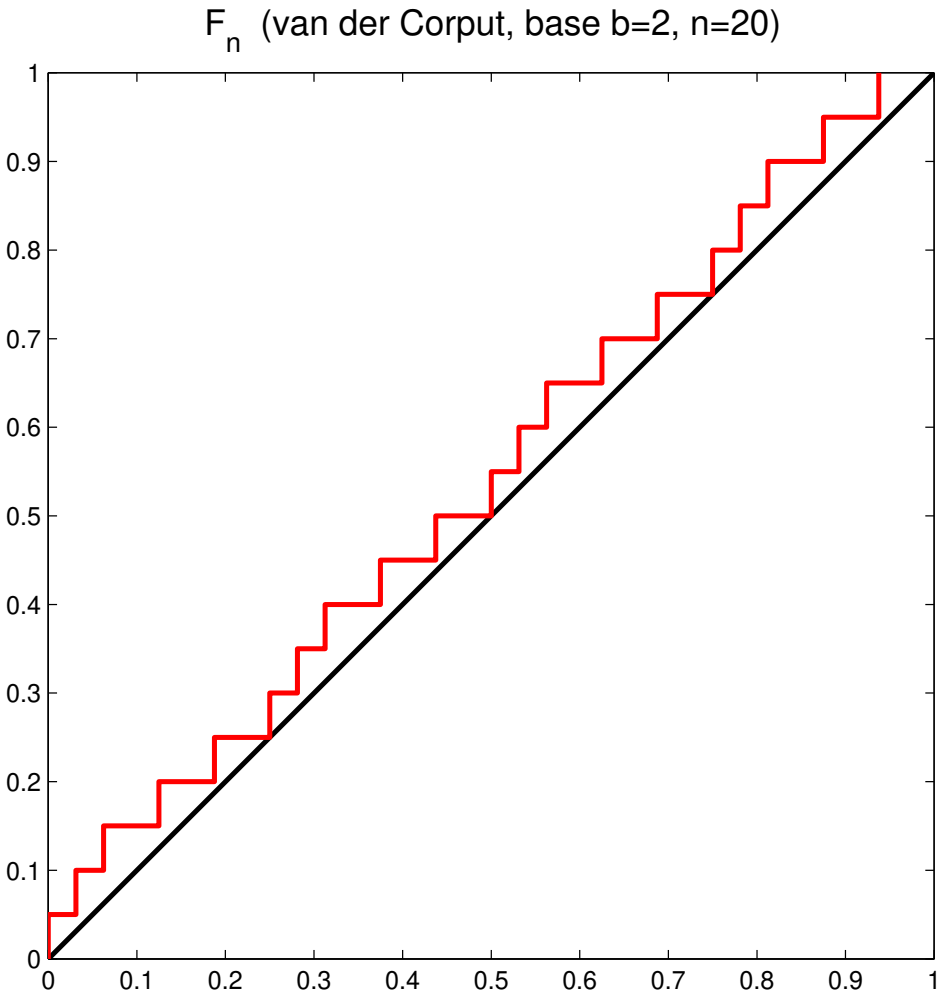


empirical c.d.f. $F_n(x)$ and $F_U(x)$
$d = 1$, $\mathbf{X}_{20}$ = first 20 points of van der Corput sequence in base 2
(voir § 2.4)



Why is it important?

For $d = 1$, f with bounded variation on $[0,1]$ ($V(f) \triangleq \int_0^1 |\mathrm{d}f(u)| < \infty$)

$$\boxed{\left| \int_0^1 f(u)\,\mathrm{d}u - \frac{1}{n}\sum_{i=1}^n f(x_i) \right| \leq D_n^*(\mathbf{X}_n)\, V(f)}$$

➠ Koksma (1942/1943) inequality (cannot be improved)
(easy proof, integration by parts)

Therefore, for $d = 1$

$$\left| \int_0^1 f(u)\,\mathrm{d}u - \frac{1}{n}\sum_{i=1}^n f(x_i) \right| \leq \frac{V(f)}{2n} \quad \text{for } \mathbf{X}_n^* \text{ such that } x_i = \frac{2i-1}{2n}\ \forall i$$

whereas MC error $\simeq \frac{\sigma(f)}{n^{1/2}}$

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In dimension $d \geq 2$: $$\left| \int_{\mathbb{I}_d} f(\mathbf{u})\,\mathrm{d}\mathbf{u} - \frac{1}{n}\sum_{i=1}^n f(\mathbf{x}_i) \right| \leq D_n^*(\mathbf{X}_n)\, V(f)$$

(Koksma-Hlawka (1961) inequality, cannot be improved)
with $V(f)$ = variation in the sense of Hardy and Krause, and

$$\left| \int_{\mathbb{I}_d} f(\mathbf{u})\,\mathrm{d}\mathbf{u} - \frac{1}{n}\sum_{i=1}^n f(\mathbf{x}_i) \right| \leq \begin{cases} V(f)\, C_d\, \dfrac{(\log n)^{d-1}}{n} \\ \text{for } \mathbf{X}_n = \text{Hammersley point set} \\ V(f)\, C_d'\, \dfrac{(\log n)^{d}}{n} \\ \text{for } \mathbf{X}_n = \text{first } n \text{ elements} \\ \text{of Halton sequence (for instance) } \mathbf{X}_\infty \end{cases}$$

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voir § 2.4

- Error $\searrow$ faster than for MC, but which constant C_d ?
- n-point set $\mathbf{X}_n \neq$ first n elements of an infinite sequence $\mathbf{X}_\infty$

2.3 Discrepancy criteria

Difficulty : $D_n^*(\mathbf{X}_n)$ and $D_n(\mathbf{X}_n)$ are difficult to compute for $d \geq 2$

see, e.g., (Dobkin and Eppstein, 1993; Thiémard, 2001; Gnewuch et al., 2012) and the references therein

➠ (many!) other definitions of discrepancy

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➠ (many!) other definitions of discrepancy

One may wish to have:

① invariance by permutation of principal axes, by reflection w.r.t. center of $\mathbb{I}_d$

② a uniformity property on d' dimensional subspaces, $d' < d$

③ a geometrical interpretation

④ a sort of Koksma-Hlawka inequality

⑤ . . . and easy evaluation!

For ⑤: substitute a L_p norm for the L_∞ norm

$$D_n^*(\mathbf{X}_n) = \sup_{\mathbf{u}\in[0,1]^d} |F_n(\mathbf{u}) - F_U(\mathbf{u})| \Rightarrow \left(\int_{[0,1]^d} |F_n(\mathbf{u}) - F_U(\mathbf{u})|^p \, \mathrm{d}\mathbf{u} \right)^{1/p}$$

⇛ Analytical expression for $p = 2$, fine for ③, ④ and ⑤, but not for ① and ②

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$D_n^*(\mathbf{X}_n) = \sup_{\mathbf{u}\in[0,1]^d} |\mathrm{F}_n(\mathbf{u}) - \mathrm{F}_U(\mathbf{u})|$ ➠ $\left(\int_{[0,1]^d} |\mathrm{F}_n(\mathbf{u}) - \mathrm{F}_U(\mathbf{u})|^p \,\mathrm{d}\mathbf{u}\right)^{1/p}$

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For ②: consider projections on all d' dimensional faces, $d' < d$

$D_n^*(\mathbf{X}_n)$ ➠

$$\left(\sum_{d'=1}^{d} \sum_{i_1<\cdots<i_{d'}} \int_{[0,1]^{d'}} |\mathrm{F}_n(\{\mathbf{u}\}_{i_1,\ldots,i_{d'}}) - \mathrm{F}_U(\{\mathbf{u}\}_{i_1,\ldots,i_{d'}})|^p \,\mathrm{d}\{\mathbf{u}\}_{i_1,\ldots,i_{d'}}\right)^{1/p}$$

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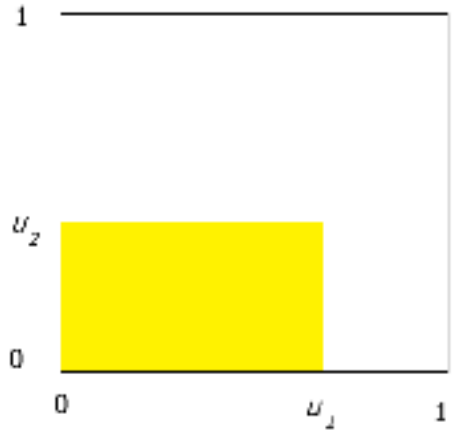
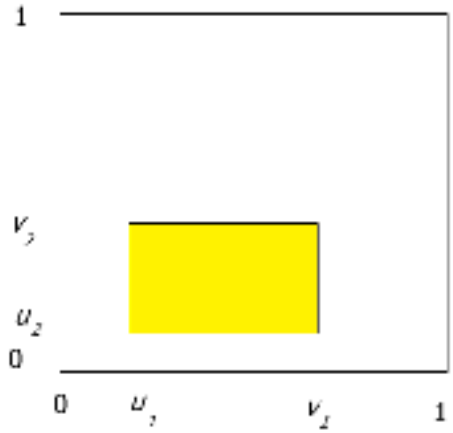
For ①: change the family of sets $\mathbb{B}$ in calculation of discrepancy

$D_n^*(\mathbf{X}_n)$: $\mathbb{B} = \prod_{\ell=1}^d [0, u_\ell)$



$D_n(\mathbf{X}_n)$: $\mathbb{B} = \prod_{\ell=1}^d [u_\ell, v_\ell)$



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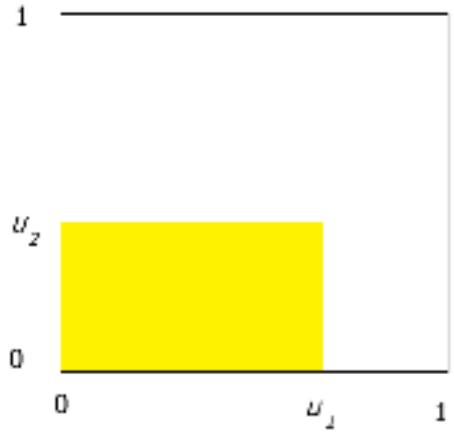

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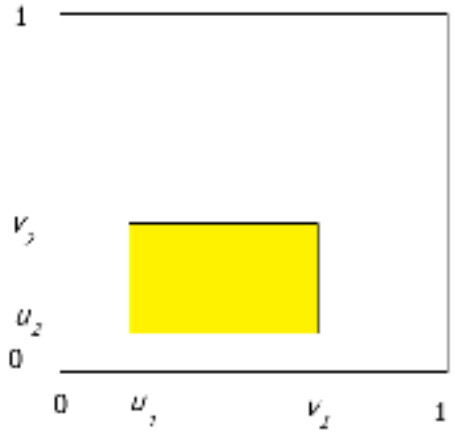
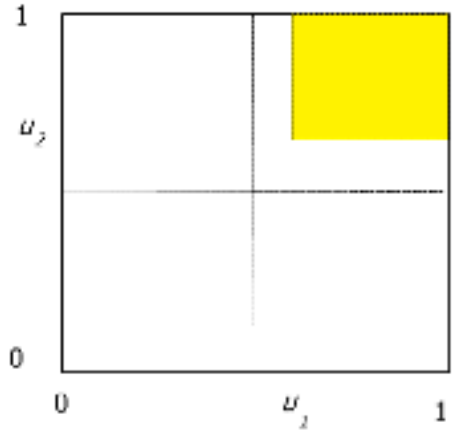
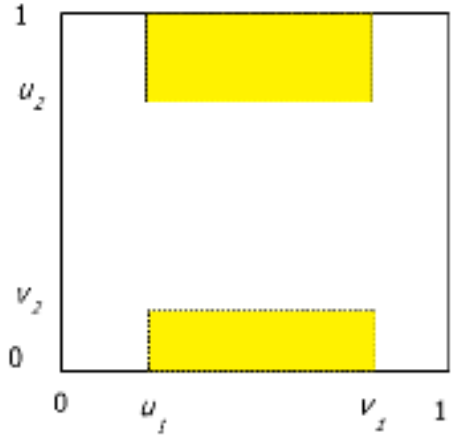


Centered discrepancy: consider the vertex of the (d' dimensional) cube closest to $\mathbf{u}$



Wrap-around discrepancy: consider $[u_i, v_i]$ if $u_i \leq v_i$ and $[u_i, 1] \cup [0, v_i]$ otherwise



They can be computed...

$$D_{Cent,L_2}(\mathbf{X}_n) = \left[\left(\frac{13}{12}\right)^d - \frac{2}{n}\sum_{k=1}^{n}\prod_{i=1}^{d}\left(1+\frac{1}{2}\left|\{\mathbf{x}_k\}_i-\frac{1}{2}\right|-\frac{1}{2}\left|\{\mathbf{x}_k\}_i-\frac{1}{2}\right|^2\right)\right.$$
$$\left.+\frac{1}{n^2}\sum_{k,k'=1}^{n}\prod_{i=1}^{d}\left(1+\frac{1}{2}\left|\{\mathbf{x}_k\}_i-\frac{1}{2}\right|+\frac{1}{2}\left|\{\mathbf{x}_{k'}\}_i-\frac{1}{2}\right|-\frac{1}{2}\left|\{\mathbf{x}_k\}_i-\{\mathbf{x}_{k'}\}_i\right|\right)\right]^{1/2}$$

$$D_{WA,L_2}(\mathbf{X}_n) = \left\{\frac{1}{n^2}\sum_{k,k'=1}^{n}\prod_{i=1}^{d}\left[\frac{3}{2}-\left|\{\mathbf{x}_k\}_i-\{\mathbf{x}_{k'}\}_i\right|\left(1-\left|\{\mathbf{x}_k\}_i-\{\mathbf{x}_{k'}\}_i\right|\right)\right]\right.$$
$$\left.-\left(\frac{4}{3}\right)^d\right\}^{1/2}$$

see Hickernell (1998a,b); Fang and Ma (2001)
they are differentiable w.r.t. $\mathbf{X}_n$ and can be minimized (Fang and Ma, 2001; Fang et al., 2003, 2005)

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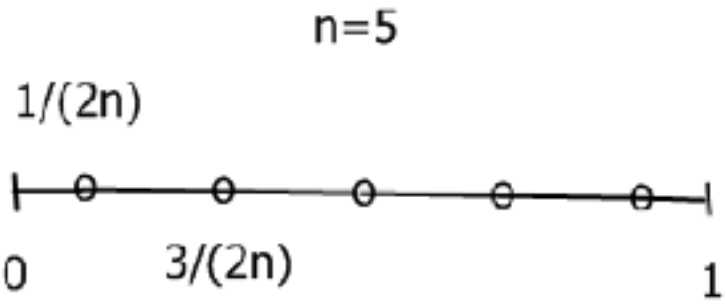
➠ However, generating low discrepancy sequences of points is much easier!

