Design of Computer Experiments — (2) with model —

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Plan I

Objectives (same as part (1))

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

1 Optimal design for Gaussian process models & kriging

1.1 Gaussian processes and kriging

Model for $f(\cdot)$: Gaussian process

$f(\mathbf{x}) = \mathbf{r}^\top(\mathbf{x})\beta + Z(\mathbf{x})$, with
$\mathbf{r}(\mathbf{x})$ a vector of known functions of $\mathbf{x}$ (the trend)
$Z(\mathbf{x})$ = realization of a random process (random field), second-order stationary, typically supposed to be Gaussian)
$\mathrm{E}\{Z(\mathbf{x})\} = 0$, $\mathrm{E}\{Z(\mathbf{x})Z(\mathbf{x}')\} = \sigma^2\, C(\mathbf{x} - \mathbf{x}'; \theta)$

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Computer experiments

Following (Sacks et al., 1989), choose $C(\delta; \theta)$ continuous at $\delta = 0$, $C(0; \theta) = 1$

➠ 2 repetitions at the same $\mathbf{x}$ yield the same $f(\mathbf{x})$
(no measurement error)

Objective = interpolation (or extrapolation): build a predictor $\eta_n(\mathbf{x})$ based on a single realization of $Z(\cdot)$

much different from prediction of other realizations of $Z(\cdot)$ (➠ simply estimate β)

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ordinary kriging
(expression for universal kriging with trend $\mathbf{r}^\top(\mathbf{x})\beta$, $\beta \in \mathbb{R}^p$, $p > 1$, are slightly more complicated):
$f(\mathbf{x}) = \beta + Z(\mathbf{x}) \rightarrow \eta_n(\mathbf{x}) = \eta_n[f](\mathbf{x})$

BLUP (Best Linear Unbiased Predictor) at $\mathbf{x}$: $\boxed{\eta_n(\mathbf{x}) = \mathbf{v}_n^\top(\mathbf{x})\mathbf{y}_n}$ with

- $\mathbf{y}_n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))^\top$
- $\mathbf{v}_n(x)$ minimizes $\mathrm{E}\{(\mathbf{v}_n^\top \mathbf{y}_n - [\beta + Z(\mathbf{x})])^2\}$
- with the constraint $\mathrm{E}\{\mathbf{v}_n^\top \mathbf{y}_n\} = \beta \sum_{i=1}^n \{\mathbf{v}_n\}_i = \mathrm{E}\{f(\mathbf{x})\} = \beta$, i.e., $\sum_{i=1}^n \{\mathbf{v}_n\}_i = 1$

Prediction: $\boxed{\eta_n(\mathbf{x}) = \hat{\beta}^n + \mathbf{c}_n^\top(\mathbf{x})\mathbf{C}_n^{-1}(\mathbf{y}_n - \hat{\beta}^n\mathbf{1})}$

MSE (Mean-Squared Error) proportional to

$$\boxed{\rho_n(x) = \left(1 - \left[\mathbf{c}_n^\top(x)\ 1\right]\begin{bmatrix}\mathbf{C}_n & \mathbf{1}\\ \mathbf{1}^\top & 0\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{c}_n(x)\\ 1\end{bmatrix}\right)}$$

[with $\{\mathbf{C}_n\}_{i,j} = C((X_i - X_j);\theta)$, $\{\mathbf{c}_n(x)\}_i = C((X_i - x);\theta)$, $\hat{\beta}^n = (\mathbf{1}^\top\mathbf{C}_n^{-1}\mathbf{y}_n)/(\mathbf{1}^\top\mathbf{C}_n^{-1}\mathbf{1})$ (WLS) and $\mathbf{1} = (1,\ldots,1)^\top$]

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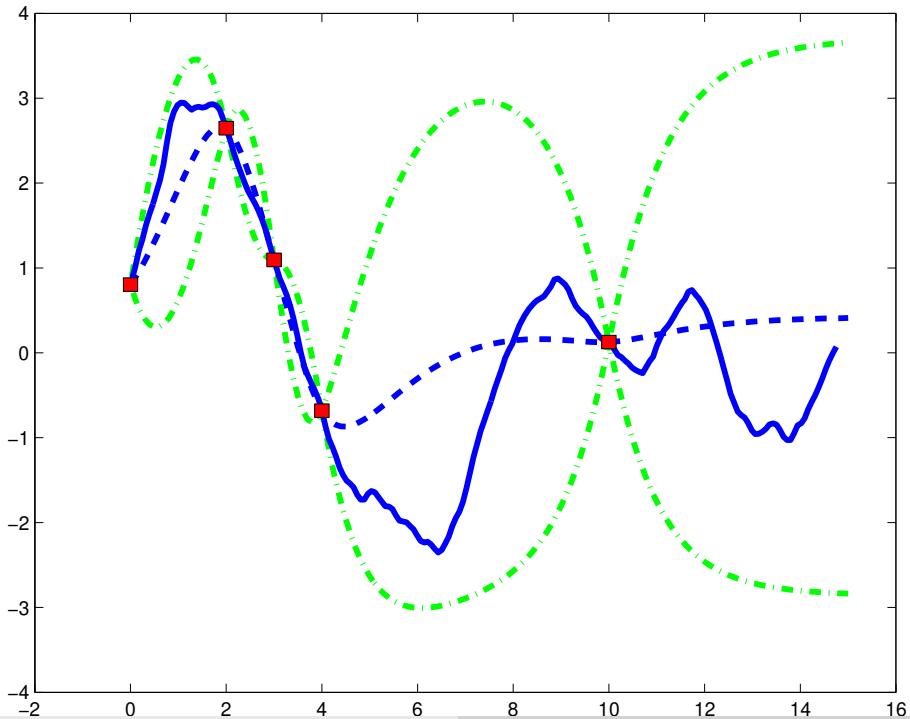
Ex. with $d = 1$, $n = 5$
(note that $\rho_n(\mathbf{x}_i) = 0$
— no measurement error)



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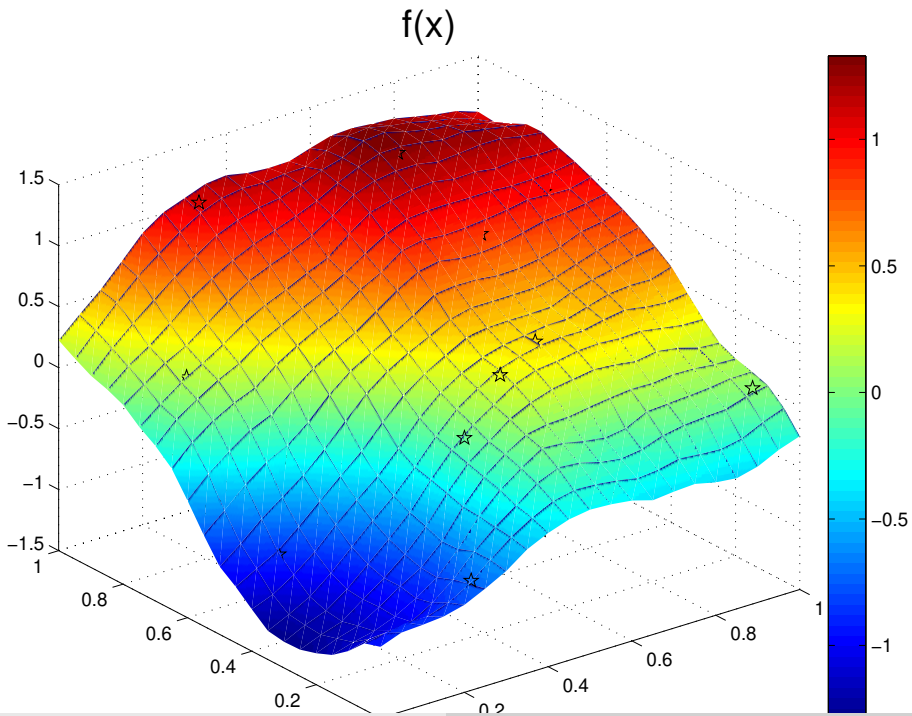
Ex. with $d = 2$, $n = 20$
($\mathbf{X}_n$ = random Lh)



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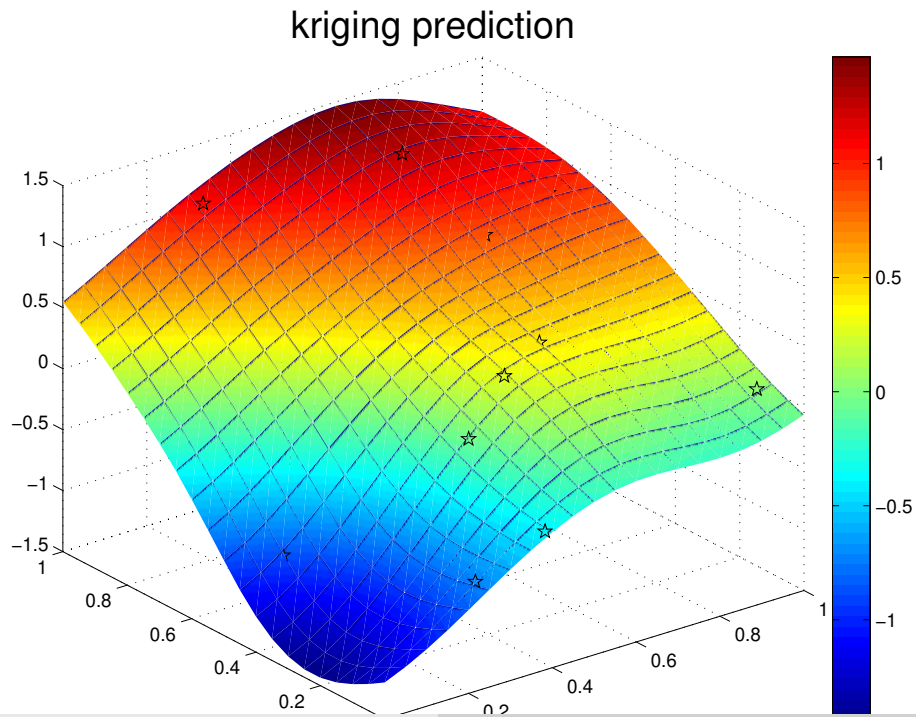

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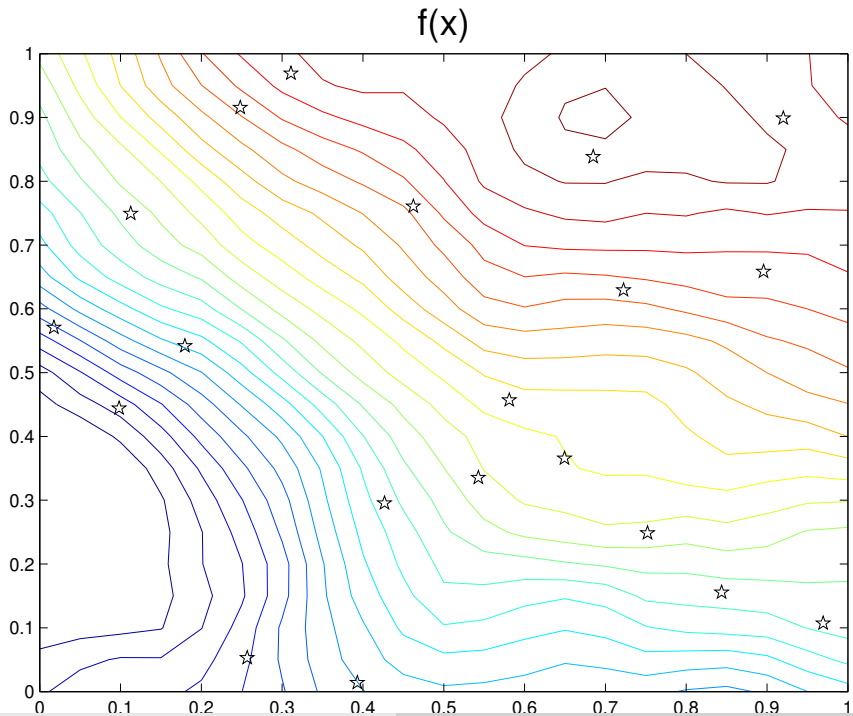

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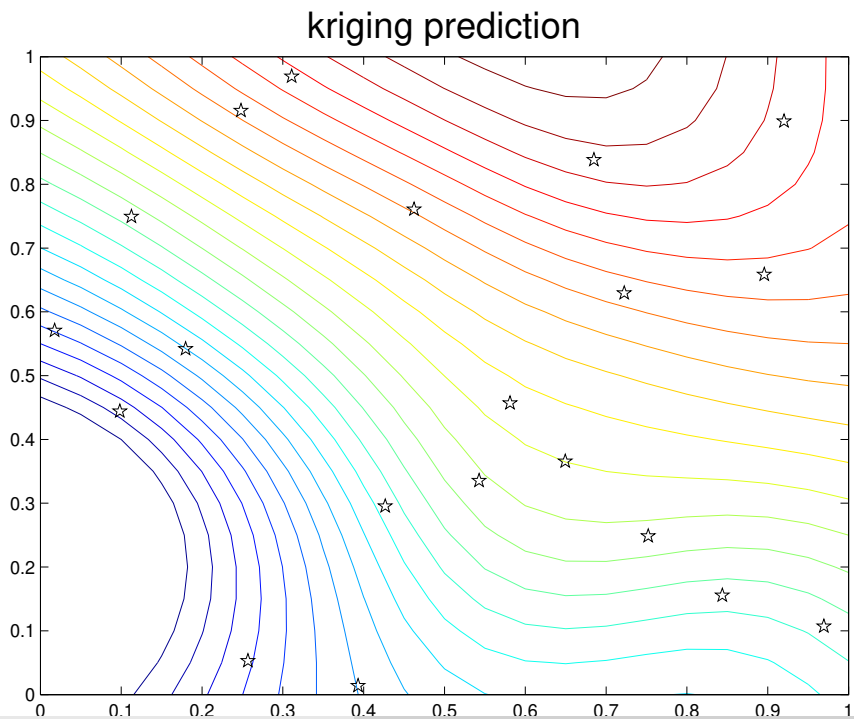

1.2 Criteria based on MSE

A natural idea: minimize $\rho_n(\mathbf{x})$ for all $\mathbf{x}$

In practice:

- minimize $\text{MMSE}(\mathbf{X}_n) = \max_{\mathbf{x}\in\mathscr{X}} \rho_n(\mathbf{x})$
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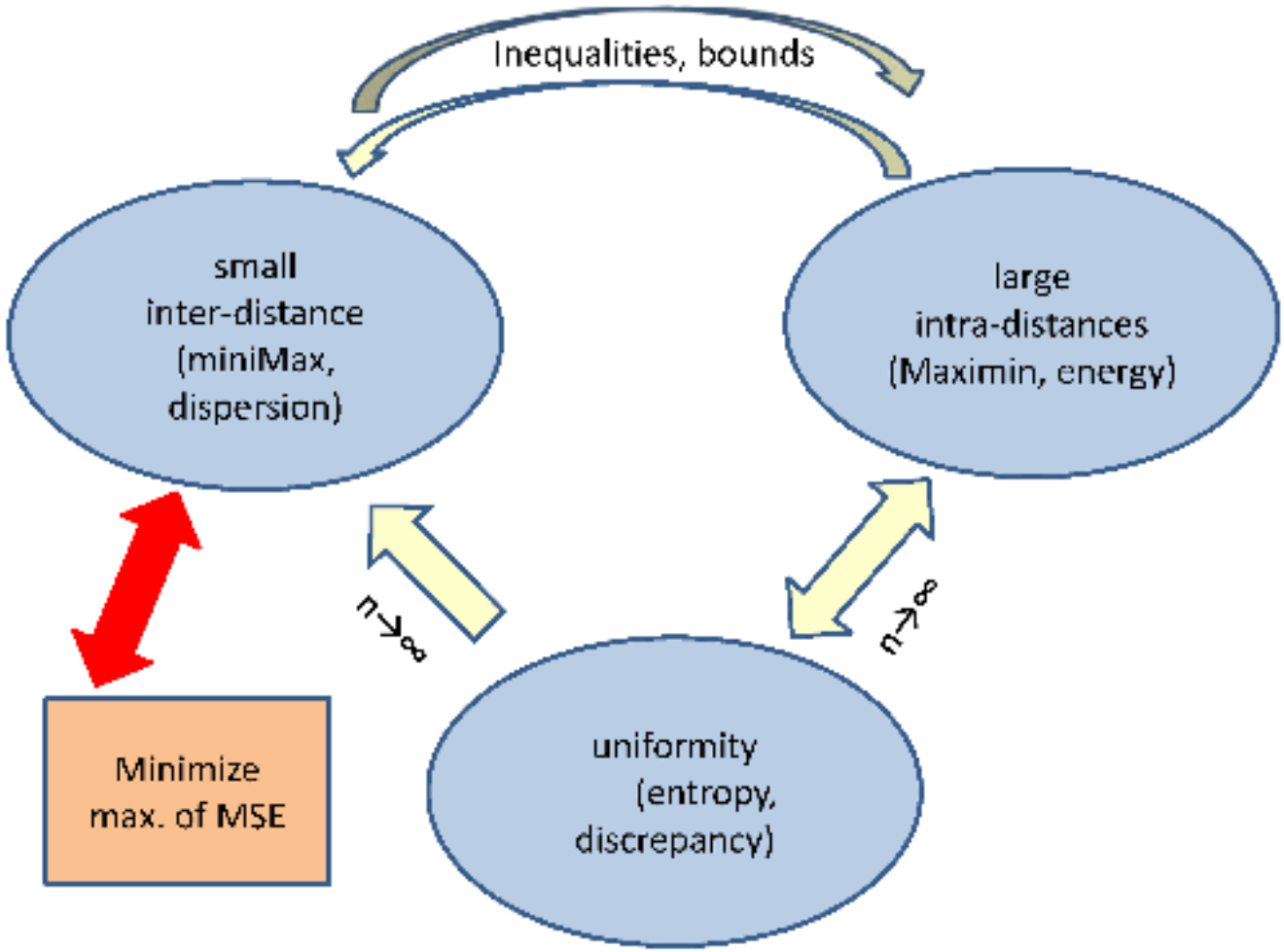
Optimal designs are typically space-filling:

Johnson et al. (1990): if $C(\mathbf{x}-\mathbf{x}') = c(\|\mathbf{x}-\mathbf{x}'\|)$ with $c(\cdot)$ decreasing, then $\mathbf{X}_n^*$ optimal for $\Phi_{mM}(\cdot)$ (miniMax optimal) tends to be optimal for $\text{MMSE}(\mathbf{X}_n)$ with covariance $C_a(\mathbf{x}-\mathbf{x}') = [C(\mathbf{x}-\mathbf{x}')]^a$ when $a \to \infty$

➠ no point $\mathbf{x}_i$ on the boundary of $\mathscr{X}$


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

$$\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$$

Calculation of MMSE($\mathbf{X}_n$):

Compute $\rho_n(\mathbf{x}^{(k)})$ for a finite Q-points set $\mathscr{X}_Q = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(Q)}\}$
(e.g., first Q point of a LDS in $\mathscr{X}$),
then MMSE($\mathbf{X}_n$) $\simeq \max_k \rho_n(\mathbf{x}^{(k)})$,
to be minimized, for instance by simulated annealing

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Calculation of IMSE($\mathbf{X}_n$) $= \int_{\mathscr{X}} \rho_n(\mathbf{x}) \mathrm{d}\mu(\mathbf{x})$ (Gauthier and P. 2014, 2016) :

Without trend ($\mathbf{r}(\mathbf{x}) = \mathbf{0}\ \forall \mathbf{x}$) ➠ $\rho_n(\mathbf{x}) = 1 - \mathbf{c}_n^\top(\mathbf{x}) \mathbf{C}_n^{-1} \mathbf{c}_n(\mathbf{x})$,
where $\{\mathbf{c}_n(\mathbf{x})\}_i = C(\mathbf{x} - \mathbf{x}_i)$, $\{\mathbf{C}_n\}_{ij} = C(\mathbf{x}_i - \mathbf{x}_j)$

$$\begin{aligned} \text{IMSE}(\mathbf{X}_n) &= 1 - \text{trace}\left[\mathbf{C}_n^{-1} \int_{\mathscr{X}} \mathbf{c}_n(\mathbf{x}) \mathbf{c}_n^\top(\mathbf{x}) \mathrm{d}\mu(\mathbf{x})\right] \\ &= 1 - \text{trace}\left[\mathbf{C}_n^{-1} \Sigma_n\right] \end{aligned}$$

Calculation for a finite Q-points set $\mathscr{X}_Q = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(Q)}\}$:

$$\begin{aligned} \text{IMSE}(\mathbf{X}_n) \simeq \widehat{\text{IMSE}}(\mathbf{X}_n) &= \sum_{k=1}^{Q} w_k \, \rho_n(\mathbf{x}^{(k)}) \\ &= 1 - \text{trace}\left[\mathbf{C}_n^{-1} \widehat{\Sigma}_n\right] \end{aligned}$$

with $\sum_{k=1}^{Q} w_k = 1$ ($w_k = 1/Q$ when μ if uniform)
and $\widehat{\Sigma}_n = \sum_{k=1}^{Q} w_k \mathbf{c}_n(\mathbf{x}^{(k)}) \mathbf{c}_n^\top(\mathbf{x}^{(k)})$

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If, moreover, $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathscr{X}_Q$, with $\mathbf{x}_i = \mathbf{x}^{(k_i)}$, $i = 1, \ldots, n$,

then $\widehat{\Sigma}_n = \{\mathbf{QWQ}\}_{\mathbb{J}_n \mathbb{J}_n}$
with $\{\mathbf{Q}\}_{k\ell} = C(\mathbf{x}^{(k)} - \mathbf{x}^{(\ell)})$, $\mathbf{W} = \text{diag}\{w_1, \ldots, w_Q\}$
and $\mathbb{J}_n = \{k_1, \ldots, k_n\}$

➠ $\text{IMSE}(\mathbf{X}_n) \simeq 1 - \text{trace}\left[\mathbf{Q}_{\mathbb{J}_n \mathbb{J}_n}{}^{-1} \{\mathbf{QWQ}\}_{\mathbb{J}_n \mathbb{J}_n}\right]$
not expensive to compute once $\mathbf{Q}$ and $\mathbf{QWQ}$ have been calculated

(a bit more complicated with a trend $\mathbf{r}^\top(\mathbf{x})\beta$)

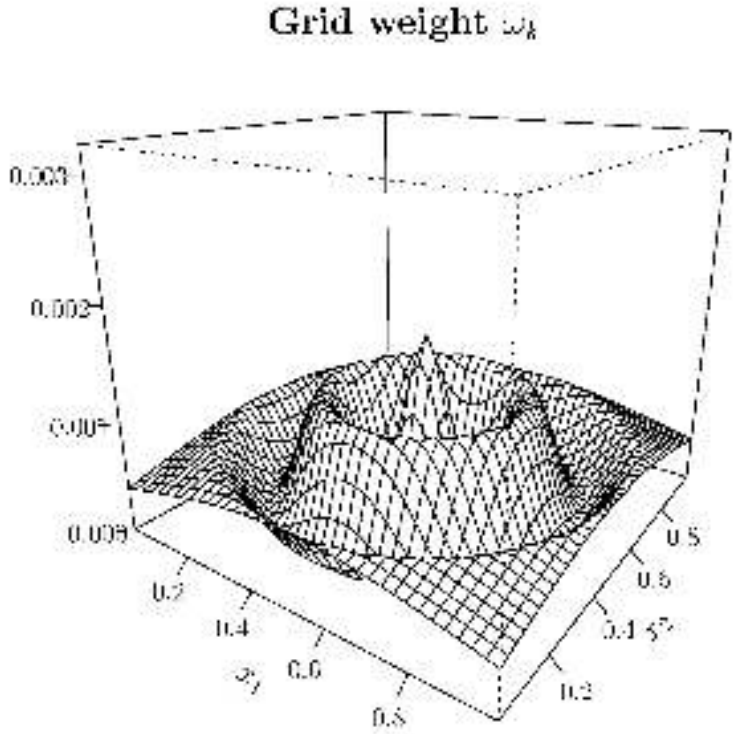
Minimization not obvious (for instance, by simulated annealing),
see § 3.3 for another approach

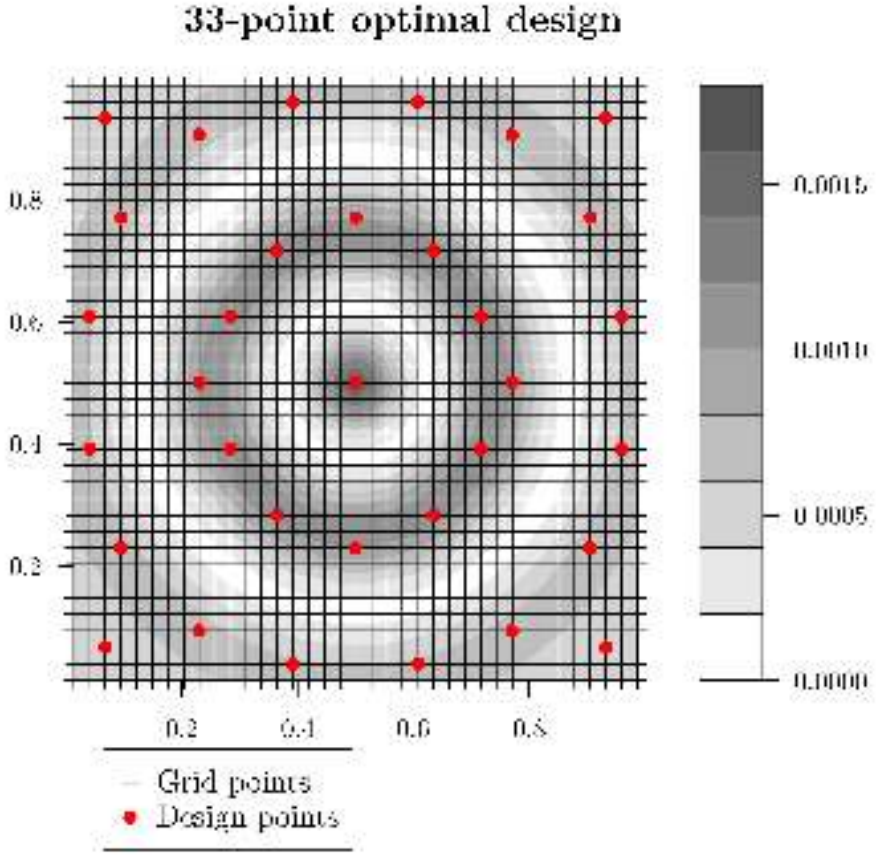
Ex. of IMSE-optimal design (Gauthier & P., 2014, 2016):

$\mathscr{X}$ = regular grid with $37^2 = 1\,369$ points

$C(\mathbf{x} - \mathbf{x}') = C_1(\{\mathbf{x}\}_1 - \{\mathbf{x}'\}_1) \times C_2(\{\mathbf{x}\}_2 - \{\mathbf{x}'\}_2)$,

$C_i(x - x') = (1 + 25/\sqrt{3}|x - x'|) \exp[-25/\sqrt{3}|x - x'|]$ (Matérn 3/2)





(measure of interest μ)

Sequential construction of an optimal design:

For IMSE: nothing special, at step $n+1$, $\mathbf{X}_{n+1} = \{\mathbf{X}_n, \mathbf{x}_{n+1}\}$ with

$$\boxed{\mathbf{x}^*_{n+1} = \arg\min_{\mathbf{x}\in\mathscr{X}} \text{IMSE}(\{\mathbf{X}_n, \mathbf{x}\})}$$

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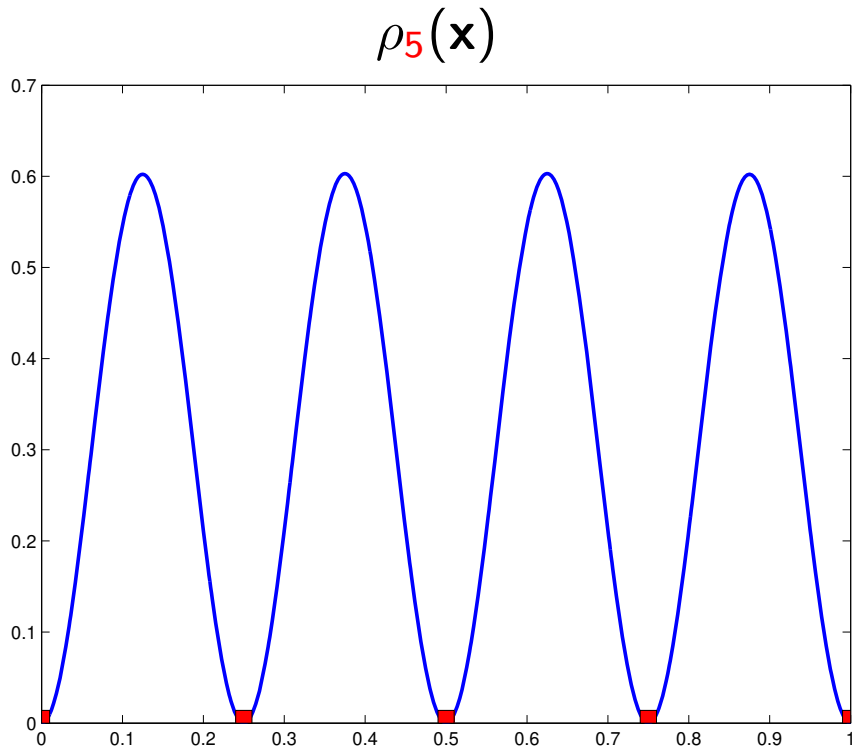