2.4 **Low discrepancy sequences (LDS)** (Niederreiter, 1992, Chap. 3)

$\mathbf{X}_n$ has low discrepancy if $D_n^*(\mathbf{X}_n^*)$ is small
(or $D_n(\mathbf{X}_n^*)$, or another discrepancy)

In dimension 1:

$\mathbf{X}_n^*$ such that $x_i = \frac{2i-1}{2n}$, $i = 1, \ldots, n$



gives $n \times D_n^*(\mathbf{X}_n^*) = 1/2$ for all n

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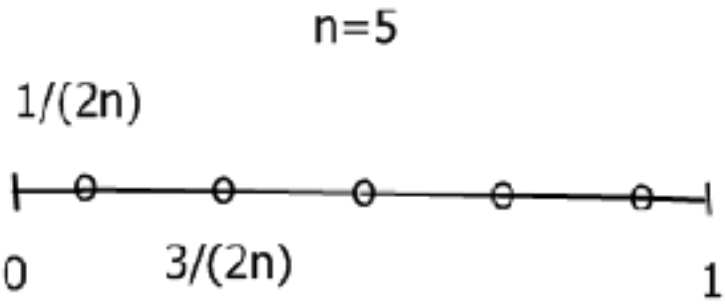

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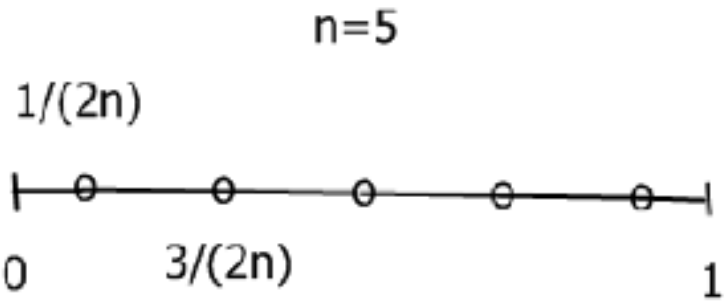

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$n \times D_n^*(\mathbf{X}_\infty)$ necessarily fluctuates: $D_n^*(\mathbf{X}_\infty) > c\frac{\log n}{n}$ infinitely often
(best constant known $c = 0.06$)

We know sequences $\mathbf{X}_\infty$ such that $\boxed{D_n^*(\mathbf{X}_\infty) = \mathcal{O}\left(\frac{\log n}{n}\right)}$

- fractional parts (mainly for $d = 1$)
  for given $n \leftrightarrow$ Lattices
- van der Corput sequences ($d = 1$)
- ➠ Halton sequences ($d > 1$)
- (t, m, d)-nets and (t, d)-sequences (Sobol', Faure)

⏩ → van der Corput

Fractional parts

For $d = 1$: $\boxed{x_k \triangleq \{kz\} = kz - \lfloor kz \rfloor}$, $k = 1, 2 \ldots$, with z irrational (fractional part of kz)

For instance, $z = \varphi = (\sqrt{5} + 1)/2 \simeq 1.618034 =$ Golden section

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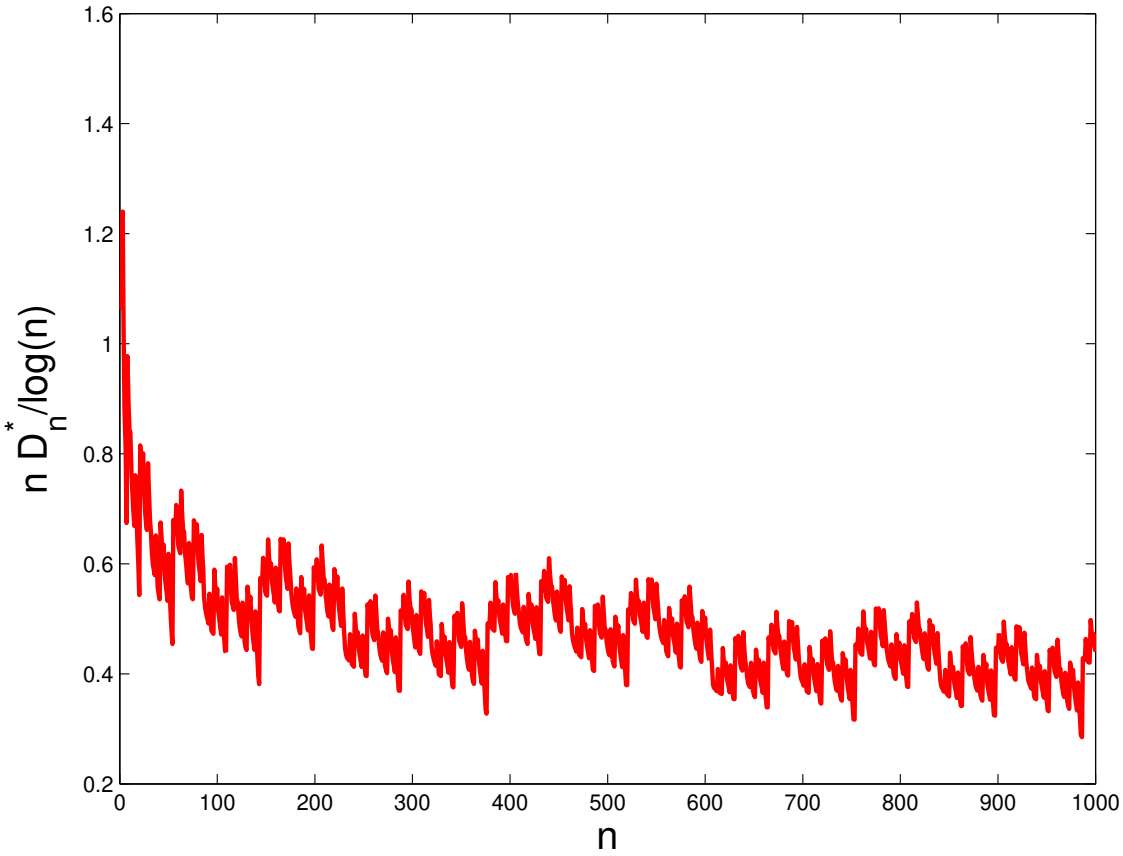
$(n/\log n) \times D_n^*$



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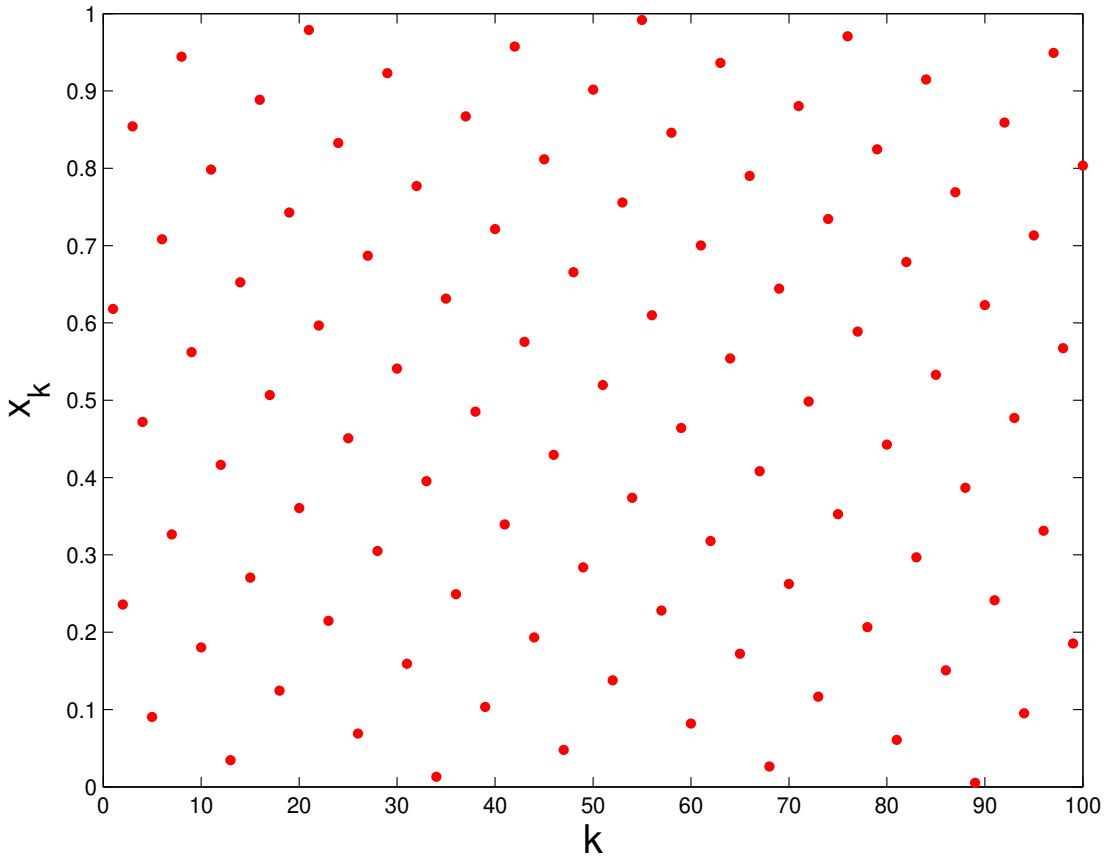
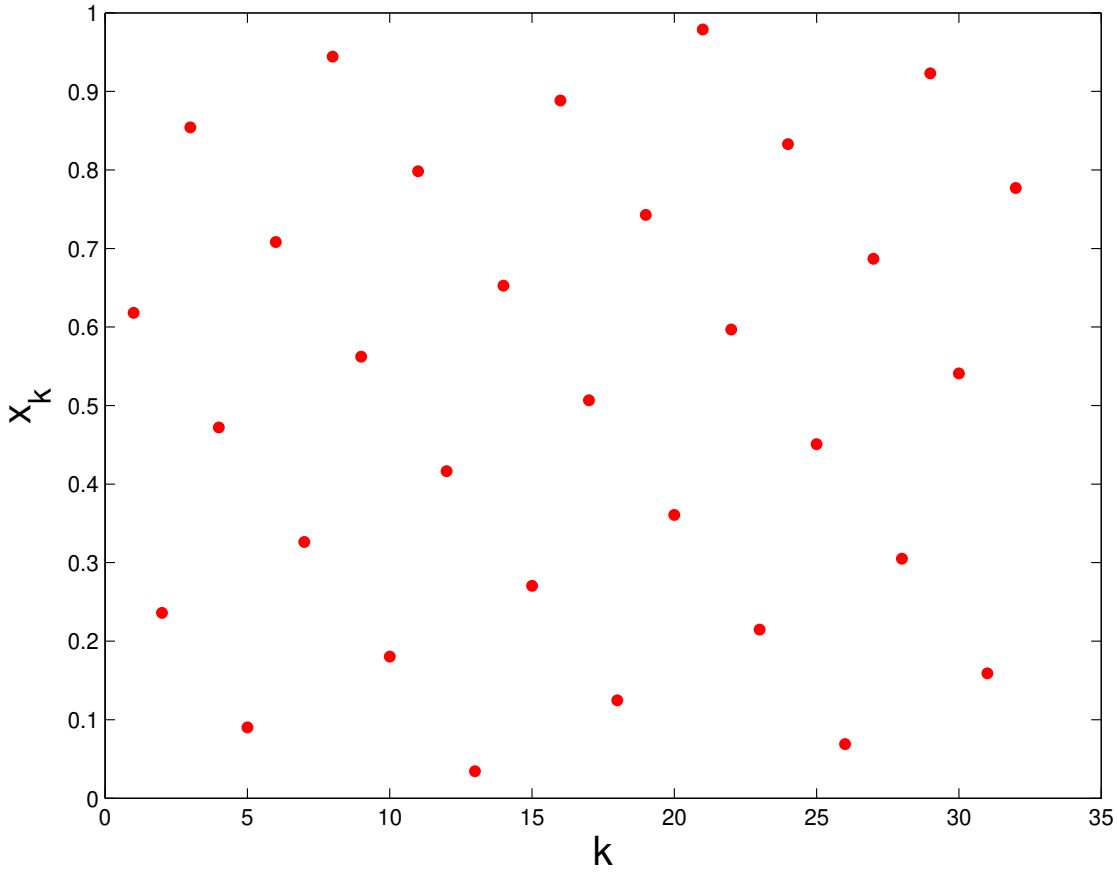
first 100 points x_k



For $d > 1$:

$$x_k = \{k\varphi\},\ k = 1, \ldots, 32$$



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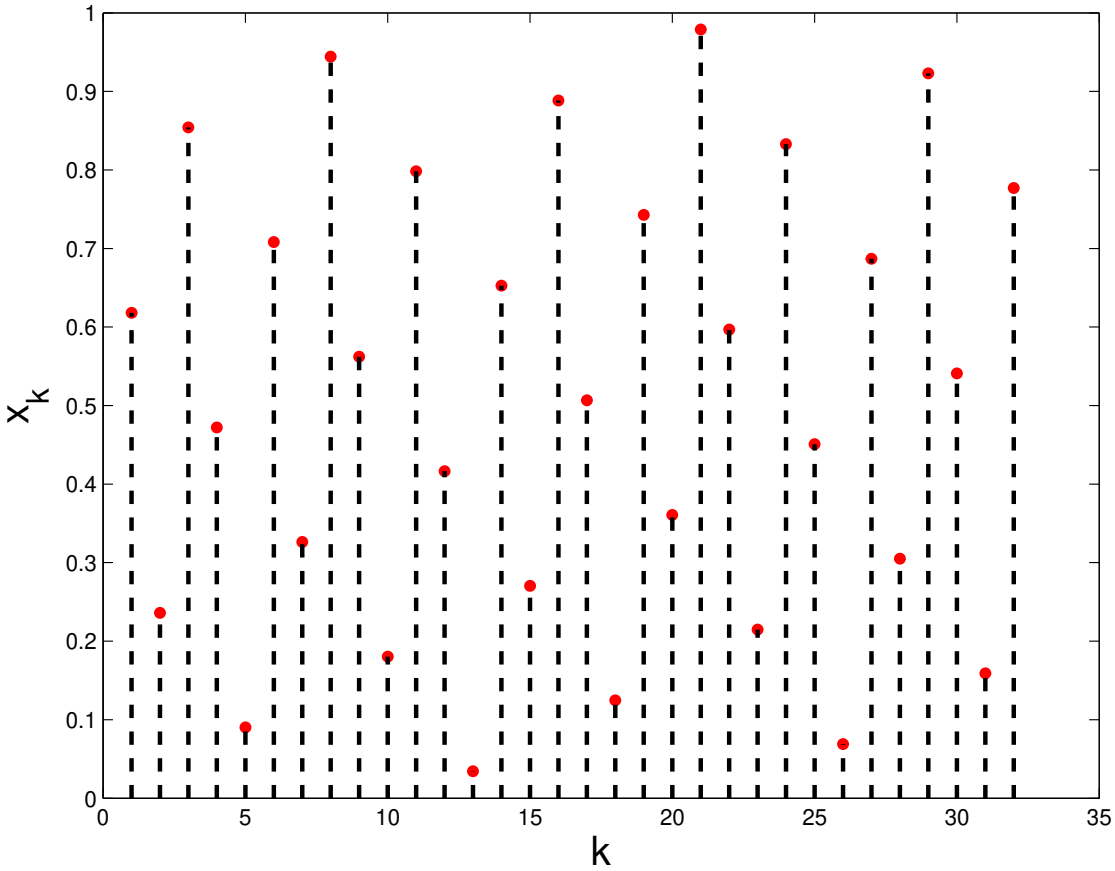
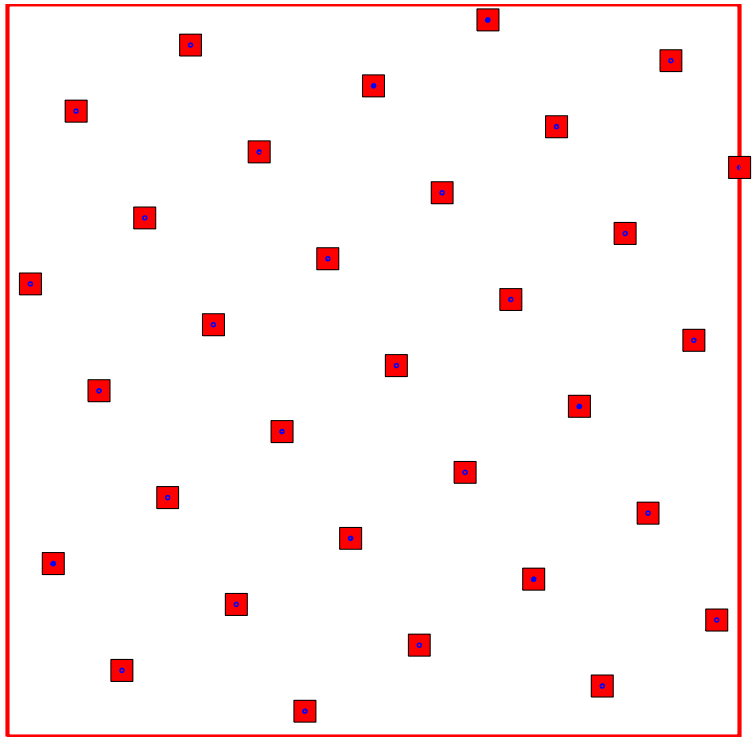