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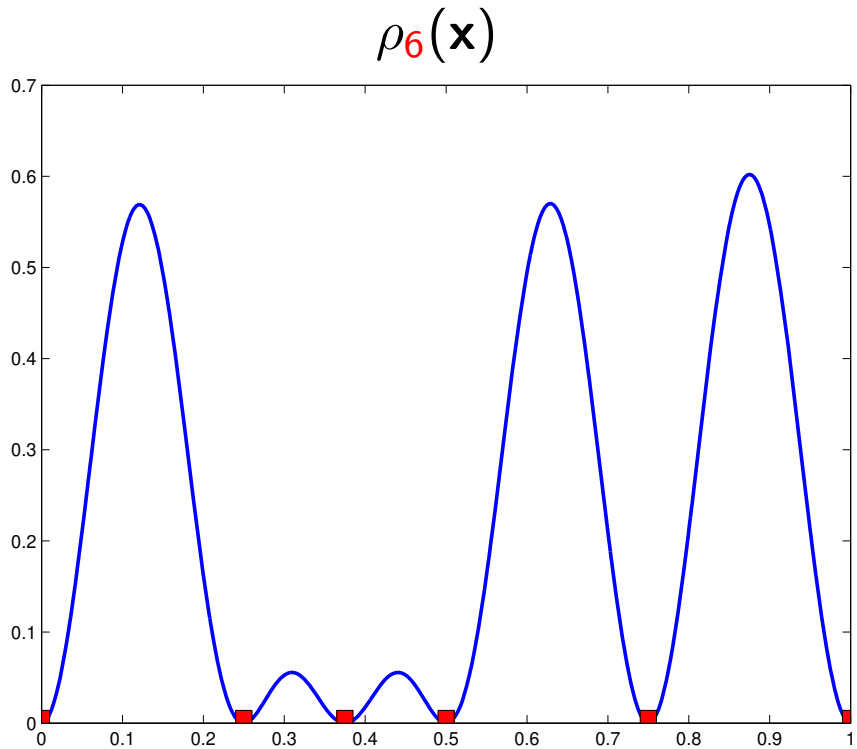

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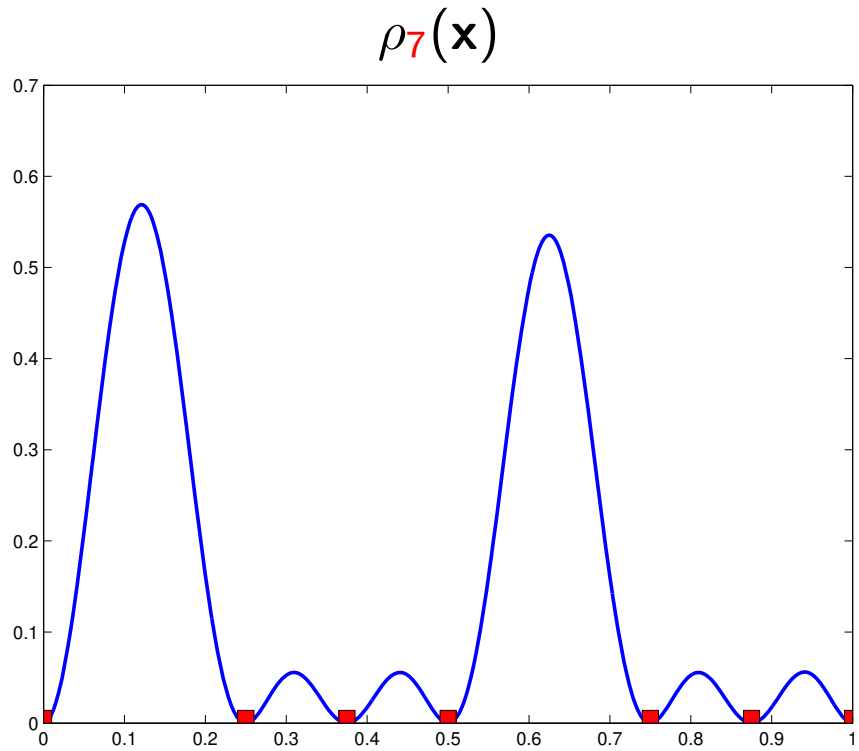

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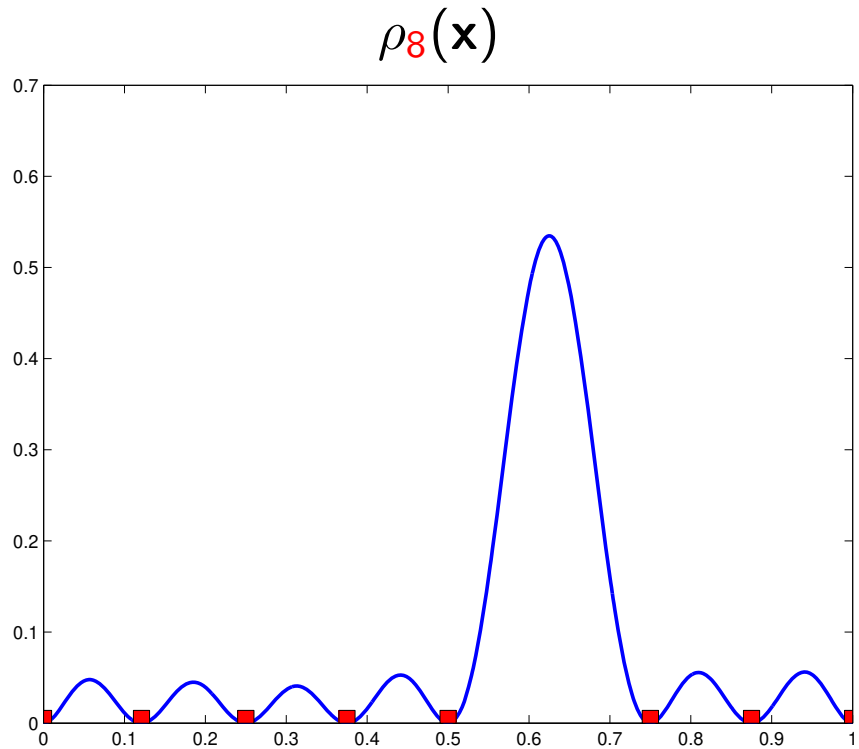

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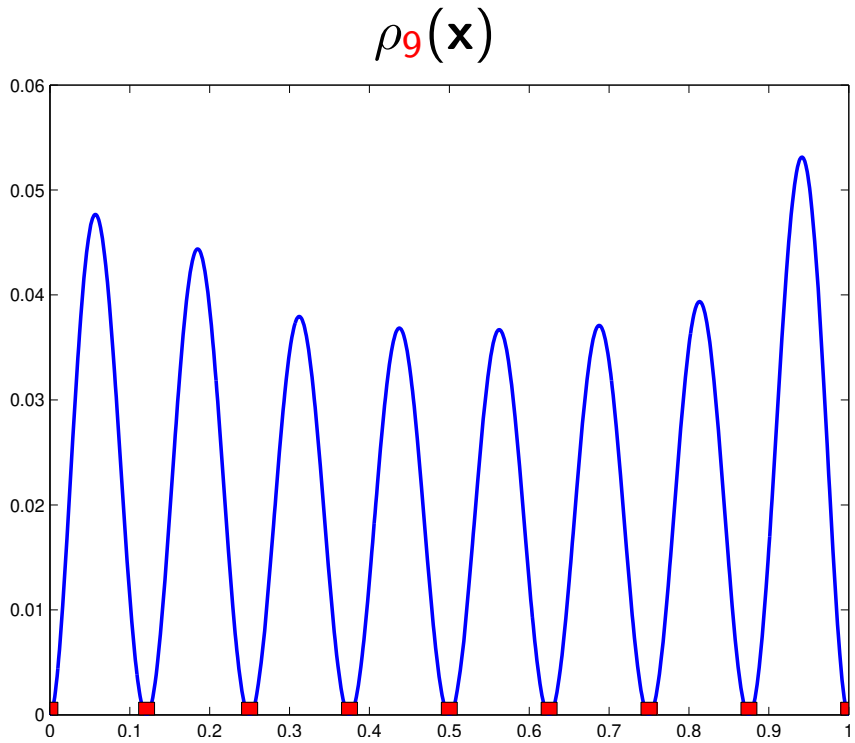

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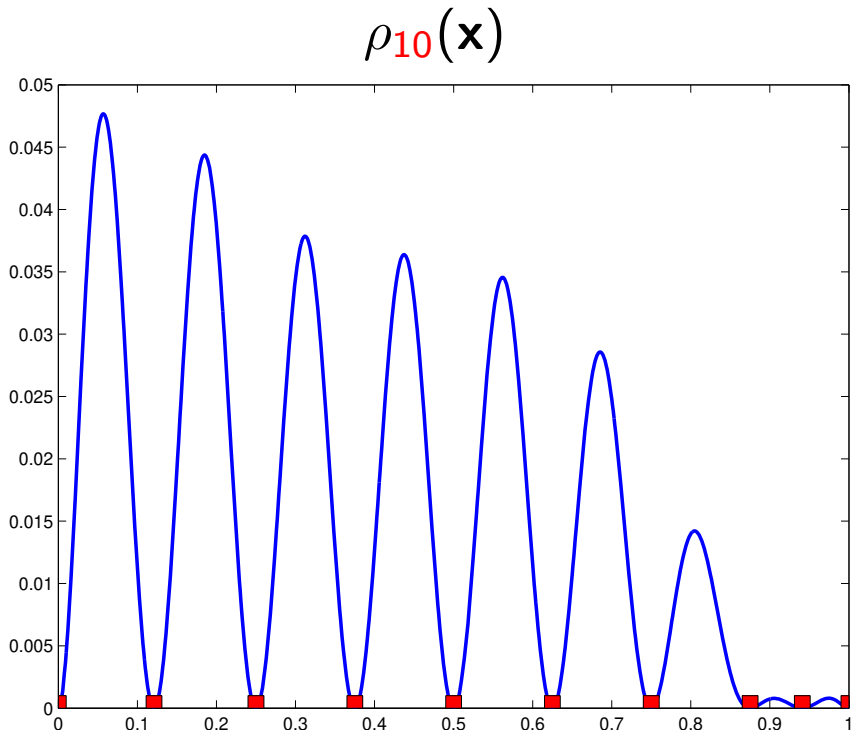

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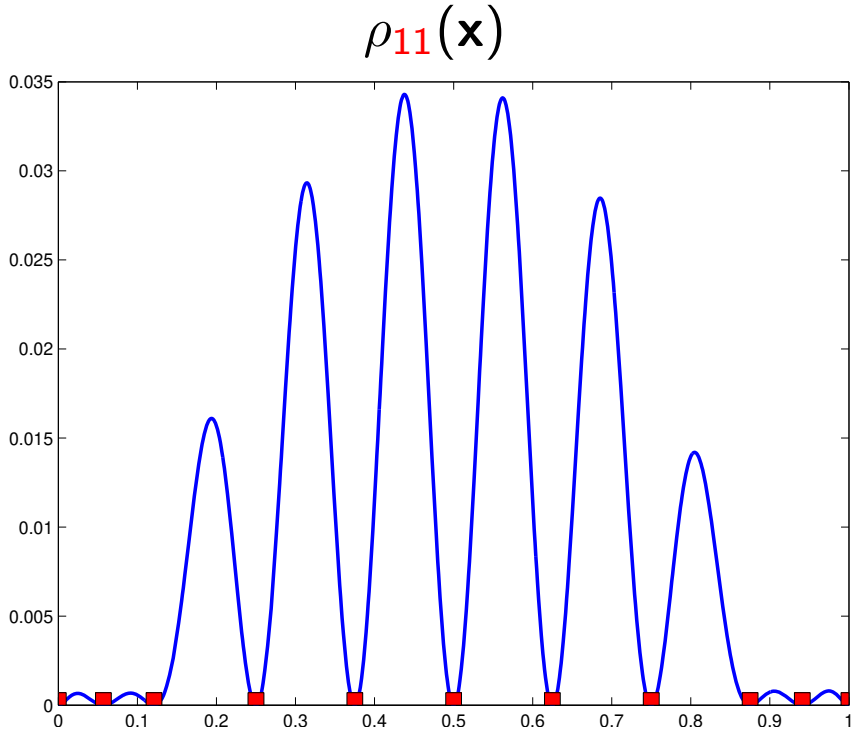

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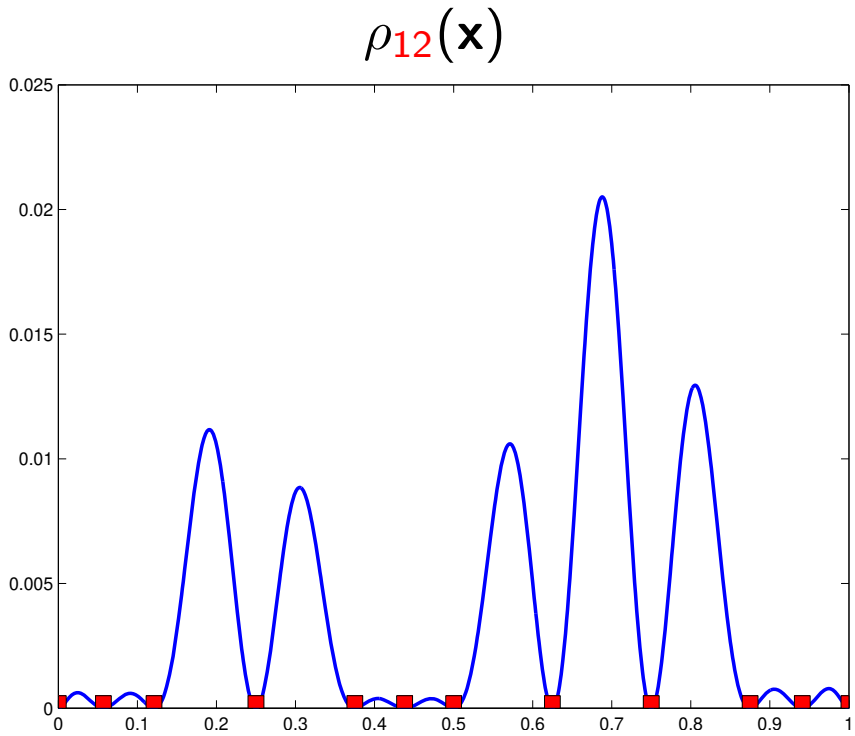

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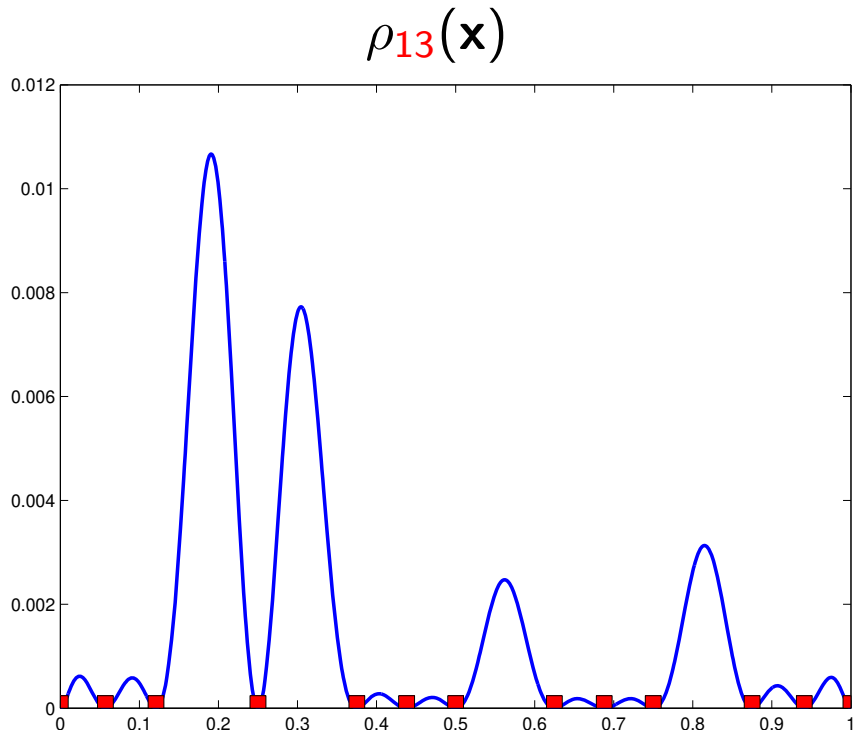

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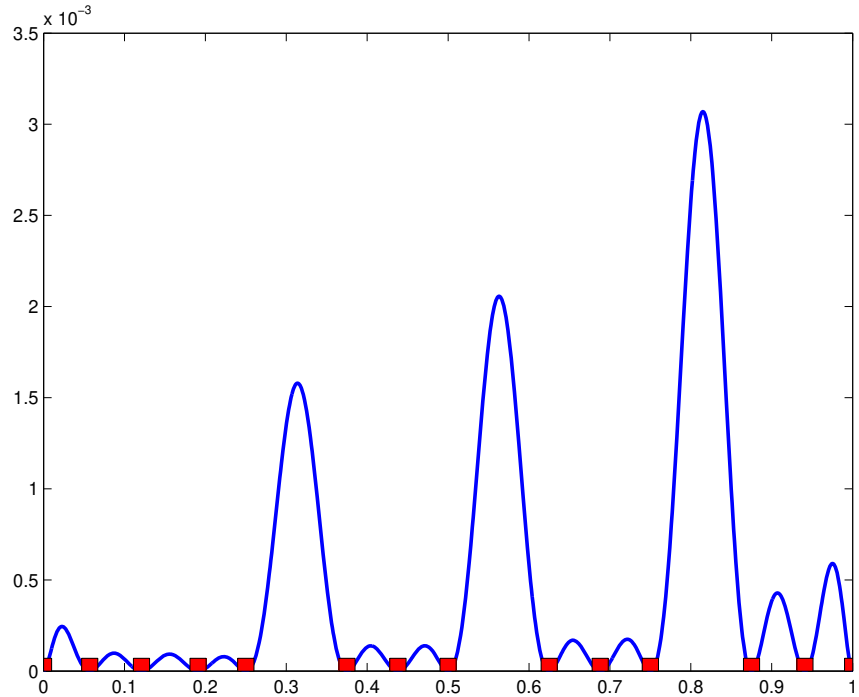

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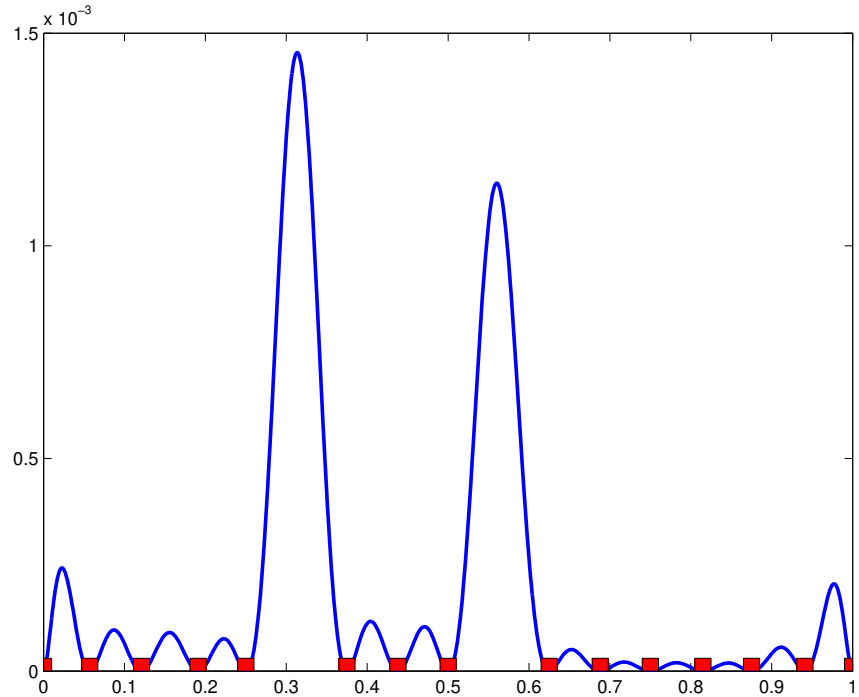

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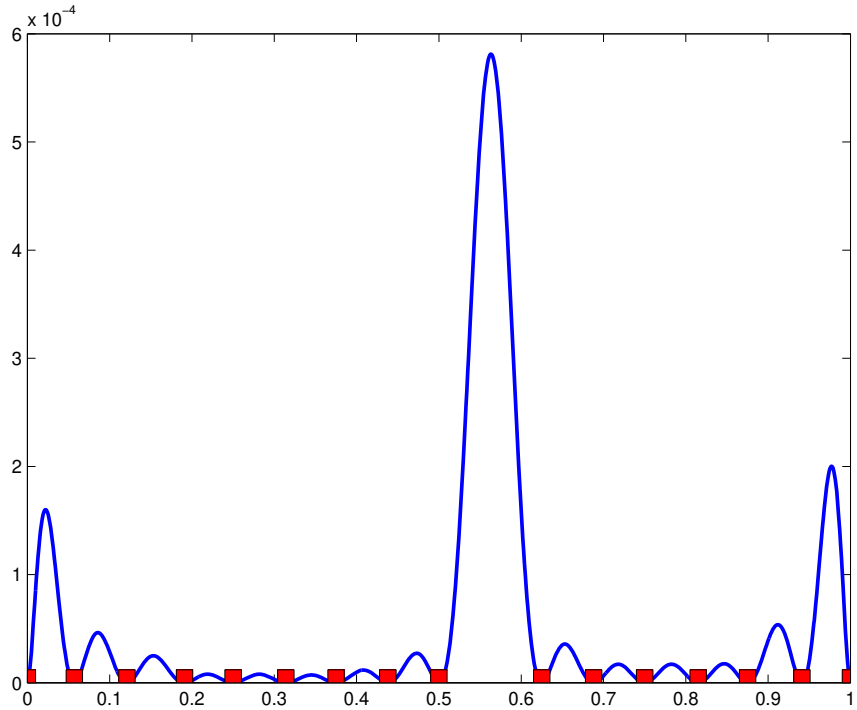

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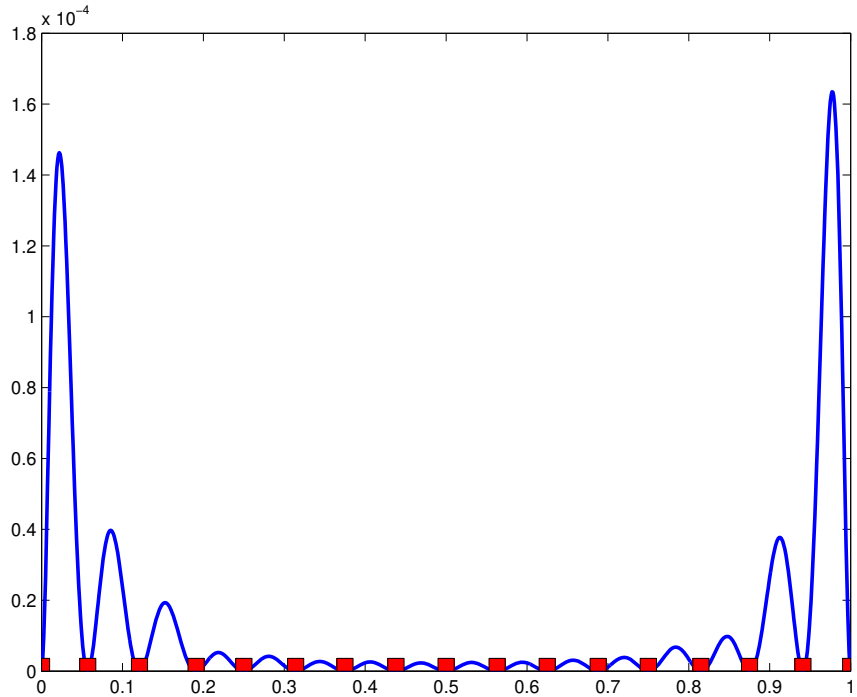

1.3 **Maximum Entropy Sampling** (Shewry and Wynn, 1987)

Without trend ($\mathbf{r}(\mathbf{x}) = \mathbf{0}\ \forall \mathbf{x}$) :

- $\mathbf{z}_Q \triangleq$ vector with components $Z(\mathbf{x}^{(k)})$, $\mathbf{x}^{(k)} \in \mathscr{X}_Q$
- $\mathbf{z}_n \triangleq$ vector with components $Z(\mathbf{x}_i)$, $i = 1, \ldots, n$ (observations)
- $H_1(\mathbf{z}) \triangleq -\int \varphi(\mathbf{z}) \log[\varphi(\mathbf{z})]\, \mathrm{d}\mathbf{z}$ Shannon entropy of $\varphi(\mathbf{z})$
  $= $ measure of "dispersion"

  $H_1(\mathbf{z}_1|\mathbf{z}_2) \triangleq$ conditional entropy of $\mathbf{z}_1$ given $\mathbf{z}_2$
  $= \int \left[-\int \varphi(\mathbf{z}_1|\mathbf{z}_2) \log[\varphi(\mathbf{z}_1|\mathbf{z}_2)]\, \mathrm{d}\mathbf{z}_1 \right] \varphi(\mathbf{z}_2)\, \mathrm{d}(\mathbf{z}_2)$

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Minimize $\mathrm{E}\{H_1(\mathbf{y}_Q|\mathbf{y}_n)\}$ w.r.t. $\mathbf{X}_n \Leftrightarrow$ maximize $H_1(\mathbf{y}_n)$

$Z(\mathbf{x})$ is Gaussian ➠ $\boxed{\text{maximize } \det[\mathbf{C}_n]}$

= intra-distances criterion

Sequential construction of an optimal design:

$$\mathbf{x}_{n+1} = \arg\max_{\mathbf{x}\in\mathscr{X}} \det[\mathbf{C}_{n+1}] = \arg\max_{\mathbf{x}\in\mathscr{X}} \underbrace{\det\begin{bmatrix} \mathbf{C}_n & \mathbf{c}_n(\mathbf{x}) \\ \mathbf{c}_n^\top(\mathbf{x}) & 1 \end{bmatrix}}_{=\det[\mathbf{C}_n]\underbrace{(1-\mathbf{c}_n^\top(\mathbf{x})\mathbf{C}_n^{-1}\mathbf{c}_n(\mathbf{x}))}_{=\rho_n(\mathbf{x})}}$$