For $d > 1$:

$$\mathbf{x}_k = (k/n, \{k\varphi\})^\top$$



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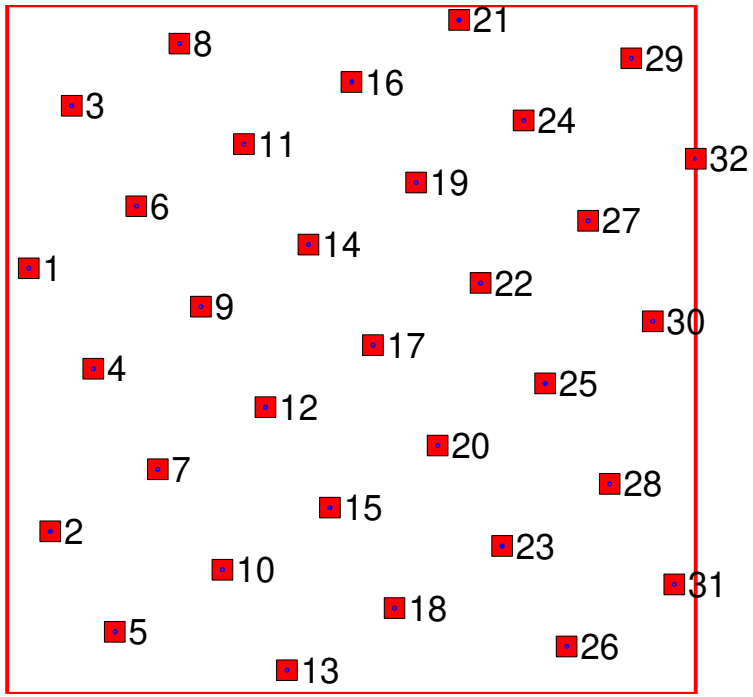

➠ Replace k/n (monotonically increasing and only valid for $k = 1, \ldots, n$) by $\{kz\}$, z irrational $\rightarrow \mathbf{x}_k \in [0,1]^2$, $k = 1, 2, 3 \ldots$

➠ repeat... $\rightarrow$ recursively $\mathbf{x}_k \in [0,1]^d$, for any given d

Take $\mathbf{x}_k \triangleq \{k\mathbf{z}\}$, $\mathbf{z}$ irrational vector in $\mathbb{R}^d$
(with independent components over rationals: $\mathbf{q}^\top \mathbf{z} \neq 0$, $\forall \mathbf{q} \in \mathbb{Q}^d$)

- sequence $\mathbf{X}_\infty$ uniformly distributed in $[0,1]^d$

  (Kuipers and Niederreiter, 1974, p. 48)

- $\forall \epsilon > 0$, $D_n(\mathbf{X}_\infty) = \mathcal{O}\left(\frac{(1+\log n)^{d+1+\epsilon}}{n}\right)$ for almost all $\mathbf{z}$

Interesting, but does not say which $\mathbf{z}$ we should take

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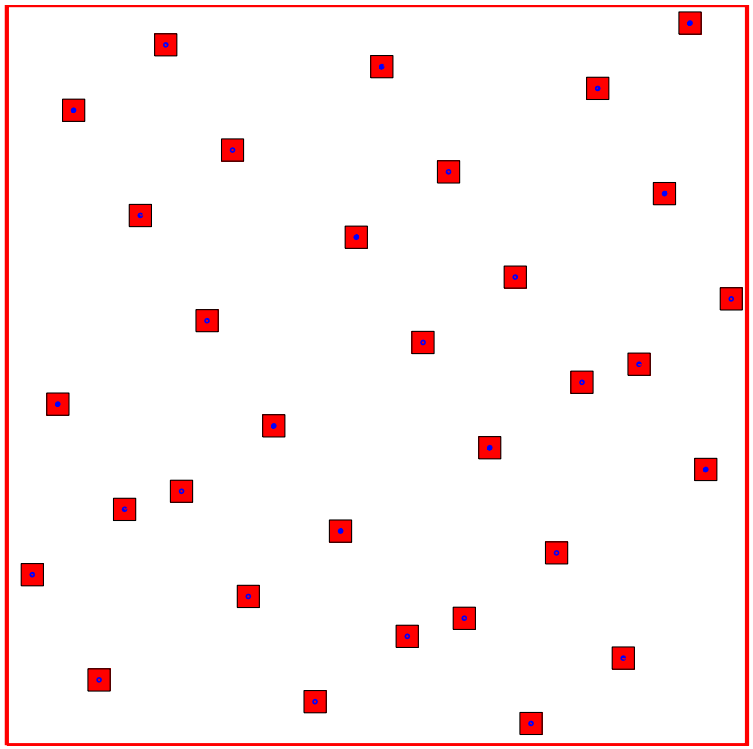
Interesting, but does not say which $\mathbf{z}$ we should take

$d = 2$, $n = 32$, $\mathbf{z} = (\varphi, (\sqrt{2}-1)^2)^\top$



Take $\mathbf{x}_k \triangleq \{k\mathbf{z}\}$, $\mathbf{z}$ irrational vector in $\mathbb{R}^d$
(with independent components over rationals: $\mathbf{q}^\top \mathbf{z} \neq 0$, $\forall \mathbf{q} \in \mathbb{Q}^d$)

➠ sequence $\mathbf{X}_\infty$ uniformly distributed in $[0,1]^d$

(Kuipers and Niederreiter, 1974, p. 48)

➠ $\forall \epsilon > 0$, $D_n(\mathbf{X}_\infty) = \mathcal{O}\left(\frac{(1+\log n)^{d+1+\epsilon}}{n}\right)$ for almost all $\mathbf{z}$

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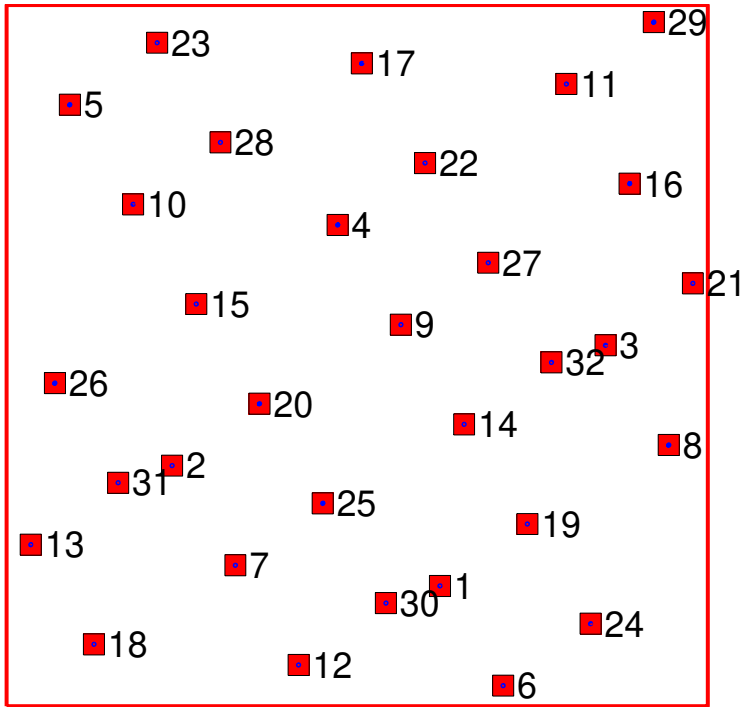

Lattices: $\mathbf{z} = \mathbf{g}/n$, with $\mathbf{g} \in \mathbb{Z}^d$

- $\mathbf{x}_k \triangleq \left\{ \frac{k}{n} \mathbf{g} \right\}$ (with repetitions if $k \geq n$)
  - n points $\neq$ if $\gcd(g_1, \ldots, g_d, n) = 1$
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For $d = 2$, $\mathbf{g} = (1, \ F_{m-1})^\top$ for $n = F_m$ is a very good choice,
with (F_m) = Fibonacci sequence: $F_1 = F_2 = 1$, $F_{k+1} = F_k + F_{k-1}$, $k \geq 2$

Since $F_{m-1}/F_m \to 1/\varphi$ for $m \to \infty$, the construction is similar to
$\mathbf{x}_k = (\frac{k}{n}, \ \left\{ \frac{k}{\varphi} \right\})^\top = (\frac{k}{n}, \ \{k\varphi\})^\top$, $k = 1, \ldots, n$

➤ Strong connection with optimal design for Fourier regression (sin, cos) (Bates et al., 1996; Riccomagno et al., 1997)

➤ The exist constructions (non explicit) with good properties (good lattice points) ➠ tables (Maisonneuve, 1972)

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Ex: $d = 2$, $n = 21 = F_8$

$$\mathbf{g} = (1, F_7)$$

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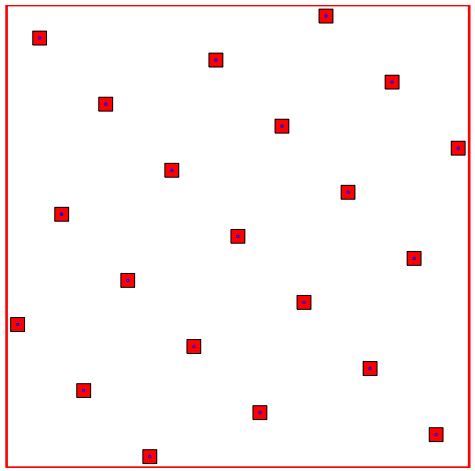

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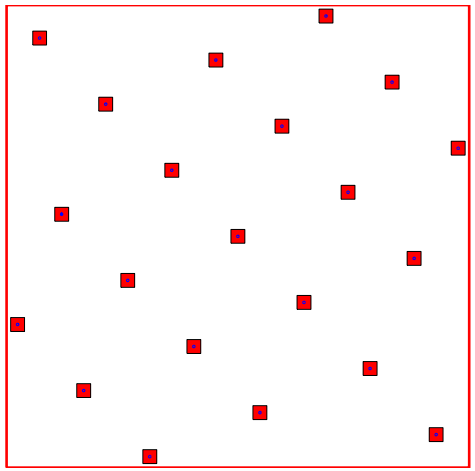
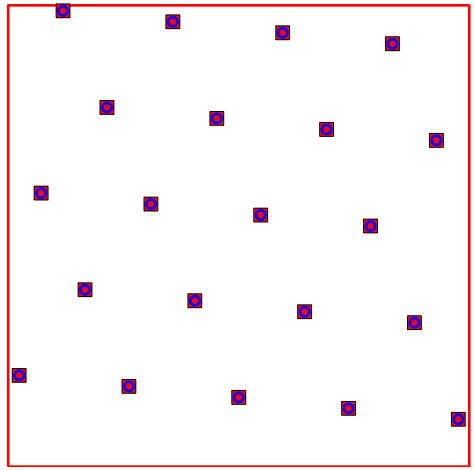


$\Phi_{Mm} = 0.2302$
$\Phi_{mM} = 0.2217$
$D_{Cent,L_2} = 0.0536$
$D_{WA,L_2} = 0.0633$

$\mathbf{g} = (1, g^*)$
(optimal for Φ_{Mm})



- Can only generate n points:
  - infinite sequence in $[0,1]^d$ if $\mathbf{x}_k \triangleq \{u_k\,\mathbf{g}\}$

  with (u_k) a (scalar) LDS (Hickernell, 1998b)

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We only considered the rank-on rule, there also exist

rank r rule: $\mathbf{x}_{k_1,\ldots,k_r} \triangleq \left\{ \frac{k_1}{n_1}\mathbf{g}_1 + \frac{k_2}{n_2}\mathbf{g}_2 + \cdots + \frac{k_r}{n_r}\mathbf{g}_r \right\}$, $k_j \in \{1,\ldots,n_j\}$

Copy rule: divide $[0,1]^d$ into k^d cubes with edge length $1/k$, construct a lattice in each

van der Corput (1935) LDS

$\boxed{d = 1}$

Let $\mathcal{Z}_b = \{0, 1, \ldots, b-1\}$ be the alphabet for base $b \geq 2$
(e.g., $\mathcal{Z}_2 = \{0, 1\}$, $\mathcal{Z}_3 = \{0, 1, 2\}$)

- Any $k = 0, 1, \ldots, b^m - 1$ can be written as $k = \sum_{\ell=0}^{m-1} a_\ell b^\ell$
with m characters $a_0, a_1, \ldots, a_{m-1}$ (dependent on k)
(that is, $k = \underline{a_{m-1} a_{m-2} \cdots a_2 a_1 a_0}_b$)

- To k, we associate $\Phi_b(k) = \sum_{\ell=0}^{m-1} a_\ell b^{-(\ell+1)}$
  - The van der Corput sequence in base b is defined by $\boxed{x_k \triangleq \Phi_b(k)}$

base $b = 2$ (van der Corput, 1935)

k	k in base 2	$\phi_b(k)$ in base 2	$\phi_2(k)$
0	0	0.0	0
1	1	0.1	1/2
2	10	0.01	1/4
3	11	0.11	3/4
4	100	0.001	1/8
5	101	0.101	5/8
k	$\underline{a_{m-1}\cdots a_1 a_0}_2$	$0.a_0 a_1 \cdots a_{m-1}$	$\sum_{\ell=0}^{m-1} a_\ell 2^{-(\ell+1)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

$$\Rightarrow \quad nD_n^*(\mathbf{X}_\infty) = nD_n(\mathbf{X}_\infty) \leq 1 + \frac{\log n}{\log 8}$$

base $b = 3$

k	k in base 3	$\phi_3(k)$
0	0	0
1	1	1/3
2	2	2/3
3	10	1/9
4	11	4/9
5	12	7/9
6	20	2/9
7	21	5/9
8	22	8/9
⋮	⋮	⋮

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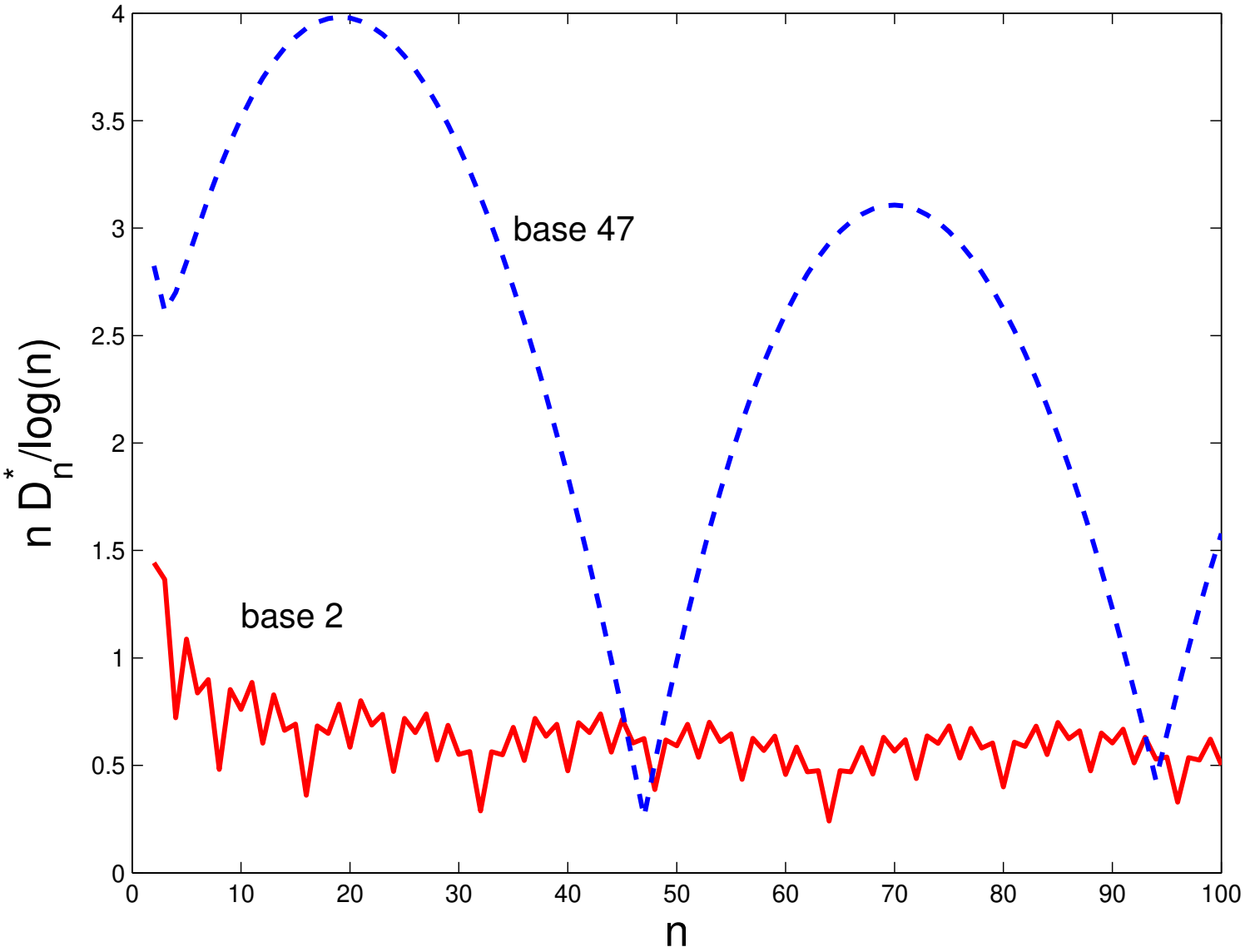
⋮	⋮	⋮