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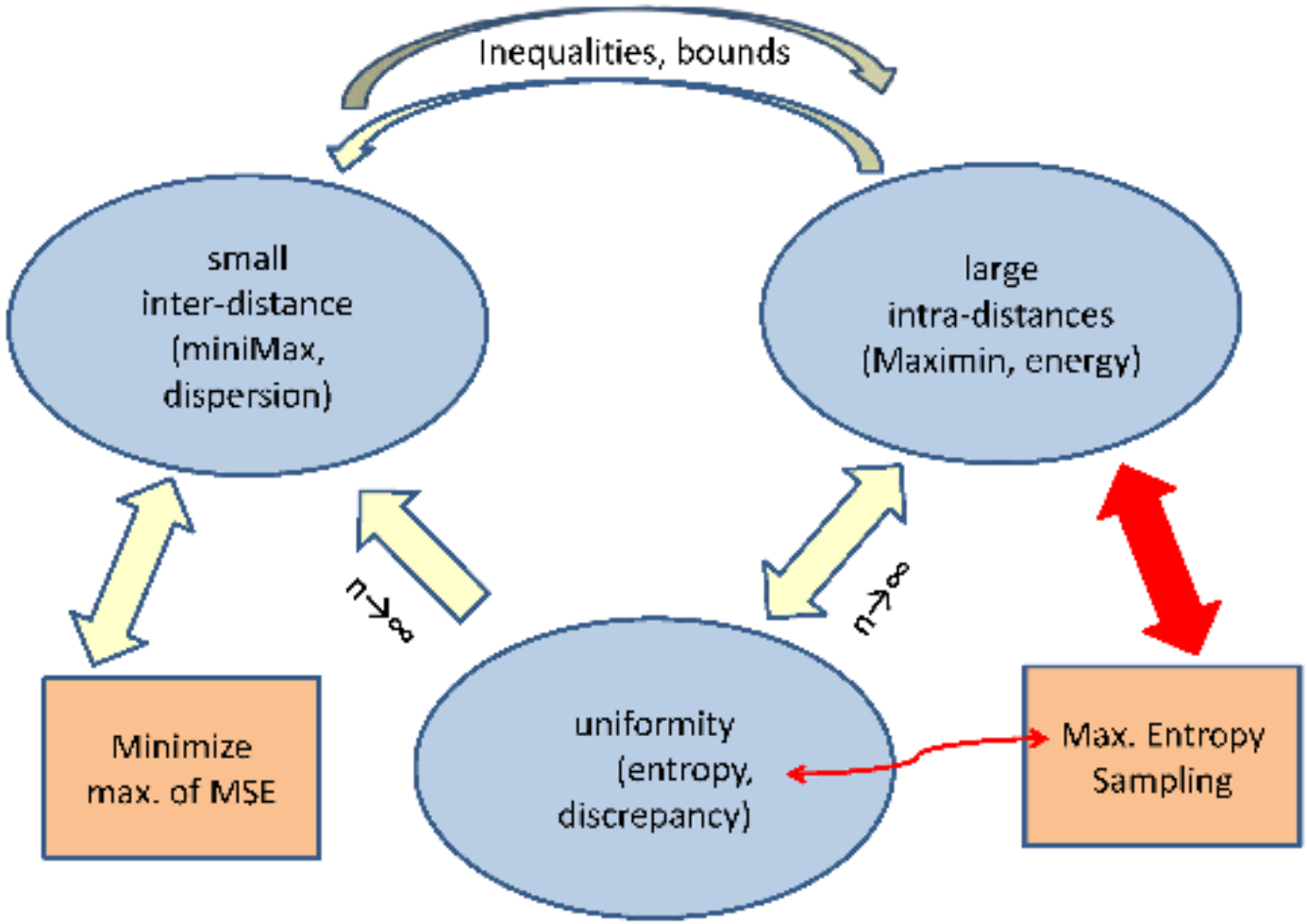
The designs obtained are typically space-filling:

Johnson et al. (1990) : if $C(\mathbf{x}-\mathbf{x}') = c(\|\mathbf{x}-\mathbf{x}'\|)$ with $c(\cdot)$ decreasing, then $\mathbf{X}_n^*$ optimal for $\Phi_{Mm}(\cdot)$ (Maximin optimal) tends to be optimal for $\det[\mathbf{C}_n]$ with covariance $C_a(\mathbf{x}-\mathbf{x}') = [C(\mathbf{x}-\mathbf{x}')]^a$ when $a \to \infty$

$\Rightarrow$ there are design points $\mathbf{x}_i$ on the boundary of $\mathscr{X}$


Inequalities, bounds
small
inter-distance
(miniMax,
dispersion)
large
intra-distances
(Maximin, energy)
$n \to \infty$
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Minimize
max. of MSE
uniformity
(entropy,
discrepancy)
Max. Entropy
Sampling

2 Optimal design for linear regression

2.1 Linear regression

Observations $\boxed{y_i = y(\mathbf{x}_i) = \mathbf{r}^\top(\mathbf{x}_i)\gamma + \varepsilon_i}$, $\gamma \in \mathbb{R}^p$

with (ε_i) i.i.d., $\mathrm{E}\{\varepsilon_i\} = 0$, $\mathrm{var}\{\varepsilon_i\} = \sigma^2 \ \forall i$

Estimation of γ by Least-Squares (LS)

$$\hat{\gamma}_n = (\mathbf{R}_n^\top \mathbf{R}_n)^{-1}\mathbf{R}_n^\top \mathbf{y}_n, \text{ with } \mathbf{y}_n = (y_1, \ldots, y_n)^\top \text{ and } \mathbf{R}_n = \begin{pmatrix} \mathbf{r}^\top(\mathbf{x}_1) \\ \vdots \\ \mathbf{r}^\top(\mathbf{x}_n) \end{pmatrix}$$

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$\mathrm{E}\{\hat{\gamma}_n\} = \gamma$ (unbiased)

$$\text{Covariance} = \mathrm{cov}(\hat{\gamma}_n) = \sigma^2(\mathbf{R}_n^\top \mathbf{R}_n)^{-1} = \frac{\sigma^2}{n}\left[\underbrace{\frac{1}{n}\sum_{i=1}^{n}\mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)}_{\mathbf{M}_n}\right]^{-1}$$

$\text{cov}(\hat{\gamma}_n) = \frac{\sigma^2}{n}\mathbf{M}_n^{-1}$, with

$$\boxed{\mathbf{M}_n = \mathbf{M}(\mathbf{X}_n) = \frac{1}{n}\sum_{i=1}^{n}\mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)} \in \mathbb{R}^{p\times p}$$

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Optimal design $\mathbf{X}_n^*$: maximizes a scalar function $\Phi(\cdot)$ of $\mathbf{M}_n$ (with $\Phi(\cdot)$ Loewner increasing)

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  (minimize sum of squared lengths of axes of confidence ellipsoids for γ)
- more generally, *L*-optimality: maximize $-\mathrm{trace}[\mathbf{L}\mathbf{M}_n^{-1}]$
  (we only consider the case $\mathbf{L}$ symmetric positive definite)

- *D*-optimality: maximize $\log\det \mathbf{M}_n$
  (minimize volume of confidence ellipsoids for γ)
  Very much used:
  - a *D*-optimal design is invariant by reparametrization:

$$\det \mathbf{M}'_n(\beta(\gamma)) = \det \mathbf{M}_n(\gamma) \det^{-2} \left(\frac{\partial \beta}{\partial \gamma^\top} \right)$$

  - ➠ often leads to repeat the same experimental conditions (replications)
    (we assumed i.i.d. errors $\varepsilon_i \Rightarrow$ several observations at the same $\mathbf{x}_i$ carry information)

⏩ Tensor-product models

2.2 Exact design

n observations at $\mathbf{x}_1, \ldots, \mathbf{x}_n$, $\mathbf{x}_i \in \mathbb{R}^d$

Maximize $\Phi(\mathbf{M}_n)$ w.r.t. $\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \in \mathbb{R}^{n \times d}$

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- If problem dimension $n \times d$ is not too big
  - ➠ "standard" algorithm (but careful with constraints and local optimas!)
- Otherwise, ➠ specific algorithm

Exchange method: at step k, exchange **one** support point $\mathbf{x}_j$ with a better one $\mathbf{x}^*$ in $\mathscr{X}$ (better for $\Phi(\cdot)$)

$$\mathbf{X}_n^k = (\mathbf{x}_1, \ldots, \boxed{\begin{array}{c}\mathbf{x}_j \\ \updownarrow \\ \mathbf{x}^*\end{array}}, \ldots, \mathbf{x}_n)$$

⏩ Approximate design

Fedorov (1972) algorithm:

At each iteration k, consider all n possible exchanges successively, each time starting from $\mathbf{X}_n^k$, retain the «best» one among these $n \rightarrow \mathbf{X}_n^{k+1}$ ➠ $\mathbf{X}_n^{k+1}$

$$\mathbf{X}_n^k = \left(\begin{array}{ccccc} \mathbf{x}_1 & , \ldots , & \mathbf{x}_j & , \ldots , & \mathbf{x}_n \\ \updownarrow & & \updownarrow & & \updownarrow \\ \mathbf{x}_1^* & & \mathbf{x}_j^* & & \mathbf{x}_n^* \end{array} \right)$$

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One iteration $\rightarrow$ n optimizations of dimension d followed by ranking n criterion values

DETMAX algorithm Mitchell (1974):

If one additional observation were allowed: optimal choice

$$\mathbf{X}_{n+1}^{k+} = (\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_n, \mathbf{x}_{n+1}^*)$$

Then, remove one support point to return to a n-points design:

➔ consider all $n+1$ possible cancellations,
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➔ consider all $n+1$ possible cancellations,
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➔ globally, exchange some $\mathbf{x}_j$ with $\mathbf{x}_{n+1}^*$

[= excursion of length 1, longer excursions are possible...]

One iteration $\rightarrow$ 1 optimization of dimension d followed by ranking $n+1$ criterion values

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- ▲ both give local optima only ▲

- DETMAX has simpler iterations than Fedorov, but usually requires more iterations
- dead ends are possible:
  - DETMAX: the point to be removed is $\mathbf{x}_{n+1}$
  - Fedorov: no possible improvement when optimizing **one** $\mathbf{x}_i$ at a time
- ▲ both give local optima only ▲
- Other methods:
  - Branch and bound: guaranteed convergence, but complicated [Welch 1982]
  - Rounding an optimal design measure (support points $\mathbf{x}_i$ and associated weights w_i^*, $i = 1, \ldots, m$, presented next in § 2.3):
    choose n integers r_i (r_i= nb. of replications of observations at x_i) such that $\sum_{i=1}^m r_i = n$ and $r_i/n \approx w_i^*$
    (e.g., maximize $\min_{i=1,\ldots,m} r_i/w_i^*$ = Adams apportionment, see [Pukelsheim & Reider 1992])

2.3 Approximate design theory

(Chernoff, 1953; Kiefer and Wolfowitz, 1960; Fedorov, 1972; Silvey, 1980; Pukelsheim, 1993) ...

$$\boxed{\mathbf{M}_n = \mathbf{M}(\mathbf{X}_n) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)}$$

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(the additive form is essential — related to the independence of observations)

If several $\mathbf{x}_i$ coincide (repetitions), with only $m < n$ different $\mathbf{x}_i$

$$\boxed{\mathbf{M}(\mathbf{X}_n) = \sum_{i=1}^{m} \frac{r_i}{n}\mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)}$$

$$\begin{aligned} \frac{r_i}{n} &= \text{proportion of observations collected at } \mathbf{x}_i \\ &= \text{«percentage of experimental effort» at } \mathbf{x}_i \\ &= \text{weight } w_i \text{ of support point } \mathbf{x}_i \end{aligned}$$

$$\mathbf{M}(\mathbf{X}_n) = \sum_{i=1}^{m} w_i \mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)$$

- design $\mathbf{X}_n \Leftrightarrow \left\{ \begin{array}{ccc} \mathbf{x}_1 & \cdots & \mathbf{x}_m \\ w_1 & \cdots & w_m \end{array} \right\}$ with $\sum_{i=1}^{m} w_i = 1$
- normalized discrete distribution on the $\mathbf{x}_i$,

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More general expression: ξ = any probability measure on $\mathscr{X}$

$$\mathbf{M}(\xi) = \int_{\mathscr{X}} \mathbf{r}(\mathbf{x})\mathbf{r}^\top(\mathbf{x})\, \xi(\mathrm{d}\mathbf{x}) \text{ with } \int_{\mathscr{X}} \xi(\mathrm{d}\mathbf{x}) = 1$$

$\mathbf{M}(\xi) \in$ convex closure of $\mathcal{M}=$ set of rank 1 matrices

$$\mathbf{M}(\delta_x) = \mathbf{r}(\mathbf{x})\mathbf{r}^\top(\mathbf{x})$$

$\mathbf{M}(\xi)$ is symmetric $p \times p \Rightarrow \in q$-dimensional space, $q = \frac{p(p+1)}{2}$

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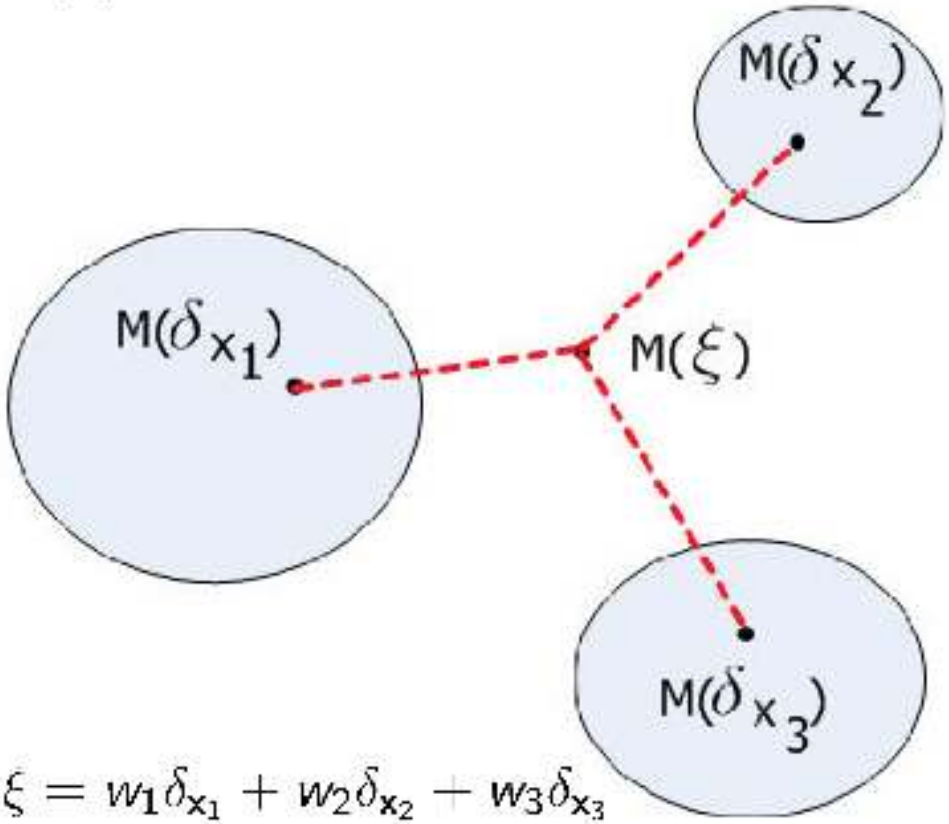

$$\xi = w_1\delta_{\mathbf{x}_1} + w_2\delta_{\mathbf{x}_2} + w_3\delta_{\mathbf{x}_3}$$

(3 points are enough for $q = 2$)

Caratheodory Theorem:

$\mathbf{M}(\xi)$ can be written as the linear combination of at most $q+1$ elements of $\mathcal{M}$:

$\mathbf{M}(\xi) = \sum_{i=1}^{m} w_i \, \mathbf{r}(\mathbf{x}_i)\mathbf{r}^\top(\mathbf{x}_i)\,, \quad m \leq \frac{p(p+1)}{2} + 1$

$\Rightarrow$ consider discrete probability measures with $\frac{p(p+1)}{2} + 1$ support points at most

(true in particular for the optimum design!)