Particular choice of b + suitable permutation of $\mathcal{Z}_b$

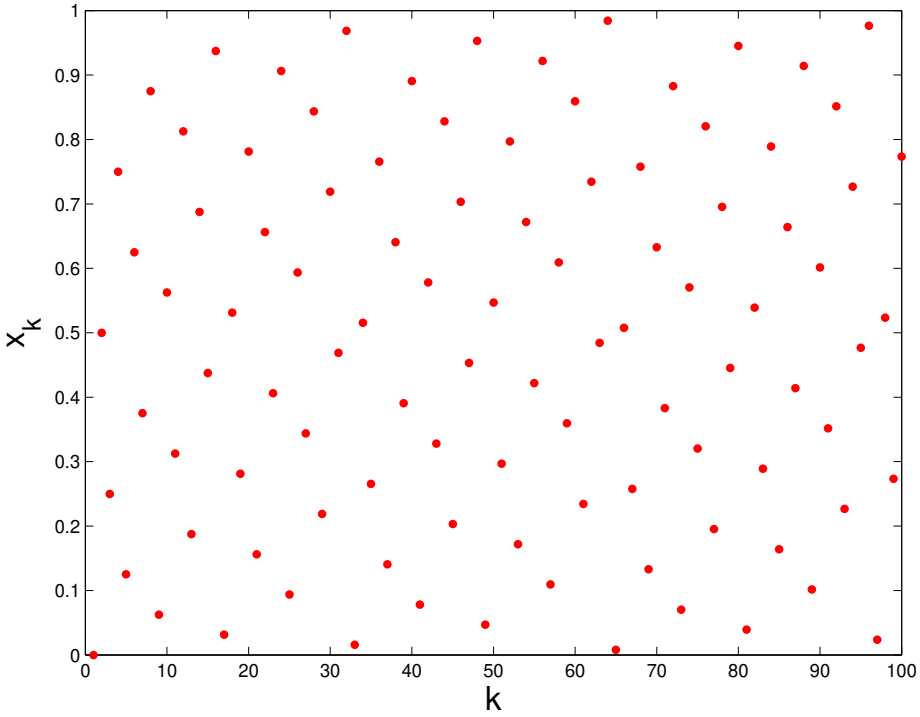
➠ best known performance for $\limsup_{n\to\infty} nD_n^*/log(n)$ $(b = 12)$ and $\limsup_{n\to\infty} nD_n/log(n)$ $(b = 36)$ (results by H. Faure (1977–20xx))

van der Corput : $(n/\log n) \times D_n^*$ for $b = 2$ and $b = 47$

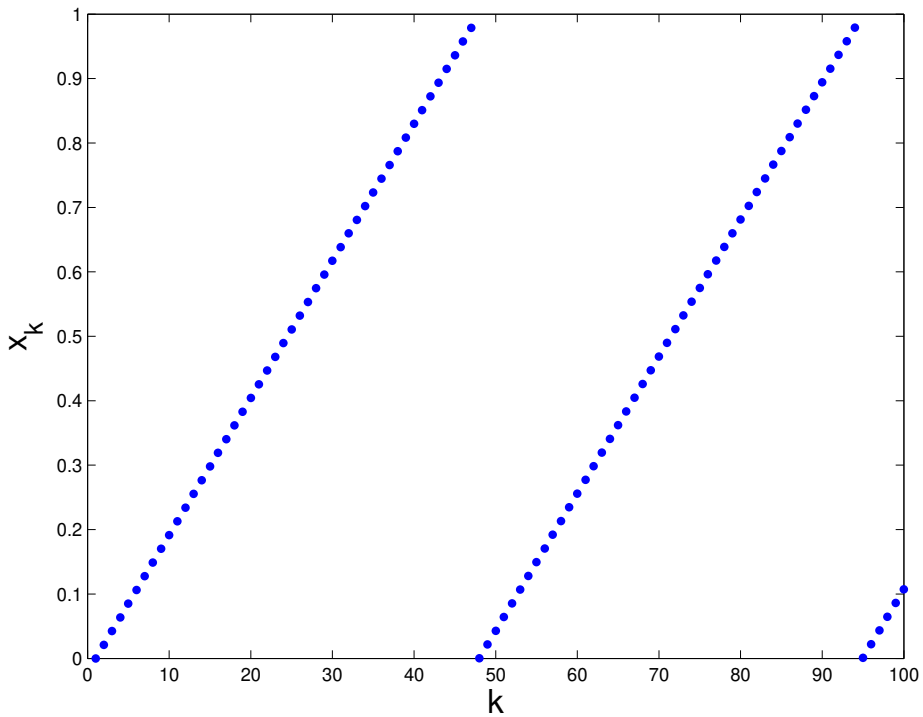


van der Corput : $x_1, x_2 \ldots, x_{100}$

$b = 2$



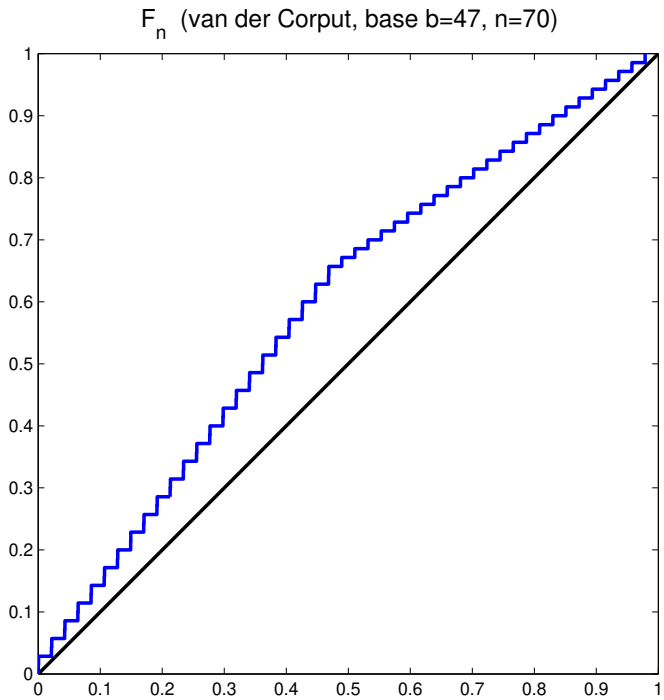
$b = 47$, $x_1, x_2 \ldots$



. . . and, moreover, $[0, 1]$ is filled in a particular order

van der Corput : $x_1, x_2 \ldots, x_{70}$

$b = 47$, empirical c.d.f.



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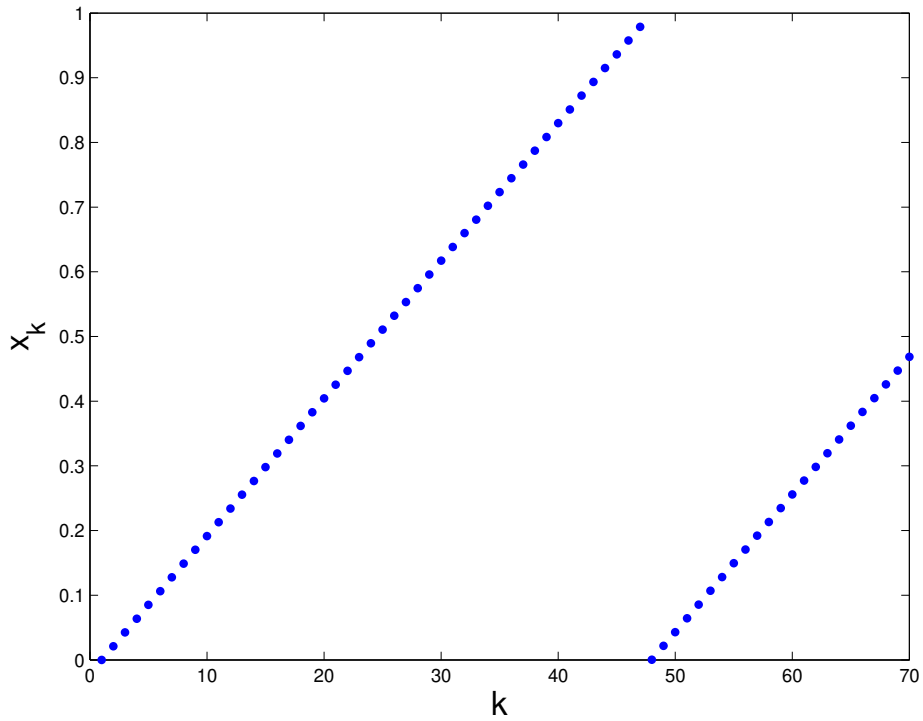

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$\boxed{d > 1}$: work separately on each component

$b_1, b_2 \ldots$ integers such that $\gcd(b_i, b_j) = 1$ for all $i \neq j$

(in practice, first prime numbers:

$2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41, 43, 47 \ldots$)

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- Hammersley: $\mathbf{x}_k \triangleq (k/n, \phi_{b_1}(k), \ldots, \phi_{b_{d-1}}(k))^\top$, $k = 1, \ldots, n$

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It is conjectured that (only proved for $d = 1, 2$)

$$D_n^*(\mathbf{X}_n) \geq B_d \frac{(\log n)^{d-1}}{n} \text{ and}$$

$$D_n^*(\mathbf{X}_\infty) \geq B'_d \frac{(\log n)^d}{n} \text{ infinitely often}$$

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. . . but what about the constant A_d?

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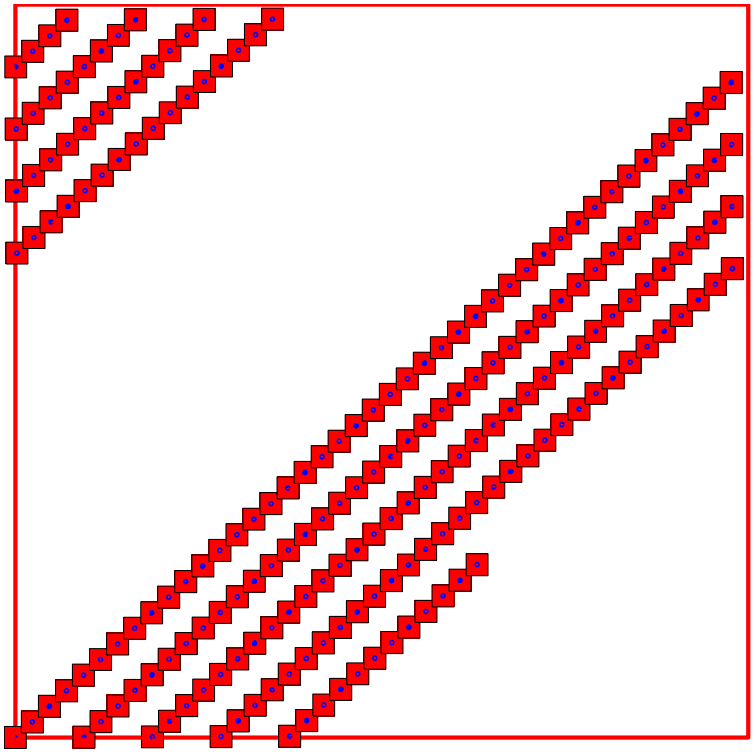
Halton LDS, $d = 15$ ($\Rightarrow b_{15} = 47$) :
$\{\mathbf{x}_k\}_{14}$ and $\{\mathbf{x}_k\}_{15}$, $k = 1, \ldots, 200$



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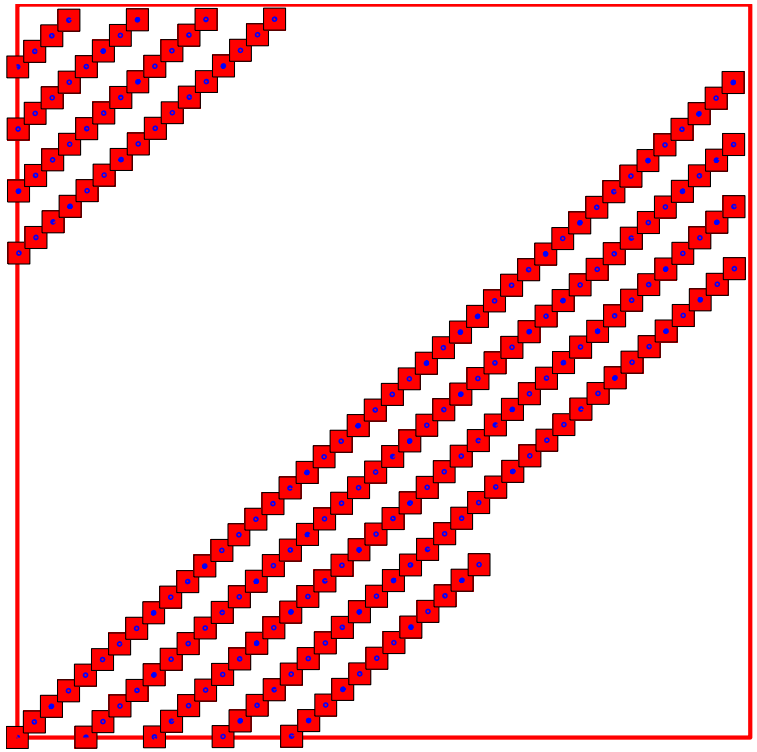

. . . not too bad in the plane $\{\mathbf{x}_k\}_{d_1}, \{\mathbf{x}_k\}_{d_2}$ if $n = b_{d_1} b_{d_2}$
(with $b_d \approx d(\log d + \log\log d)$)

2.5 (t, m, d)-nets & (t, d)-sequences (Niederreiter, 1992, Chap. 4), (Owen, 1995)

suites-(t, d)

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For a base b, consider an elementary interval (= a d-dimensional box)

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where q_j and a_j are integers, $0 \leq q_j$ and $0 \leq a_j \leq b^{q_j} - 1$

$$\mathbb{P}(\mathbf{a}, \mathbf{q}) \subset [0,1]^d \text{ and } \text{vol}[\mathbb{P}(\mathbf{a}, \mathbf{q})] = \prod_{j=1}^{d} b^{-q_j} = b^{-\sum_{j=1}^{d} q_j}$$

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More precisely: for $0 \leq t \leq m$, a $\boxed{(t, m, d)\text{-net}}$ in base b contains $n = b^m$ points, such that each elementary interval with volume b^{t-m} contains b^t points

Example: $(0, 2, 2)$-net in base 2 ($b = 2$, $d = 2$, $m = 2$, $t = 0$)

➠ $n = b^m = 4$, $b^0 = 1$ point in each elementary interval with volume $b^{t-m} = 1/4$

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$$\sum_{j=1}^{d} q_j = m - t = 2 \Rightarrow q_j \in \{0, 1, 2\}$$

	q_1	q_2	
(i)	0	2	$a_1 = 0$, $a_2 \in \{0, 1, 2, 3\}$
(ii)	2	0	$a_1 \in \{0, 1, 2, 3\}$, $a_2 = 0$
(iii)	1	1	$a_1 \in \{0, 1\}$, $a_2 \in \{0, 1\}$

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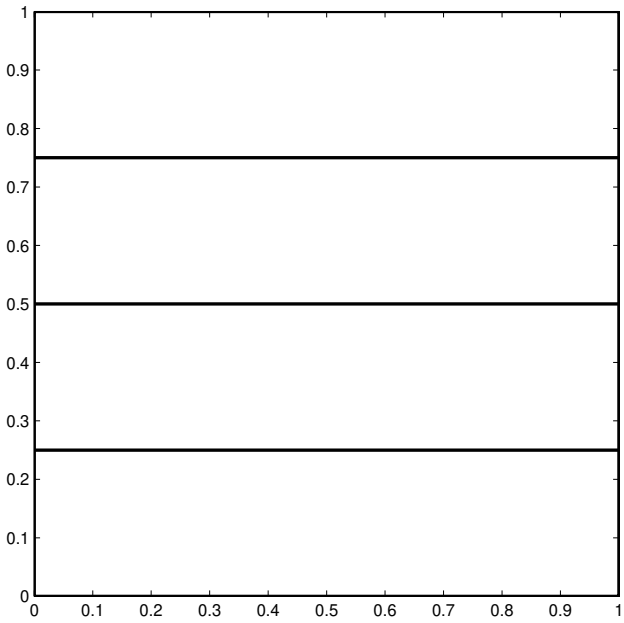
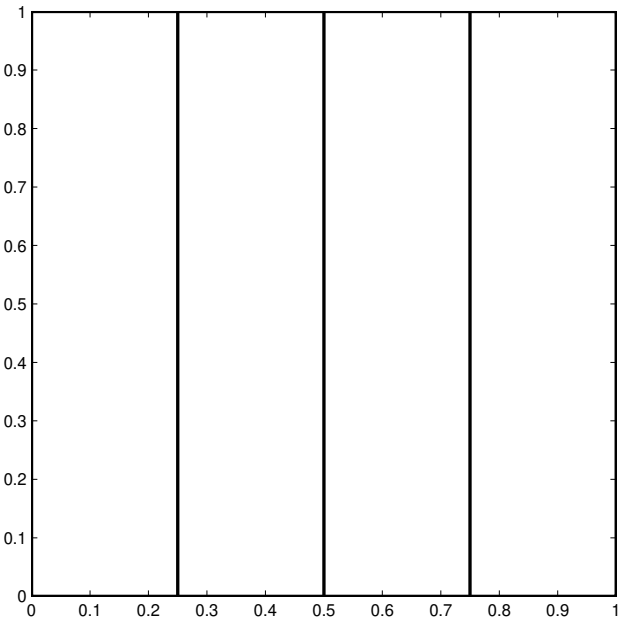
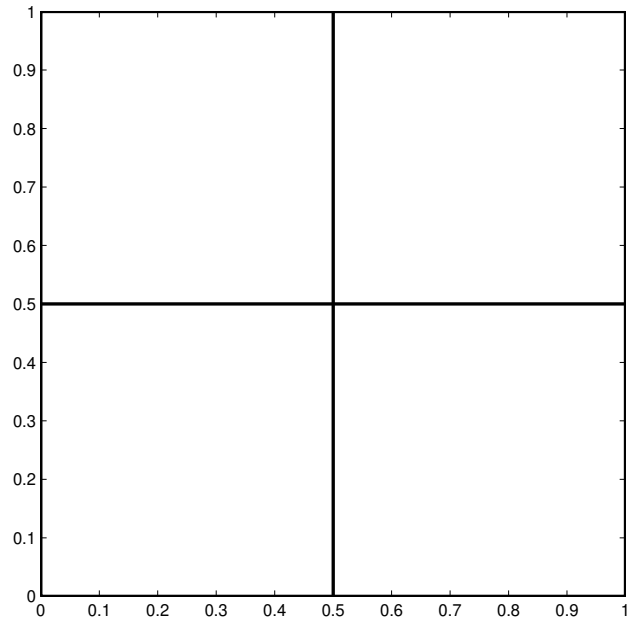


case (ii)



case (iii)



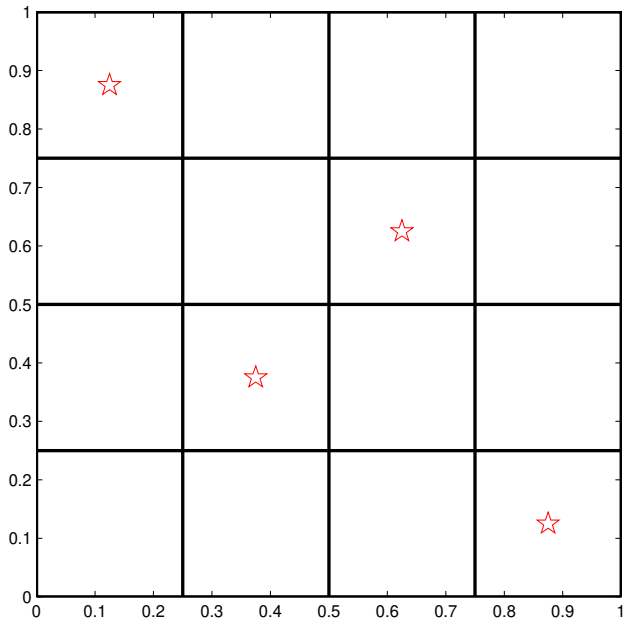
Example: $(0, 2, 2)$-net in base 2 ($b = 2$, $d = 2$, $m = 2$, $t = 0$)

➠ $n = b^m = 4$, $b^0 = 1$ point in each elementary interval with volume $b^{t-m} = 1/4$

$$\sum_{j=1}^{d} q_j = m - t = 2 \Rightarrow q_j \in \{0, 1, 2\}$$

	q_1	q_2	
(i)	0	2	$a_1 = 0$, $a_2 \in \{0, 1, 2, 3\}$
(ii)	2	0	$a_1 \in \{0, 1, 2, 3\}$, $a_2 = 0$
(iii)	1	1	$a_1 \in \{0, 1\}$, $a_2 \in \{0, 1\}$

a $(0, 2, 2)$-net in base 2



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  ➠ a $(0, 1, d)$-net in base b is a Lh with b points
- A $(0, 2, d)$-net in base b is an Orthogonal Array (OA) and a Lh with $n = b^2$ points: previous example had $b = 2$ and $d = 2$
  — but the construction is not always possible...
- no $(0, m, d)$-net in base b for $d > b + 1$ (Niederreiter, 1992, p. 62)

$\mathbf{X}_\infty =$ $\boxed{(t,d)\text{-sequence}}$ in base b if for any $k \geq 0$ and any $m \geq t$ the b^m points $\{\mathbf{x}_{kb^m}, \mathbf{x}_{kb^m+1}, \ldots, \mathbf{x}_{(k+1)b^m-1}\}$ form a (t, m, d)-net

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- van der Corput sequence in base b is a $(0, 1)$-sequence in base b
- Construction rather complicated...
  For $b = 2$, any d: Sobol' (1967) sequences, with a smaller t when $d \geq 8$ for Niederreiter (1992) sequences

(t, d)-sequences in base b rely on rather complicated algebraic constructions, but ensure a good distribution of points in $\mathbb{I}_d = [0, 1]^d$

- t and b should be as small as possible
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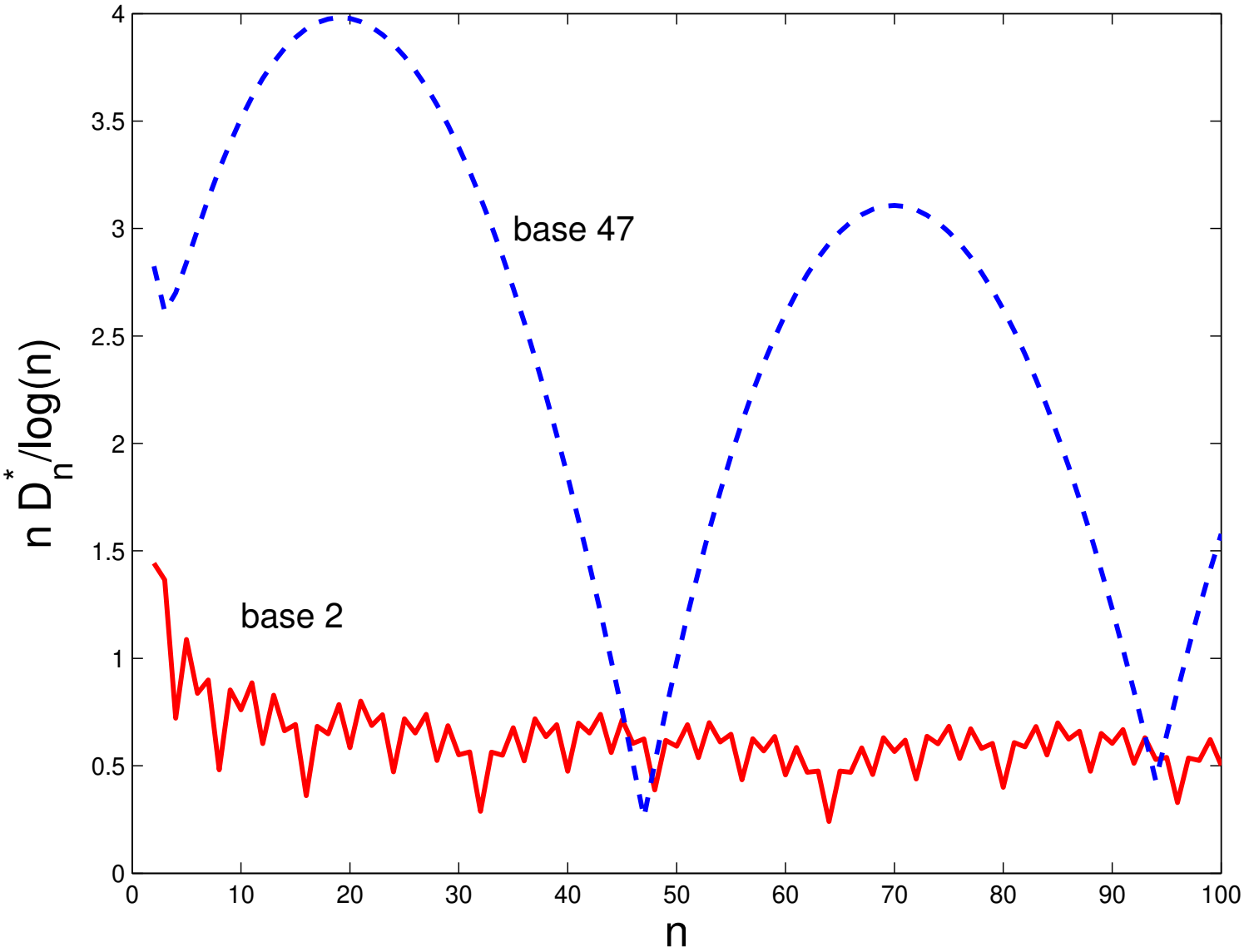
Discrepancy:

$$D_n^*(\mathbf{X}_\infty) \leq C_d \frac{(\log n)^d}{n} + \mathcal{O}\left(\frac{(\log n)^{d-1}}{n}\right)$$

bound similar to that of Halton LDS

. . . but here $C_d \searrow 0$ super-exponentially fast as $d \to \infty$!

Halton: $(n/\log n) \times D_n^*$ for $\{\mathbf{X}_n\}_1$ and $\{\mathbf{X}_n\}_{15}$



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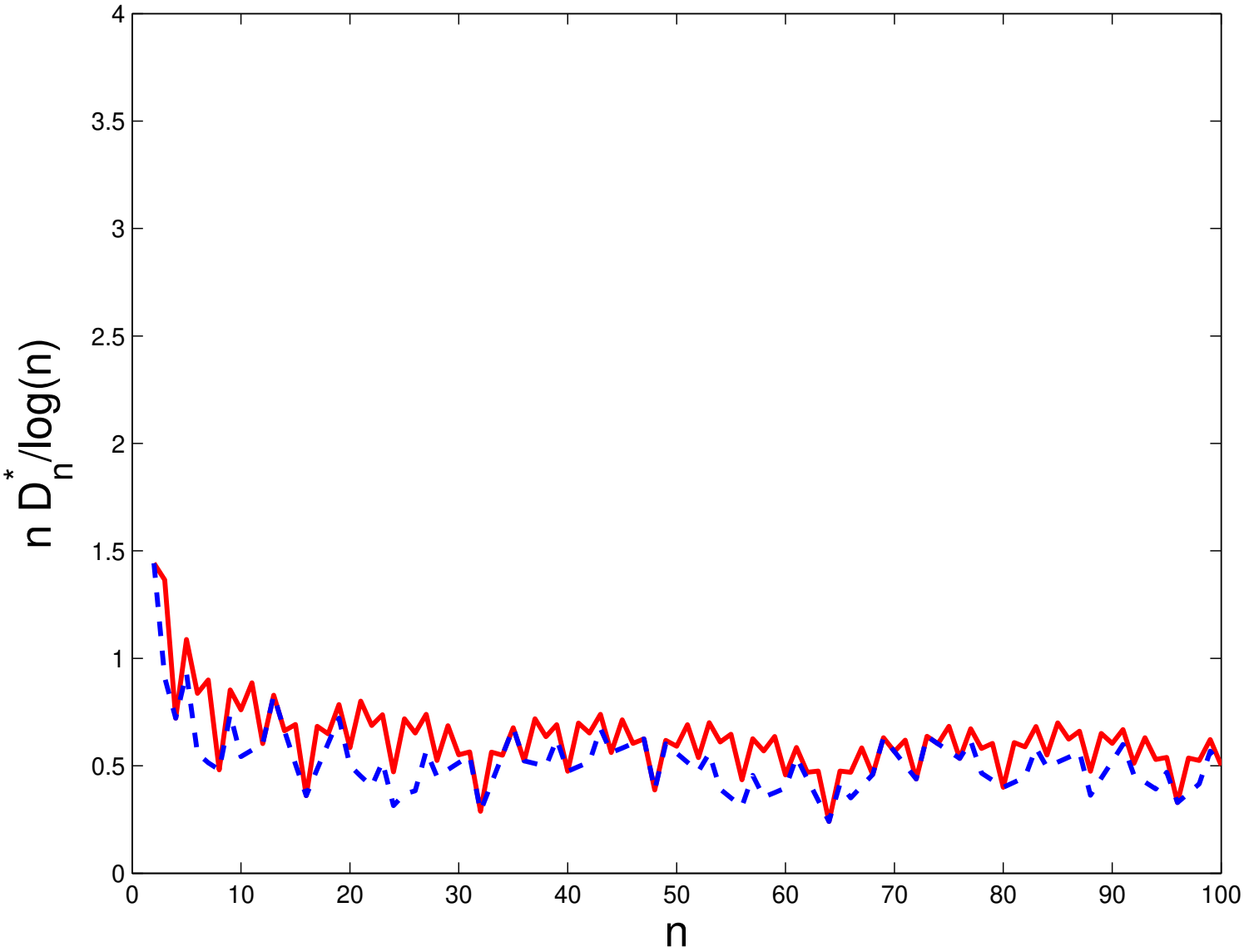