[Even better: for many criteria $\Phi(\cdot)$, if ξ^* is optimal (maximizes $\Phi[\mathbf{M}(\xi)]$) then $\mathbf{M}(\xi^*)$ is on the boundary of the convex closure of $\mathcal{M}$ and $\frac{p(p+1)}{2}$ support points are enough]

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Suppose we found an optimal $\xi^* = \sum_{i=1}^{m} w_i^* \delta_{\mathbf{x}_i}$

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Why design measures are interesting?
How does it simplify the optimization problem?

➠ Maximize $\Phi(\cdot)$ concave w.r.t. $\mathbf{M}(\xi)$ in a convex set

Ex: D-optimality: $\forall\, \mathbf{M}_1 \succ \mathbf{O}$, $\mathbf{M}_2 \succeq \mathbf{O}$, with $\mathbf{M}_2 \not\propto \mathbf{M}_2$, $\forall \alpha$, $0 < \alpha < 1$,

$\log\det[(1-\alpha)\mathbf{M}_1 + \alpha\mathbf{M}_2] > (1-\alpha)\log\det\mathbf{M}_1 + \alpha\log\det\mathbf{M}_2$

$\Rightarrow \log\det[\cdot]$ is (strictly) concave

convex set + concave criterion $\Rightarrow$ one unique optimum!

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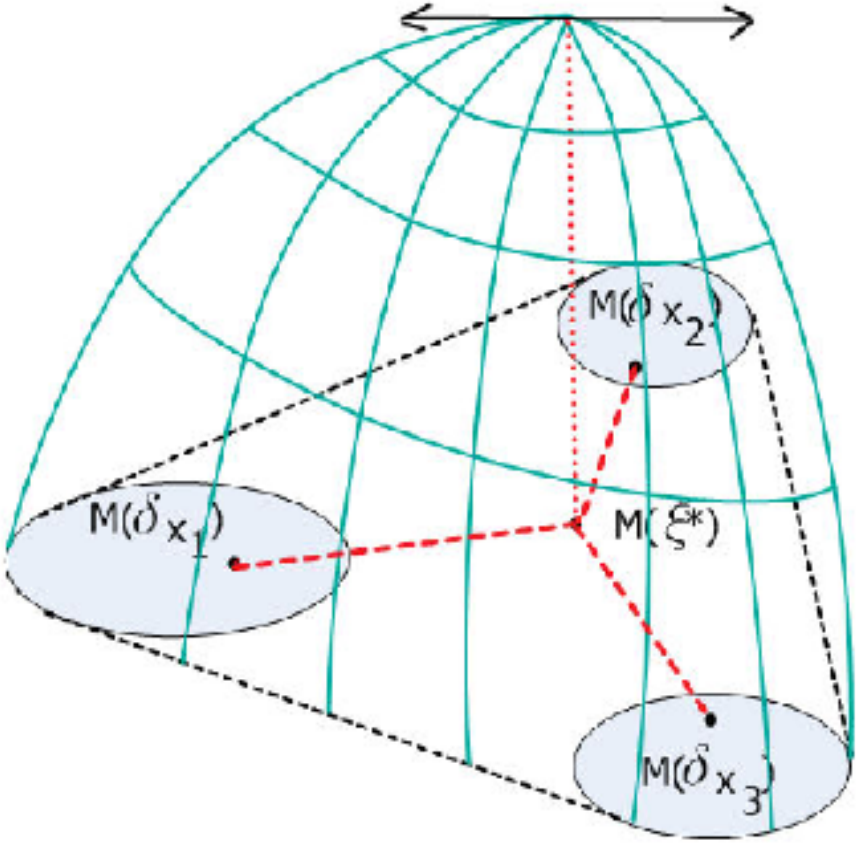

ξ^* is optimal $\Leftrightarrow$ directional derivative ≤ 0 in all directions

$\Longrightarrow$ "Equivalence Theorem" [Kiefer & Wolfowitz 1960]

Ξ = set of probability measures on $\mathscr{X}$, $\Phi(\cdot)$ concave, $\phi(\xi) = \Phi[\mathbf{M}(\xi)]$

$F_\phi(\xi;\nu) = \lim_{\alpha\to 0^+} \frac{\phi[(1-\alpha)\xi+\alpha\nu]-\phi(\xi)}{\alpha}$

$= $ directional derivative of $\phi(\cdot)$ at ξ in direction ν

Equivalence Theorem: $\boxed{\xi^* \text{ maximizes } \phi(\xi) \Leftrightarrow \max_{\nu\in\Xi} F_\phi(\xi^*;\nu) \leq 0}$

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➔ Takes a simple form when $\Phi(\cdot)$ is differentiable

$$\boxed{\xi^* \text{ maximizes } \phi(\xi) \Leftrightarrow \max_{\mathbf{x}\in\mathcal{X}} F_\phi(\xi^*;\delta_{\mathbf{x}}) \leq 0}$$

☞ Check optimality of ξ^* by plotting $F_\phi(\xi^*;\delta_{\mathbf{x}})$

Ex: *D*-optimal design

- ξ_D^* maximizes $\log\det[\mathbf{M}(\xi)]$ w.r.t. $\xi \in \Xi$
- $\Leftrightarrow \max_{\mathbf{x}\in\mathscr{X}} d(\xi_D^*, \mathbf{x}) \leq p$
- $\Leftrightarrow \xi_D^*$ minimizes $\max_{\mathbf{x}\in\mathscr{X}} d(\xi, \mathbf{x})$ w.r.t. $\xi \in \Xi$

where $d(\xi, \mathbf{x}) = \mathbf{r}^\top(\mathbf{x})\mathbf{M}^{-1}(\xi)\mathbf{r}(\mathbf{x})$

Moreover, $d(\xi_D^*, \mathbf{x}_i) = p = \dim(\theta)$ for any $\mathbf{x}_i$ = support point of ξ_D^*

Ex. : $\mathbf{r}(x) = (1 \; x \; x^2)^\top$ $(p = 3)$ i.i.d. erreurs, $\mathscr{X} = [0, 2]$

➠ $d(\xi, x)$ as a function of x

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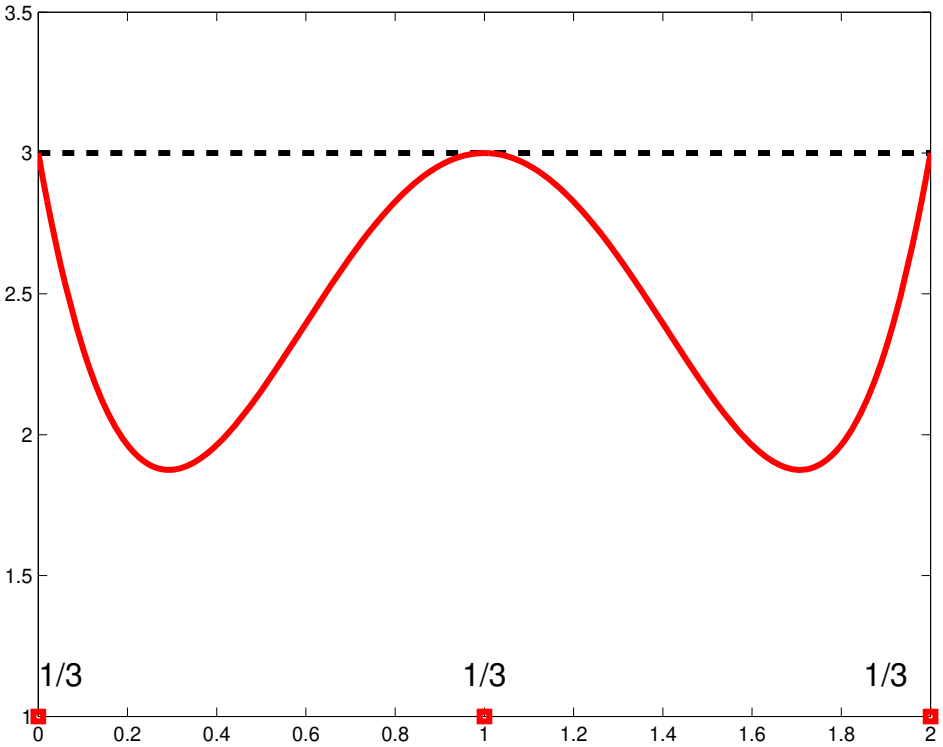
$$\xi_D^* = \left\{ \begin{array}{ccc} 0 & 1 & 2 \\ 1/3 & 1/3 & 1/3 \end{array} \right\}$$



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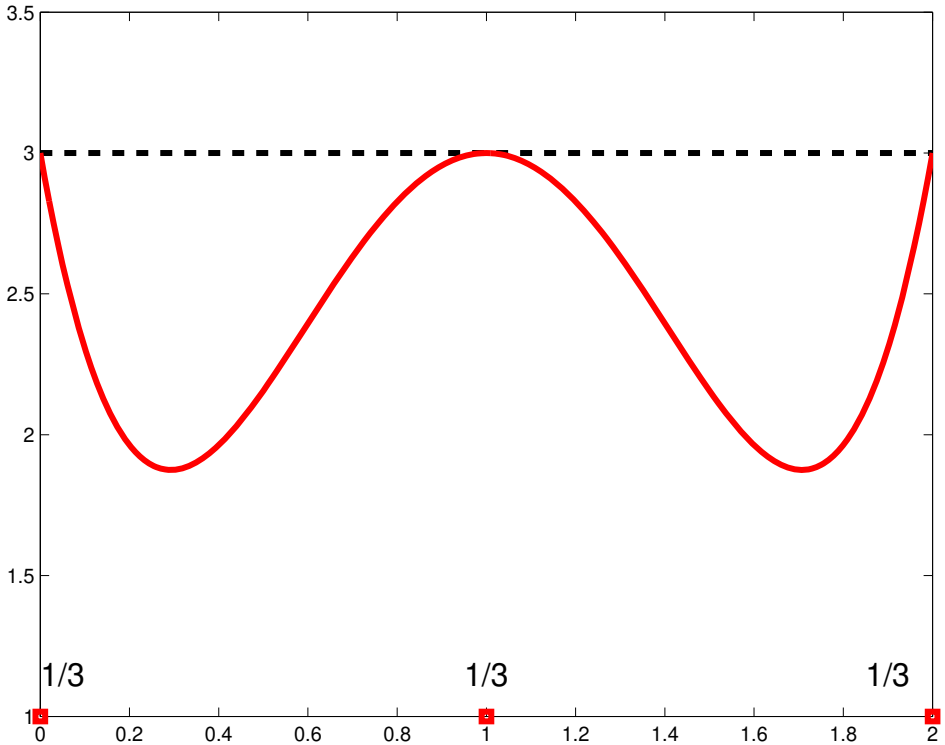
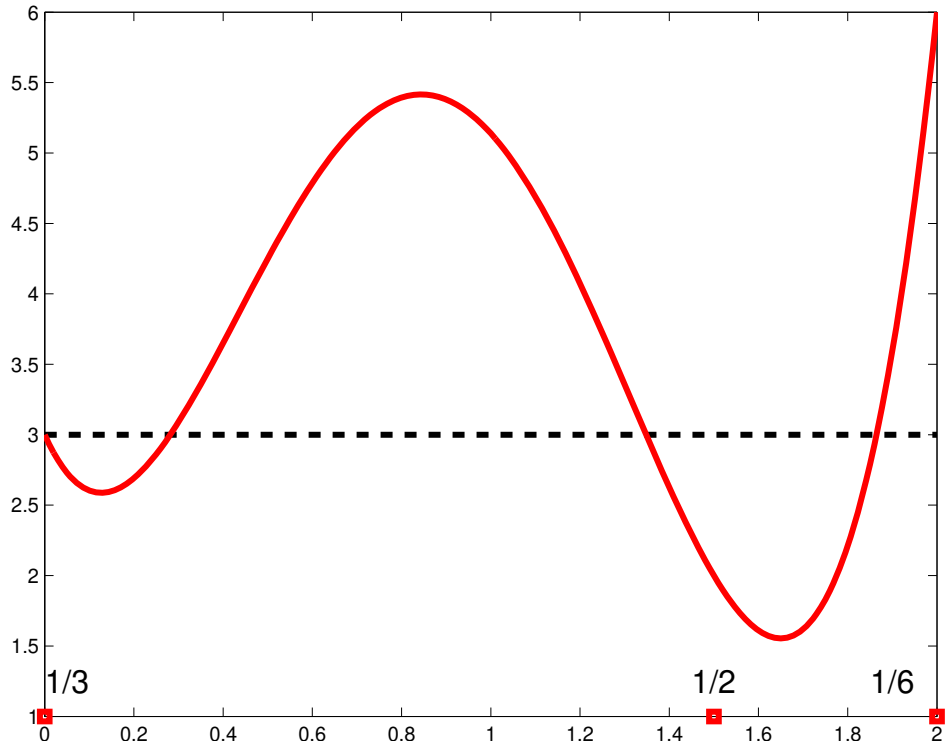
$$\xi_D^* = \left\{ \begin{array}{ccc} 0 & 1 & 2 \\ 1/3 & 1/3 & 1/3 \end{array} \right\} \qquad \xi = \left\{ \begin{array}{ccc} 0 & 1.5 & 2 \\ 1/3 & 1/2 & 1/6 \end{array} \right\}$$