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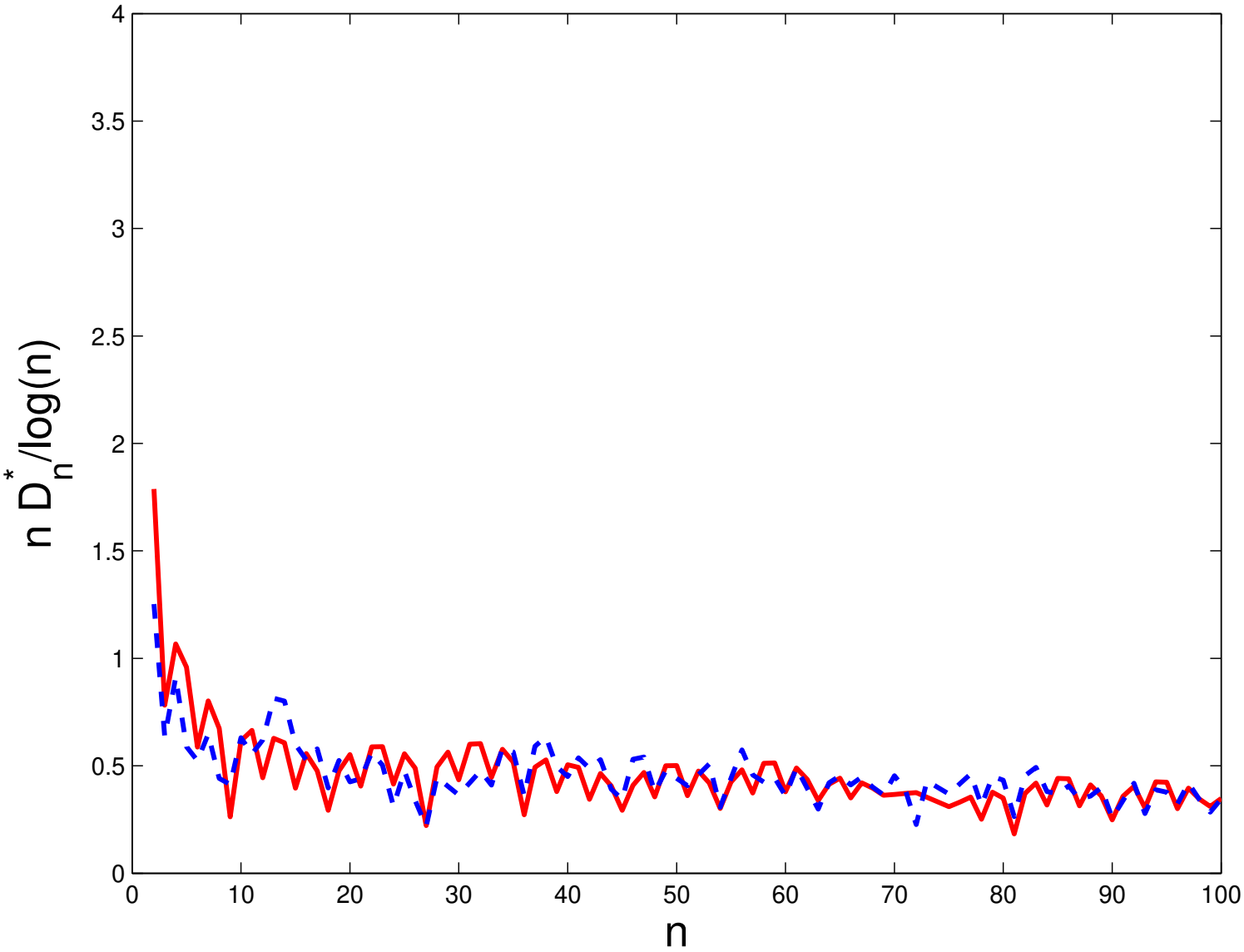
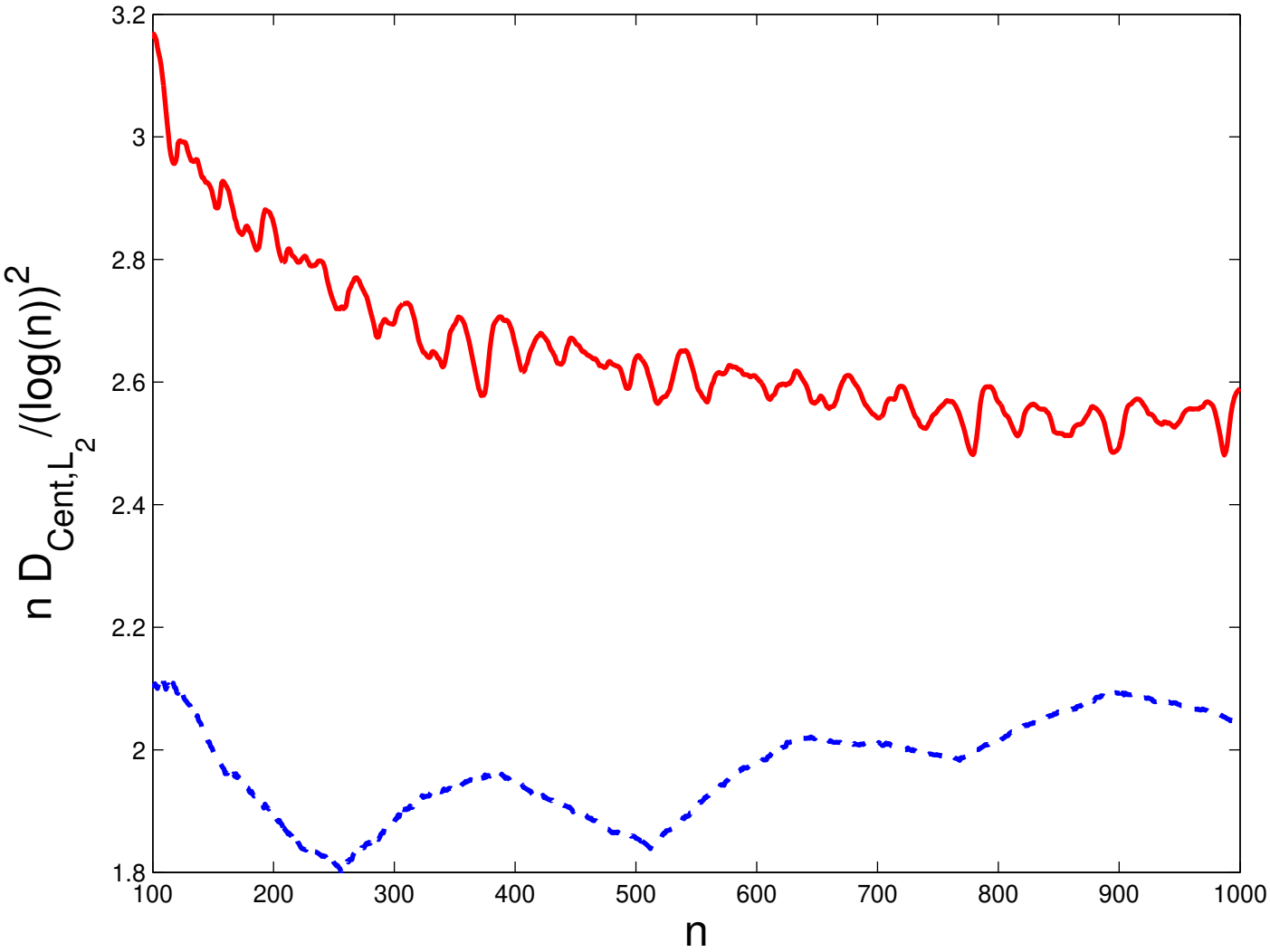


$[n/(\log n)^2] \times D_{Cent,L_2}(\mathbf{X}_n)$ for Halton and Sobol' $(d = 15)$

$(/(\log n)^2$, but no obvious normalization for $D_{Cent,L_2})$



$[n/(\log n)^2] \times D_{WA,L_2}(\mathbf{X}_n)$ for Halton and Sobol' $(d = 15)$

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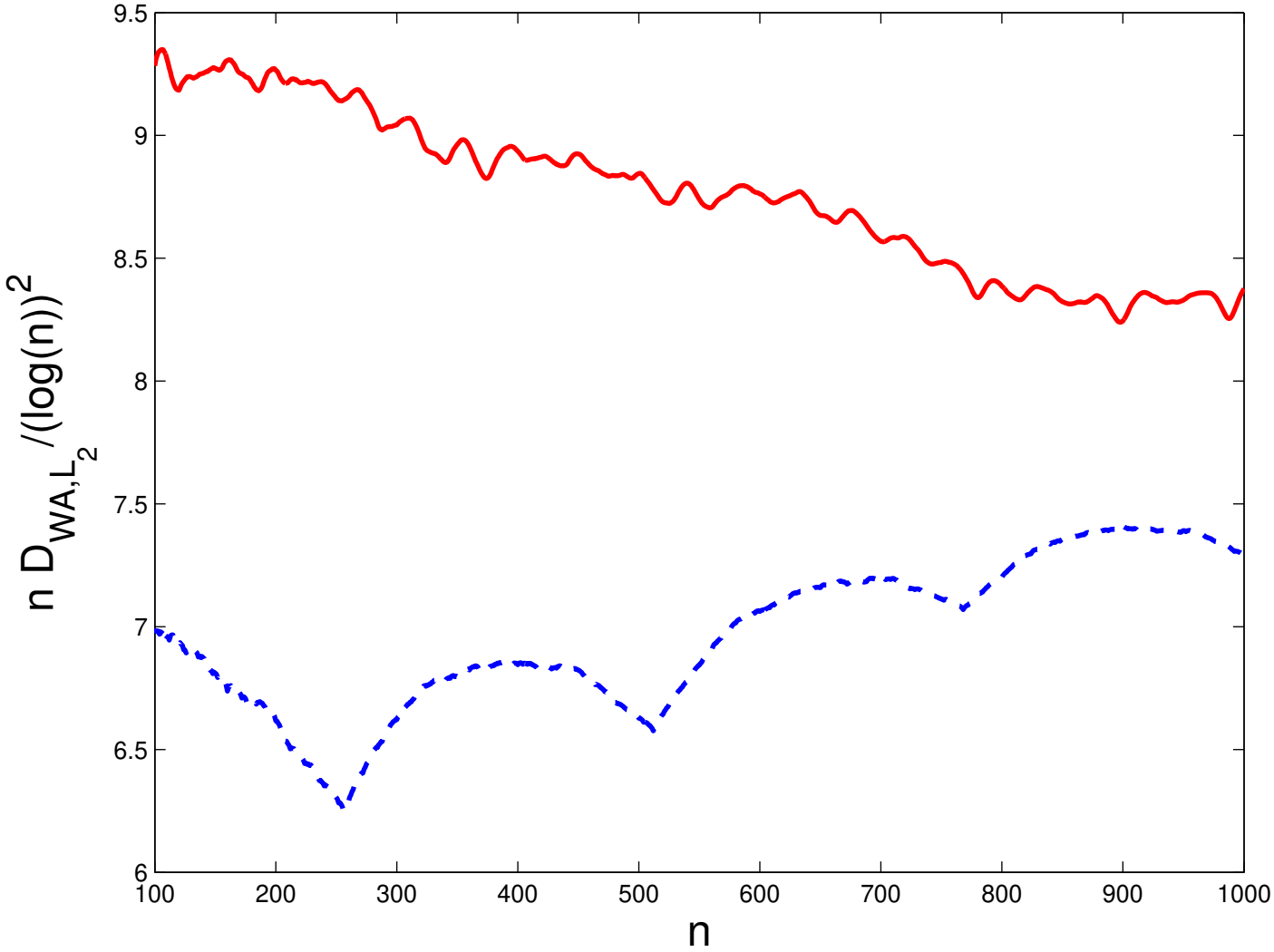

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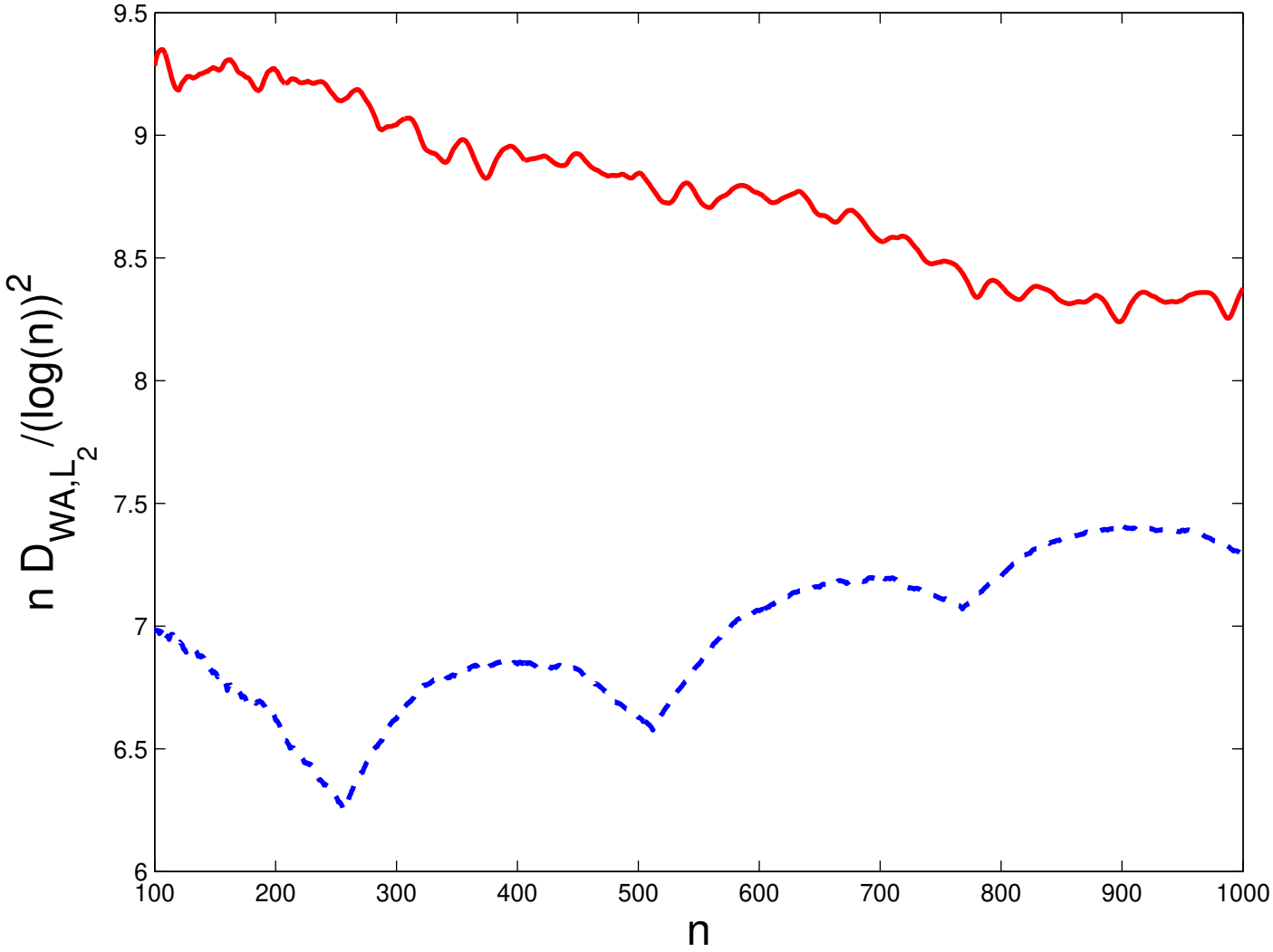
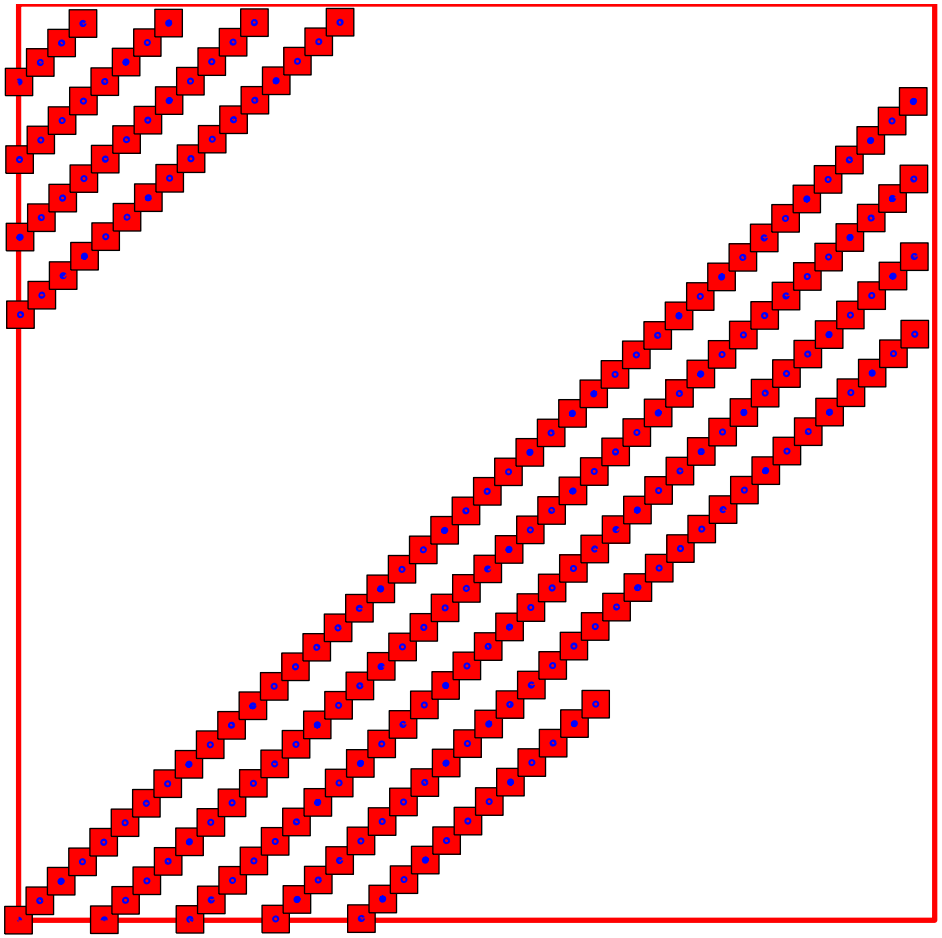


➤ $n = 1\,000$ is small: the cube $[0, 1]^{15}$ has $2^{15} = 32\,768$ vertices!

Halton, $d = 15$: $\{\mathbf{x}_k\}_{14}$ and $\{\mathbf{x}_k\}_{15}$, $k = 1, \ldots, 200$



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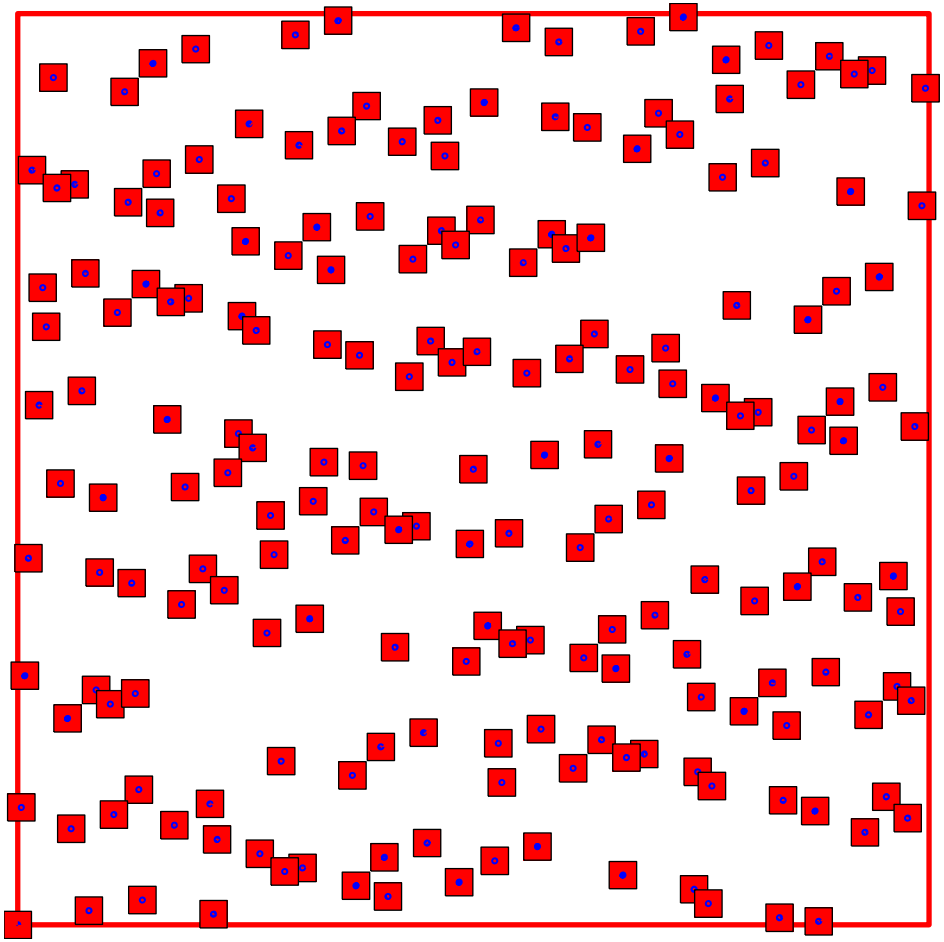

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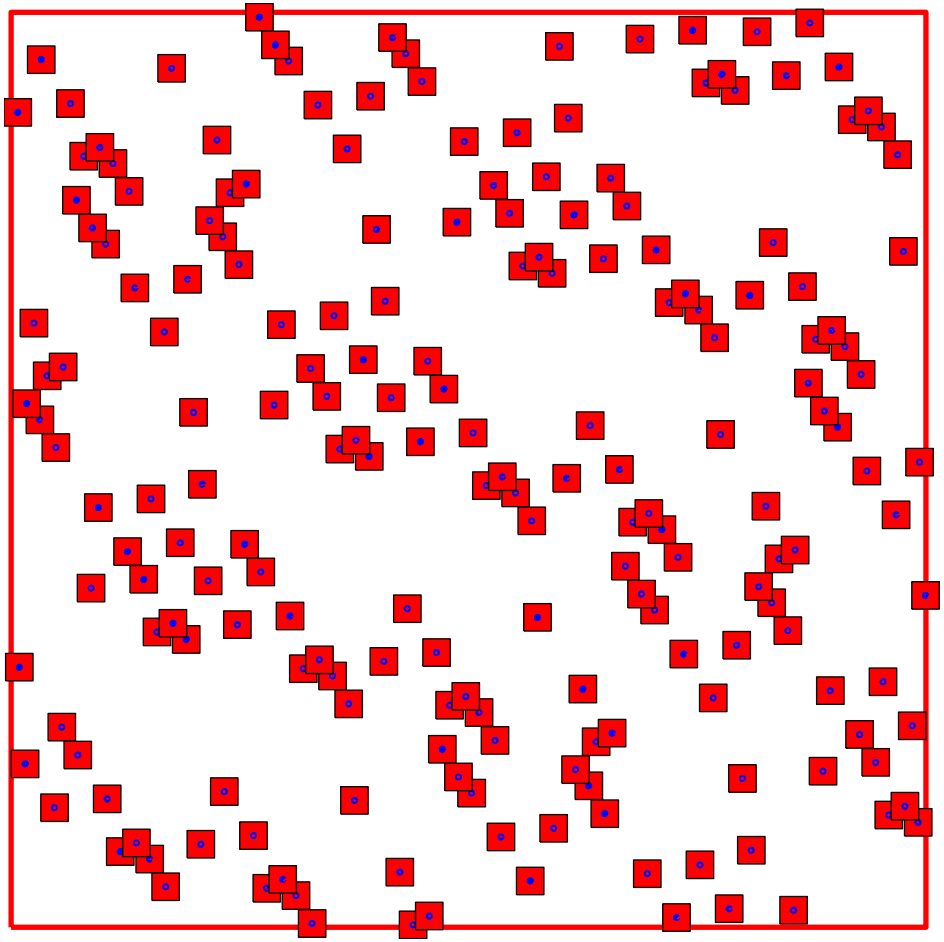

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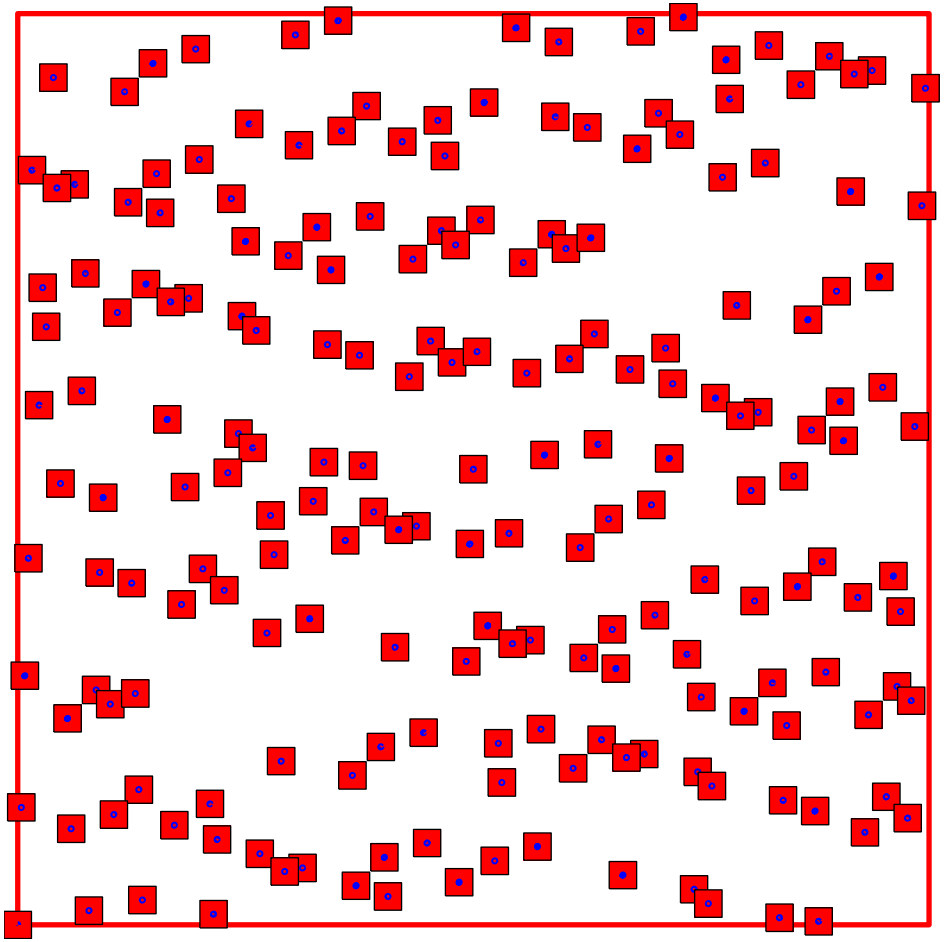

3 Dispersion & miniMax

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Discrepancy measures uniformity of the distribution of the $\mathbf{x}_k$

➠ we can also restrict our attention to the "filling" of $\mathscr{X}$ by $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$

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- $d_{\infty,n}(\mathbf{X}_n, \mathscr{X}) = d_n(\mathbf{X}_n, \mathscr{X})$ for $d = 1$

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with equality for some $\mathbf{X}_n$, for any n an d

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$$\leq A \frac{(\log n)^{(d-1)/d}}{n^{1/d}} \text{ for } \mathbf{X}_n \text{ a LDS}$$

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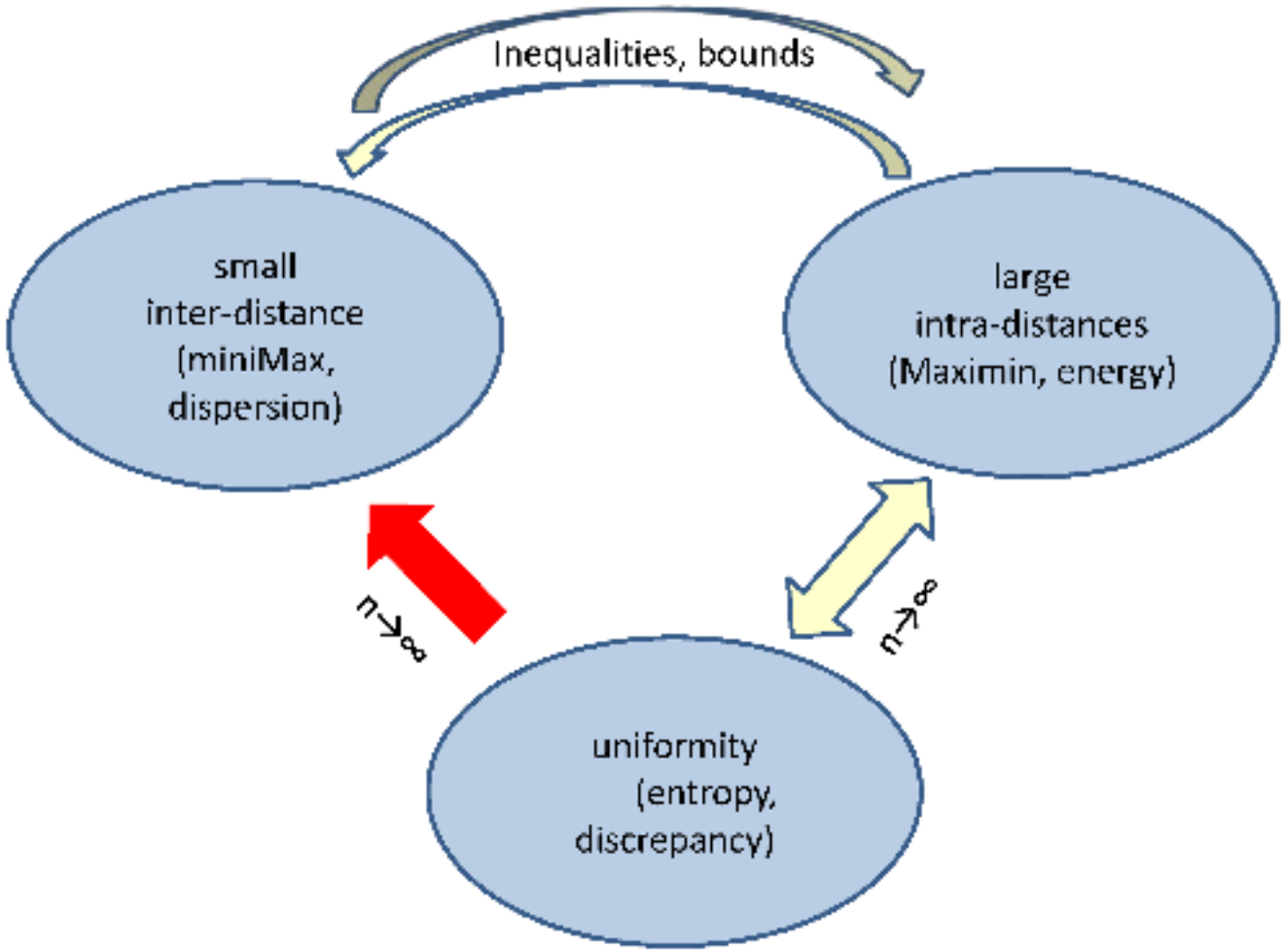
$$\Rightarrow \max\left\{ \frac{1}{(nV_d)^{1/d}}, \frac{1}{2}\, \frac{1}{\lfloor n^{1/d} \rfloor} \right\} \leq \underbrace{= \Phi^*_{mM,n}}_{\min_{\mathbf{X}_n} \Phi_{mM}(\mathbf{X}_n)} \underbrace{\leq \frac{\sqrt{d}}{2}\, \frac{1}{\lfloor n^{1/d} \rfloor}}_{\S 1.5}$$

(slightly improves the bounds of §1.5)


Inequalities, bounds
small
inter-distance
(miniMax,
dispersion)
large
intra-distances
(Maximin, energy)
$n \to \infty$
$n \to \infty$
uniformity
(entropy,
discrepancy)

3.2 **Low dispersion sequences** (Niederreiter, 1992, Chap. 6)

$\underline{d = 1}$: for any sequence $\mathbf{X}_\infty$, $\limsup_{n\to\infty} n d_n(\mathbf{X}_\infty) \geq \frac{1}{2\log 2} \simeq 0.7213$

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The bound is reached for Ruzsa sequence:

$$x_1 = 1,\ x_k = \left\{\frac{\log(2k-3)}{\log 2}\right\},\ k \geq 2$$

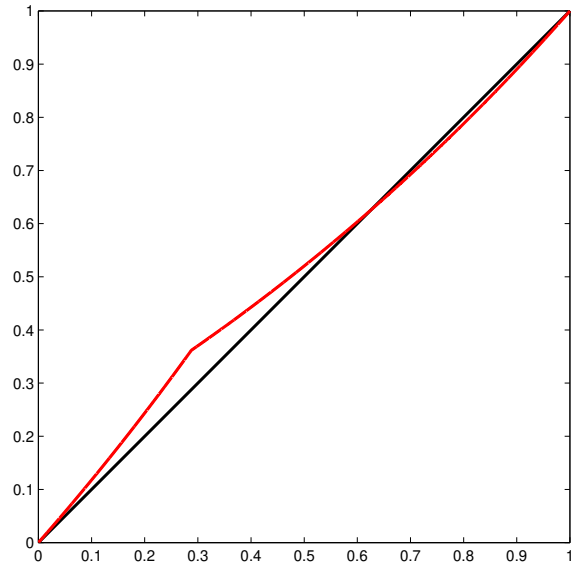
3.2 **Low dispersion sequences** (Niederreiter, 1992, Chap. 6)

$d = 1$: for any sequence $\mathbf{X}_\infty$, $\limsup_{n\to\infty} n d_n(\mathbf{X}_\infty) \geq \frac{1}{2\log 2} \simeq 0.7213$

The bound is reached for Ruzsa sequence:

$$x_1 = 1,\ x_k = \left\{\frac{\log(2k-3)}{\log 2}\right\},\ k \geq 2$$

but $D_n^*(\mathbf{X}_\infty) \not\to 0$! F_n for $n = 10\,000$ points ($D_n^* \simeq 0.0740$)



Low discrepancy ($\Leftrightarrow$ uniformity) $\Rightarrow$ low dispersion

but low dispersion $\not\Rightarrow$ low discrepancy

$\underline{d > 1}$: $\frac{1}{2} \leq \boxed{\inf_{\mathbf{X}_\infty} \limsup_{n\to\infty} n^{1/d} d_{\infty,n}(\mathbf{X}_\infty)} \leq \frac{1}{2\log 2}$

Sequences that reach the upper bound $\frac{1}{2\log 2}$ are known

The smallest value $\inf_{\mathbf{X}_\infty} \limsup_{n\to\infty} n^{1/d} d_{\infty,n}(\mathbf{X}_\infty)$ is unknown

(and best sequences $\mathbf{X}_\infty$ are unknown too)

(very) little is known about $n^{1/d} d_n(\mathbf{X}_\infty) = n^{1/d} \Phi_{mM}(\mathbf{X}_\infty)$!