KW Eq. Th. relates optimality in γ space (parameters)
to optimality in y space (observations)

$$n\text{var}[\mathbf{r}^\top(\mathbf{x})\hat{\gamma}^n)] = \sigma^2\,\mathbf{r}^\top(\mathbf{x})\mathbf{M}^{-1}(\xi)\mathbf{r}(\mathbf{x}) = \sigma^2\,d(\xi,\mathbf{x}) \text{ (i.i.d. errors)}$$

$$D\text{-optimality} \Leftrightarrow G\text{-optimality}$$

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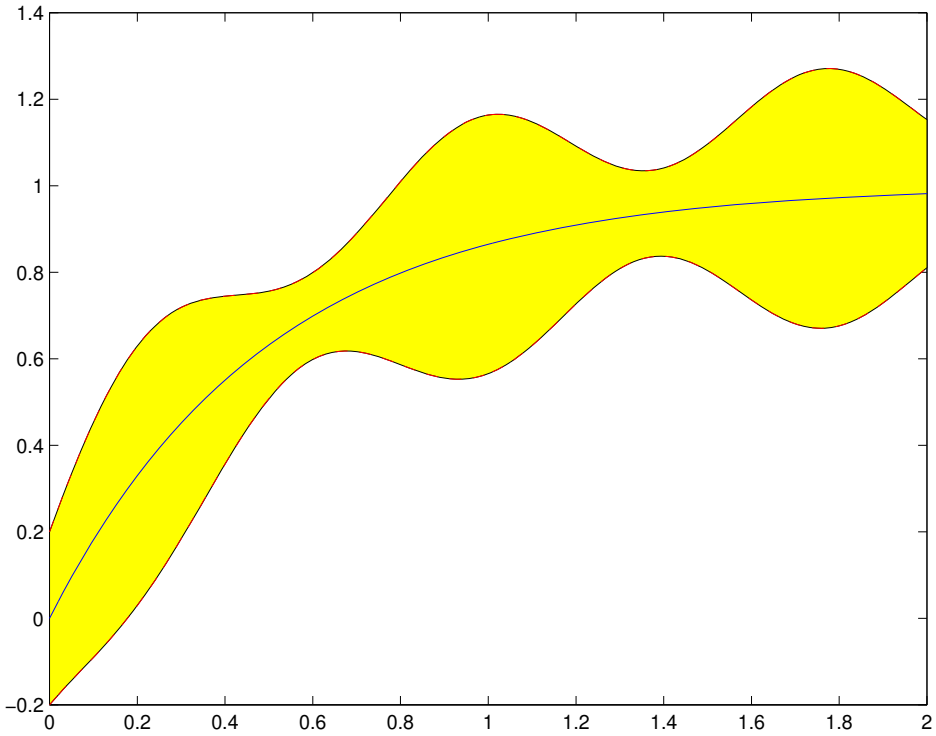
D-optimality $\Leftrightarrow$ G-optimality

➠ ξ_D^* minimizes the maximum value of prediction variance over $\mathscr{X}$

$\eta(\mathbf{x},\hat{\gamma}^n)$

$\eta(\mathbf{x},\hat{\gamma}^n) \pm$ 2 standard deviations

➠ put next observation where $d(\xi,\mathbf{x})$ is large



⏩ Tensor-product models

Construction of an optimal design measure

Central idea (▲ for a differentiable $\Phi(\cdot)$ ▲): use steepest-ascent direction

Fedorov–Wynn :

- 1 : Choose ξ^1 non degenerate ($\det \mathbf{M}(\xi^1) > 0$)
- 2 : Compute $\mathbf{x}_k^* = \arg\max_{\mathscr{X}} F_\phi(\xi^k; \delta_{\mathbf{x}})$
  If $F_\phi(\xi^k; \delta_{\mathbf{x}_k^+}) < \epsilon$, stop: ξ^k is ϵ-optimal
- 3 : $\xi^{k+1} = (1 - \alpha_k)\xi^k + \alpha_k \delta_{\mathbf{x}_k^*}$ (delta measure at $\mathbf{x}_k^*$)
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  $k \to k+1$, return to step 2

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Step size α_k?

➠ $\alpha_k = \arg\max \phi(\xi^{k+1})$
$= \frac{d(\xi^k, \mathbf{x}_k^*) - p}{p[d(\xi^k, \mathbf{x}_k^*) - 1]}$ for *D*-optimality (Fedorov, 1972)
$\to$ monotone convergence

➠ $\alpha_k > 0$, $\lim_{k\to\infty} \alpha_k = 0$, $\sum_{i=1}^{\infty} \alpha_k = \infty$
((Wynn, 1970) for *D*-optimality)

Remarks:

- Sequential design, one $\mathbf{x}_i$ at at a time enters $\mathbf{M}(\mathbf{X})$:

$$\mathbf{M}(\mathbf{X}_{k+1}) = \frac{k}{k+1}\mathbf{M}(\mathbf{X}_k) + \frac{1}{k+1}\mathbf{r}(\mathbf{x}_{k+1})\mathbf{r}^\top(\mathbf{x}_{k+1})$$

with $\mathbf{x}_{k+1} = \arg\max_{\mathbf{x}\in\mathscr{X}} F_\phi(\xi^k; \delta_\mathbf{x})$

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- **Guaranteed convergence to the optimum**
- There exist faster methods:
  - remove support points from ξ^k ($\approx$ allow α_k to be < 0) (Atwood, 1973; Böhning, 1985, 1986)
  - combine with gradient projection (or a second-order method) (Wu, 1978)
  - use a multiplicative algorithm (Titterington, 1976; Torsney, 1983, 2009; Yu, 2010) (for A and D optimality, far from the optimum)
  - combine different methods (Yu, 2011)
  - Still an active topic — especially for non differentiable $\Phi(\cdot)\ldots$

2.4 Tensor-product models

D-optimality (also true for *A*-optimality under some conditions (Schwabe, 1996))

$[\mathbf{r}^{(k)}(x)]^\top \theta^{(k)} \triangleq \sum_{i=1}^{d_k} \theta_i^{(k)} x^i$ polynomial with degree d_k, $\dim(\theta^{(k)}) = p_k = 1 + d_k$

Global model for $\mathbf{x} = (\{\mathbf{x}\}_1, \{\mathbf{x}\}_2, \ldots, \{\mathbf{x}\}_d)^\top$:

$\mathbf{r}^\top(\mathbf{x})\gamma = \prod_{k=1}^{d} [\mathbf{r}^{(k)}(x)]^\top \theta^{(k)}$,

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Example:

$$\begin{aligned}
\mathbf{r}^\top(\mathbf{x})\gamma &= (\theta_0^{(1)} + \theta_1^{(1)}\{\mathbf{x}\}_1 + \theta_2^{(1)}\{\mathbf{x}\}_1^2) \times (\theta_0^{(2)} + \theta_1^{(2)}\{\mathbf{x}\}_2 + \theta_2^{(2)}\{\mathbf{x}\}_2^2) \\
&= \gamma_0 + \gamma_1\{\mathbf{x}\}_1 + \gamma_2\{\mathbf{x}\}_2 + \gamma_{12}\{\mathbf{x}\}_1\{\mathbf{x}\}_2 + \gamma_{11}\{\mathbf{x}\}_1{}^2 + \gamma_{22}\{\mathbf{x}\}_2{}^2 \\
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\end{aligned}$$

D-optimal design (approximate theory) = tensor product of d one-dimensional *D*-optimal designs

(true for any type of model, not only polynomials)

Polynomial of degree k: D-optimal design supported on $k+1$ points,
(on $[-1,1]$, roots of $(1-t^2)P_k'(t)$, with $P_k(t) \triangleq k$-th Legendre polynomial)
all with equal weight $1/(k+1)$

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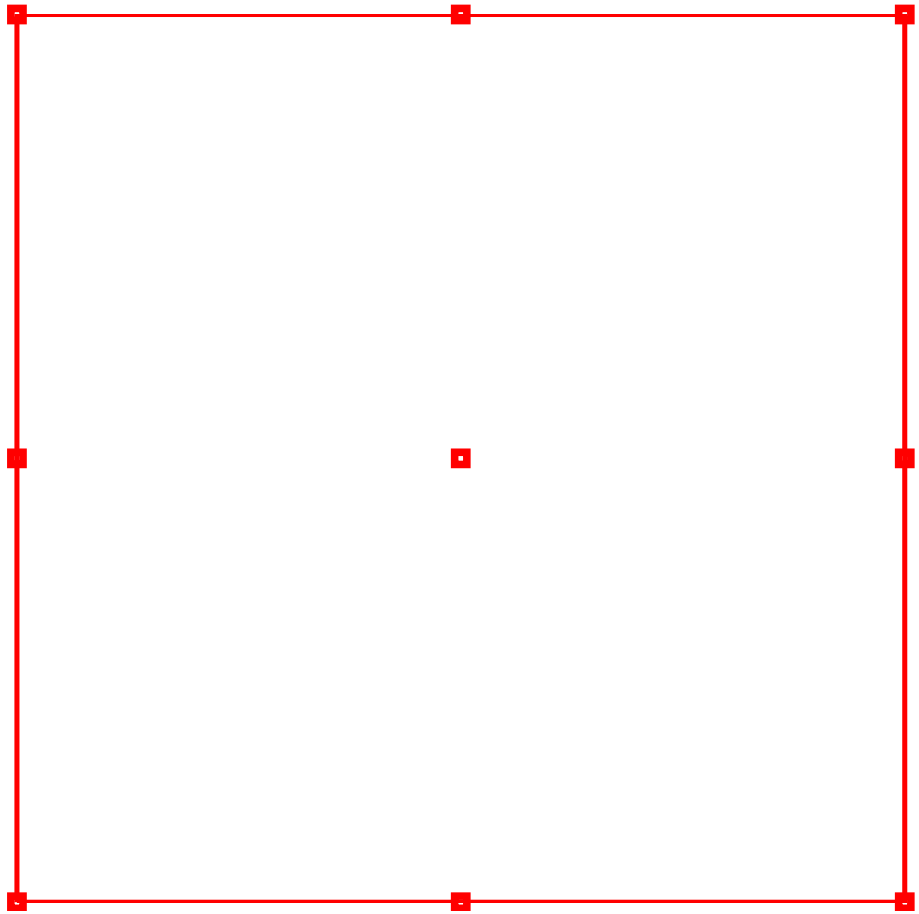
dimension 2, $d_1 = d_2 = 2$
9 points, weights $=1/9$



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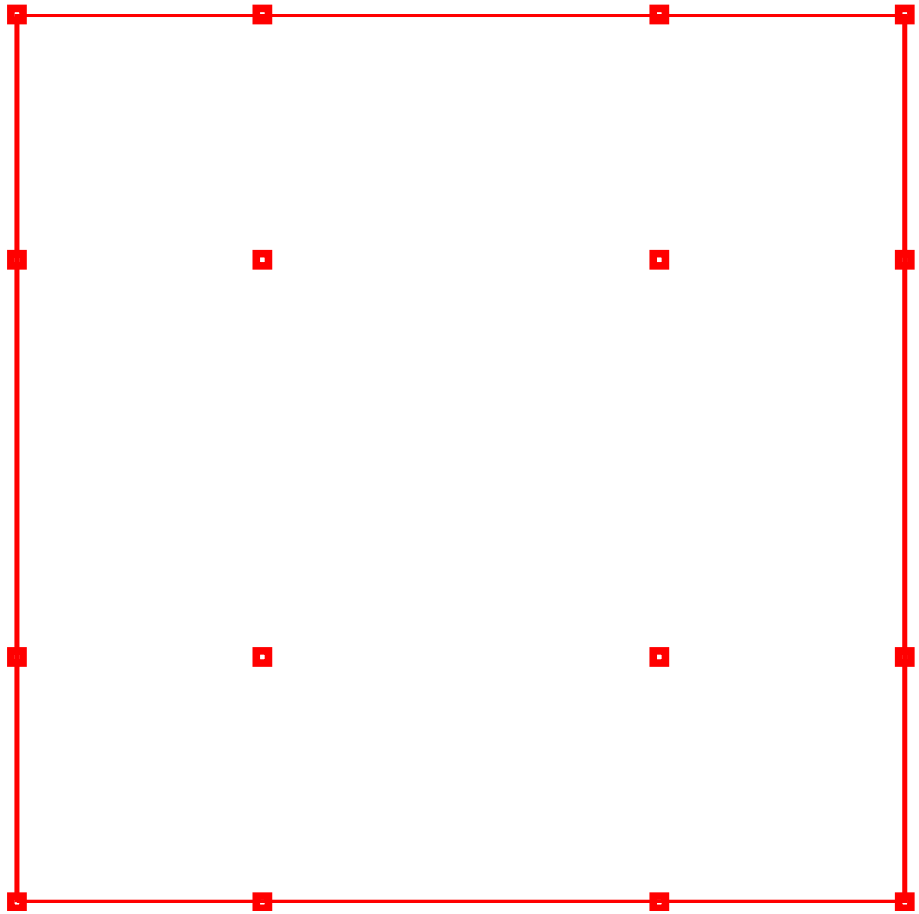
dimension 2, $d_1 = d_2 = 3$
16 points, weights $=1/16$