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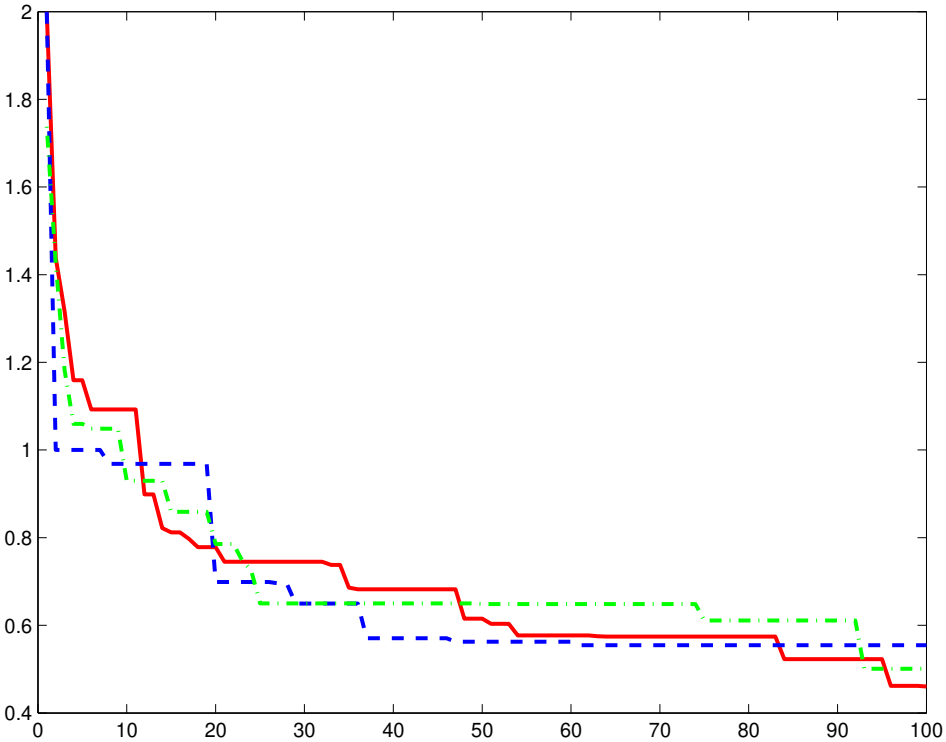
Upper bounds (rather pessimistic):

- Halton in base $(b_1, \ldots, b_d)$ ⇛ $\boxed{d_{\infty,n}(\mathbf{X}_\infty) < \frac{\max_{1\leq i\leq d} b_i}{n^{1/d}}}$
- (t,d)-sequence in base b ⇛ $\boxed{d_{\infty,n}(\mathbf{X}_\infty) < \frac{b^{1+t/d}}{n^{1/d}}}$

Ex. : $d = 4$, n from 1 to 100, $\Phi_{mM}(\mathbf{X}_n)$ for Halton ($\mathbf{b} = (2, 3, 5, 7)$), Sobol ($t = 3$, $b = 2$) and Faure ($t = 0$, $b = 5$)



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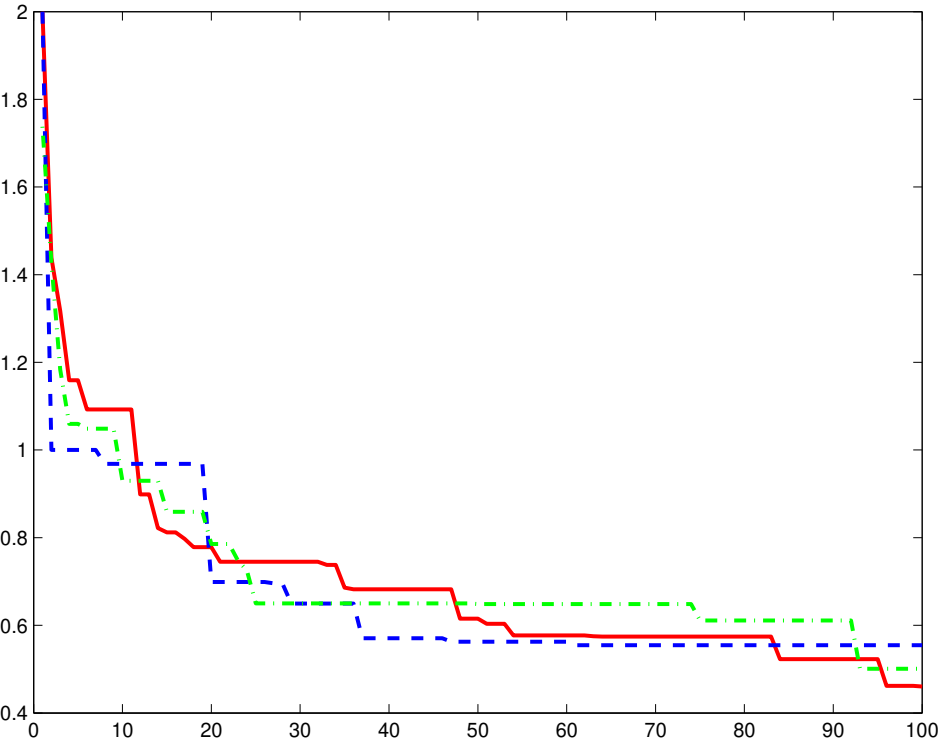

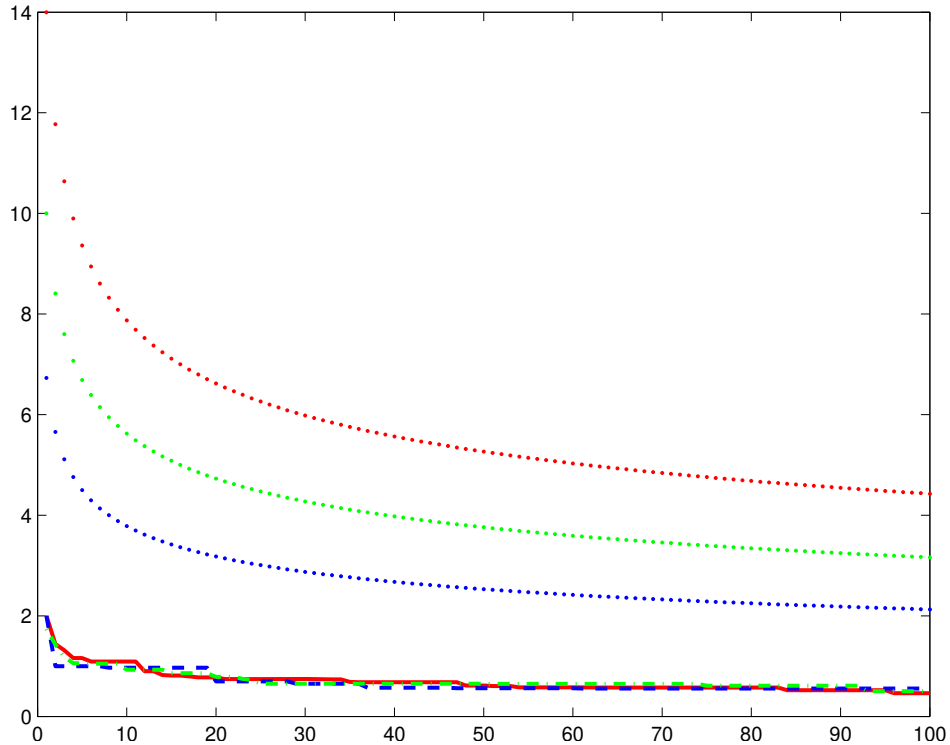

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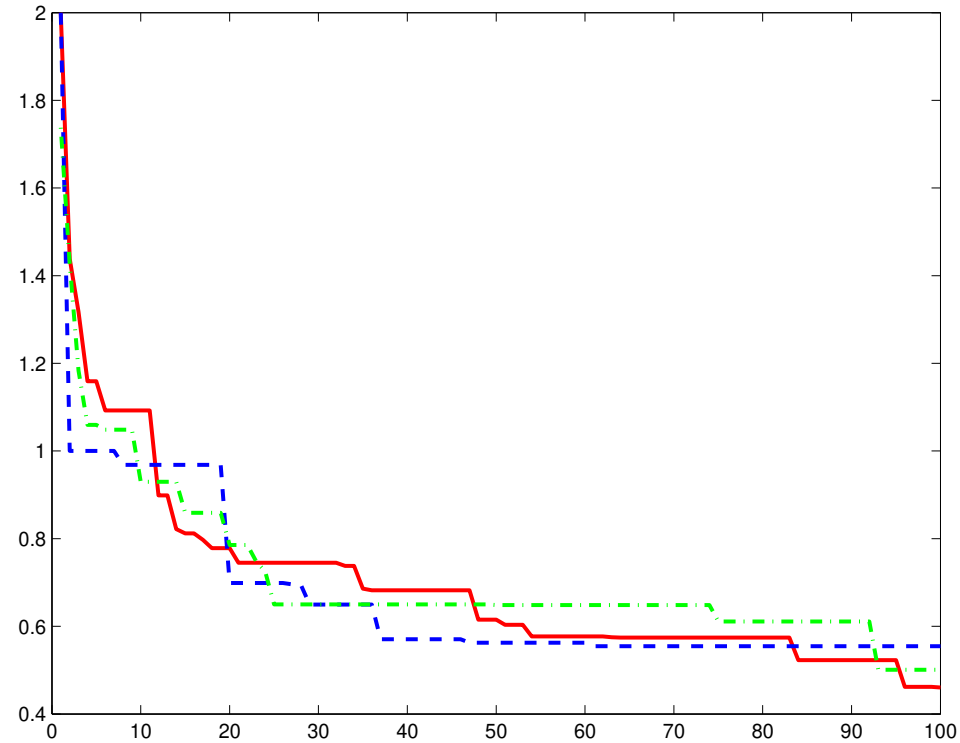

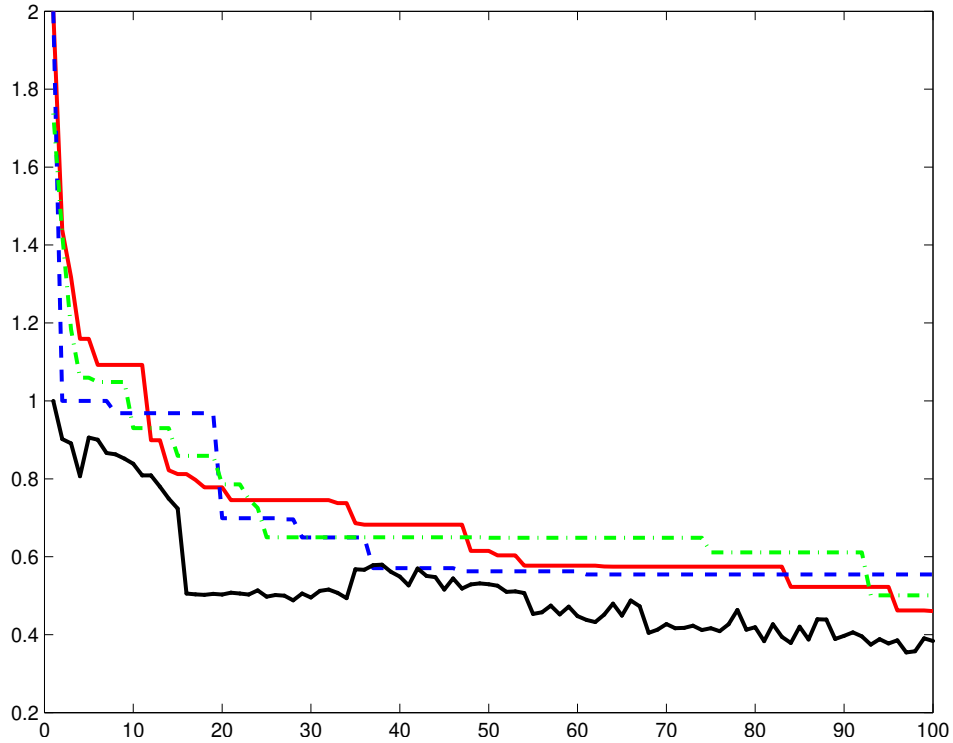

running `kmeans` algorithm on 10 000 points of Sobol' LDS (with centers initialized at the first n points)

4 Conclusions part (1) — without model

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  $\Phi_{mM}(\cdot)$ is rather compelling, its evaluation is not trivial but possible

  can be optimized by clustering (with Chebyshev centers) for small d,

  by stochastic approximation otherwise
- Low discrepancy sequences:

  easy to generate

  the sequence is well distributed (not necessary to choose n *a priori*)

  can be used for any compact $\mathscr{X}$ (with non empty interior)

  (generate points in a cube containing $\mathscr{X}$, and reject points not in $\mathscr{X}$)

The curse of dimensionality is always present!

$d = 50$, Faure $(0, d)$-sequence ➠ b prime $\geq d \rightarrow b = 53$

If we want to ensure that there is a point in each box cut along q dimensions, then

$\sum_{j=1}^{d} q_j = q = m - t = m$

➠ $n = b^q$

$q = 2$ ➠ $n = 2809$

$q = 50$ ➠ $n \simeq 1.6360\ 10^{86}$

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$d = 50$, (t, d)-sequence in base 2, with smallest possible $t \rightarrow t = 77$
If we want that each elementary interval cut along each dimension contains some points, then $n = b^m$ with $\sum_{j=1}^{d} q_j = d = m - t$ ➠ $m = 127$ and $n \simeq 1.7014\ 10^{38}$

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See (Owen, 1998) for possible constructions, such as

$$\mathbf{X}_n = \{\mathbf{X}_n\}_{1:d} = \begin{pmatrix} \{\mathbf{X}_n\}_{1:s} \\ \{\mathbf{X}_n\}_{s+1:d} \end{pmatrix}$$

with e.g. $\{\mathbf{X}_n\}_{1:s}$ a LDS sequence
$\{\mathbf{X}_n\}_{s+1:d}$ a Lh

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