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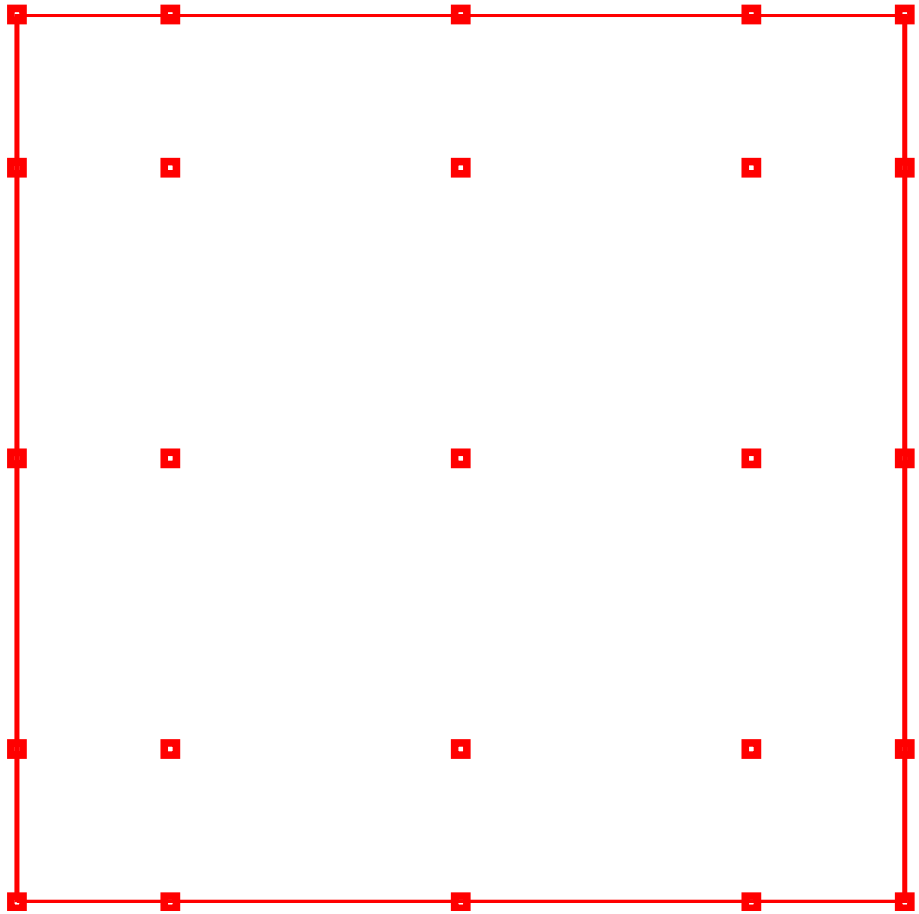
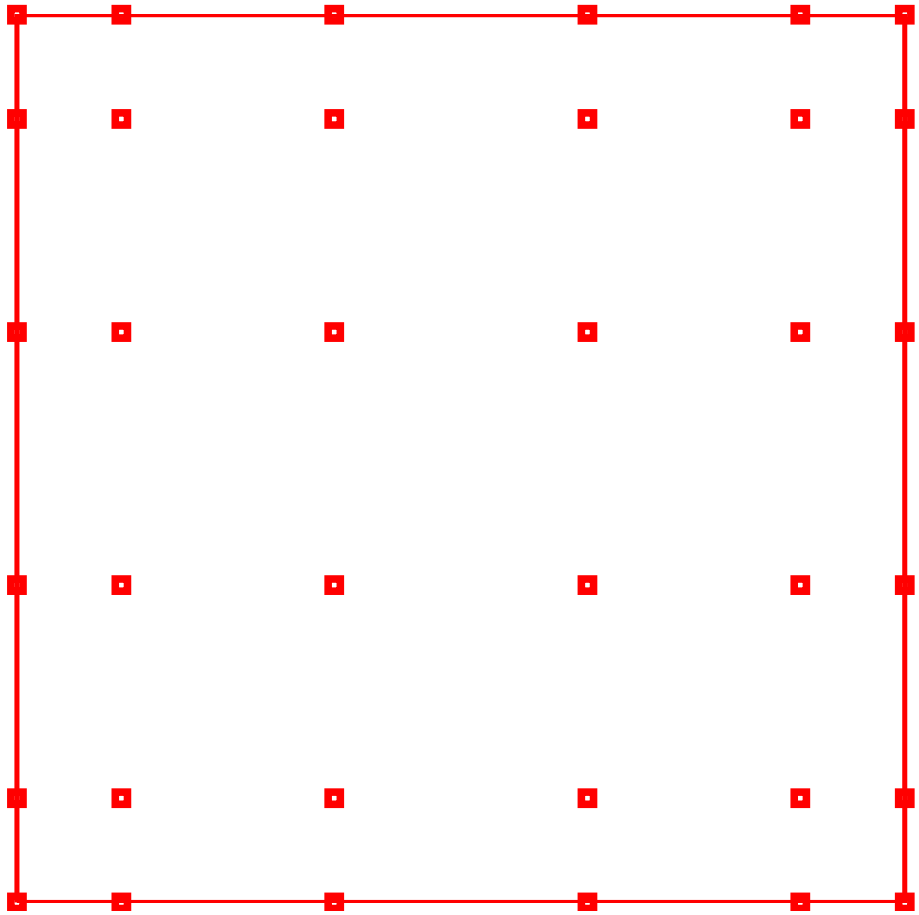
all with equal weight $1/(k+1)$

dimension 2, $d_1 = d_2 = 4$
25 points, weights $=1/25$



Polynomial of degree k: D-optimal design supported on $k+1$ points,
(on $[-1,1]$, roots of $(1-t^2)P_k'(t)$, with $P_k(t) \triangleq k$-th Legendre polynomial)
all with equal weight $1/(k+1)$

dimension 2, $d_1 = d_2 = 5$
36 points, weights $=1/36$



Sum of polynomials?

$$\mathbf{r}^\top(\mathbf{x})\gamma = \sum_{k=1}^{d} [\mathbf{r}^{(k)}(x)]^\top \theta^{(k)},$$

total degree $\max_{k=1}^{d} d_k$, $\dim(\gamma) = (\sum_{k=1}^{d} p_k) - 1 = \sum_{k=1}^{d} d_k + d - 1$

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Example:

$$\begin{aligned} \mathbf{r}^\top(\mathbf{x})\gamma &= (\theta_0^{(1)} + \theta_1^{(1)}\{\mathbf{x}\}_1 + \theta_2^{(1)}\{\mathbf{x}\}_1^2) + (\theta_0^{(2)} + \theta_1^{(2)}\{\mathbf{x}\}_2 + \theta_2^{(2)}\{\mathbf{x}\}_2^2) \\ &= \gamma_0 + \gamma_1\{\mathbf{x}\}_1 + \gamma_2\{\mathbf{x}\}_2 + \gamma_{11}\{\mathbf{x}\}_1{}^2 + \gamma_{22}\{\mathbf{x}\}_2{}^2 \end{aligned}$$

(no interaction term)

Again, *D*-optimal design (approximate theory) = tensor product of d one-dimensional *D*-optimal designs (Schwabe, 1996)

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Again, *D*-optimal design (approximate theory) = tensor product of d one-dimensional *D*-optimal designs (Schwabe, 1996)

Difficult to apply in big dimension:

d polynomials of degree k ➠ $(k+1)^d$ support points!

but a general lesson, and possible extension towards Gaussian process models and kriging

2.5 Consequences for space-filling design

D-optimality + polynomials ➠ more points close to the boundary as degree increases

Erdös-Turan theorem: roots r of orthonormal polynomials on $[0,1]$ are asymptotically distributed with the arcsine law, with density $\varphi_0(r) = \frac{1}{\pi\sqrt{r\,(1-r)}}$

➠ **Should we put more points close to the boundary ?**

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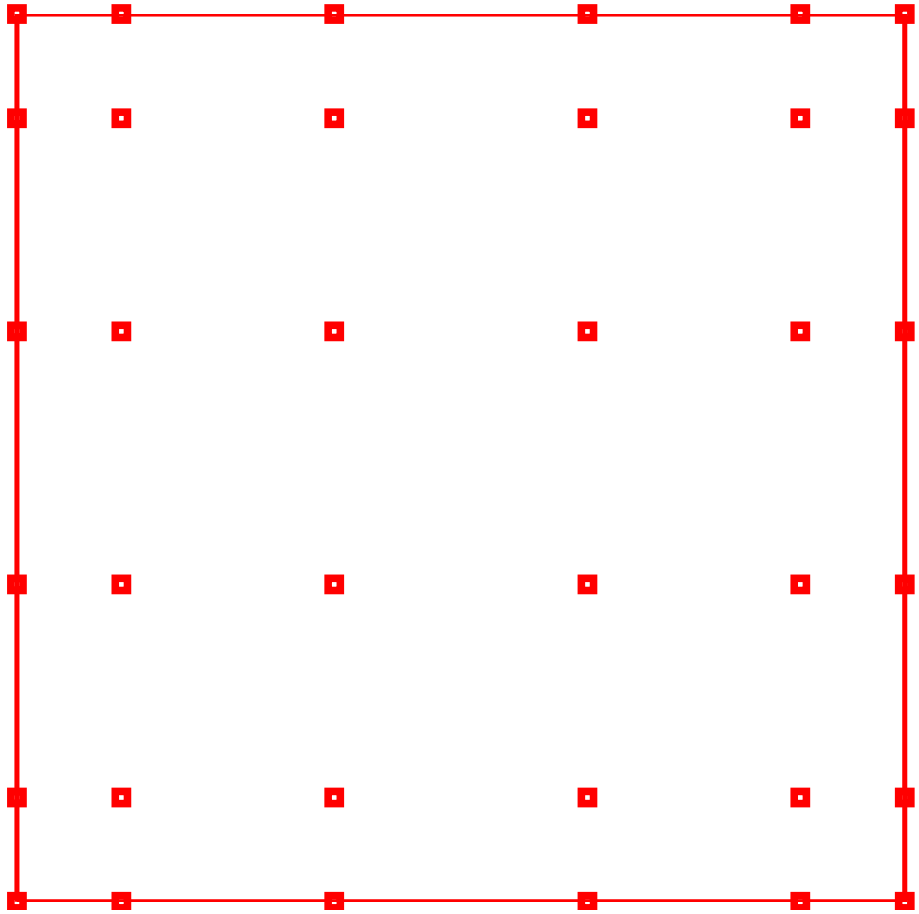
In order to counter the boundary effect Dette and Pepelyshev (2010):

- Take a "standard" space-filling design (e.g., Maximin, Lh Maximin, LDS),
- for each $j = 1, \ldots, d$, transform j-th coordinates $\{\mathbf{x}_i\}_j$ with $T : x \mapsto z = T(x) = \frac{1+\cos(\pi\, x)}{2}$ ($x \sim$ uniform $\rightarrow z \sim$ arcsine),
- Use the transformed design $\mathbf{Z}_n = (\mathbf{z}_1, \ldots, \mathbf{z}_n)$

dimension 2, 5-degree polynomials:
D-optimal design has 36 points, weights $=1/36$



dimension 2, $n = 36$

Transformed (arcsine) Maximin-optimal design

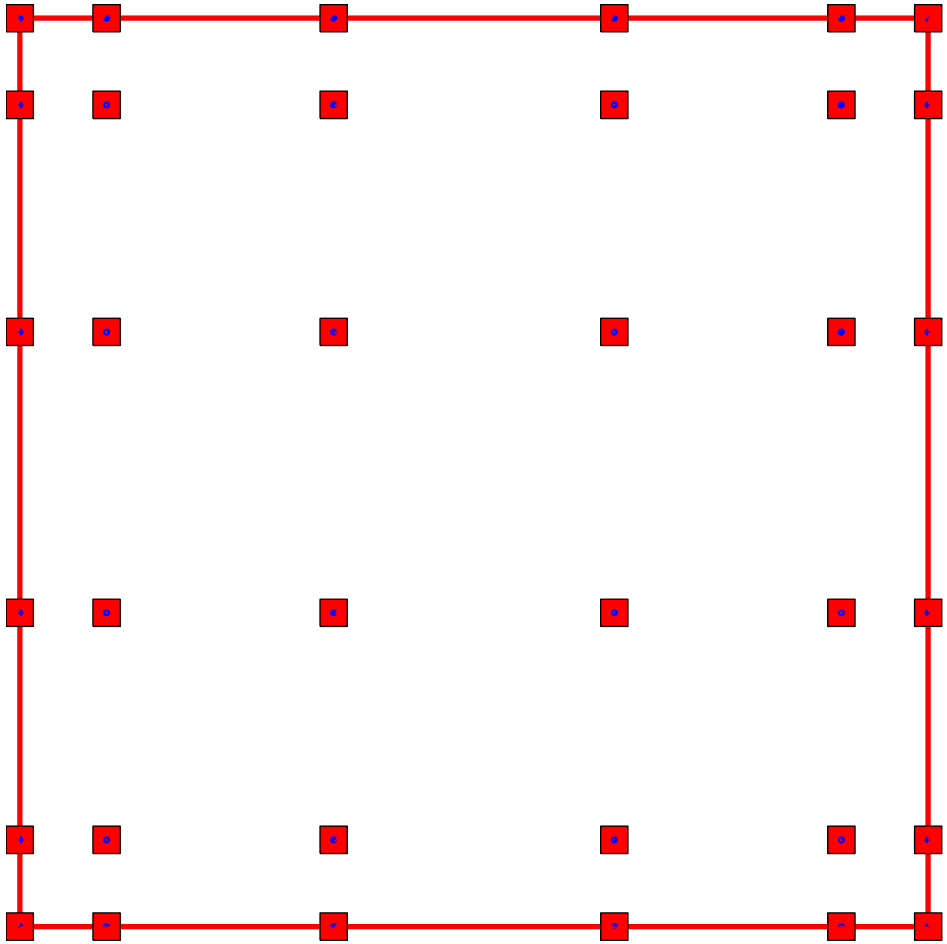
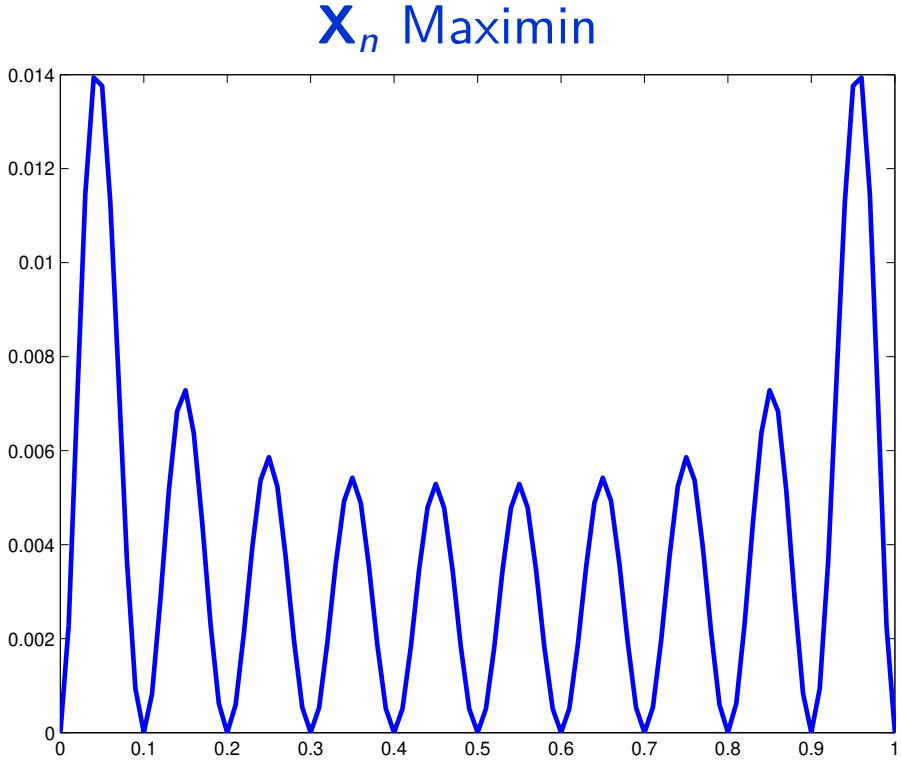


Illustration of boundary effect: $d = 1$, $n = 11$ observations in $[0, 1]$, ordinary kriging with covariance $C(t) = \exp(-50\, t^2)$ ➠ plot of $\rho_n(x)$



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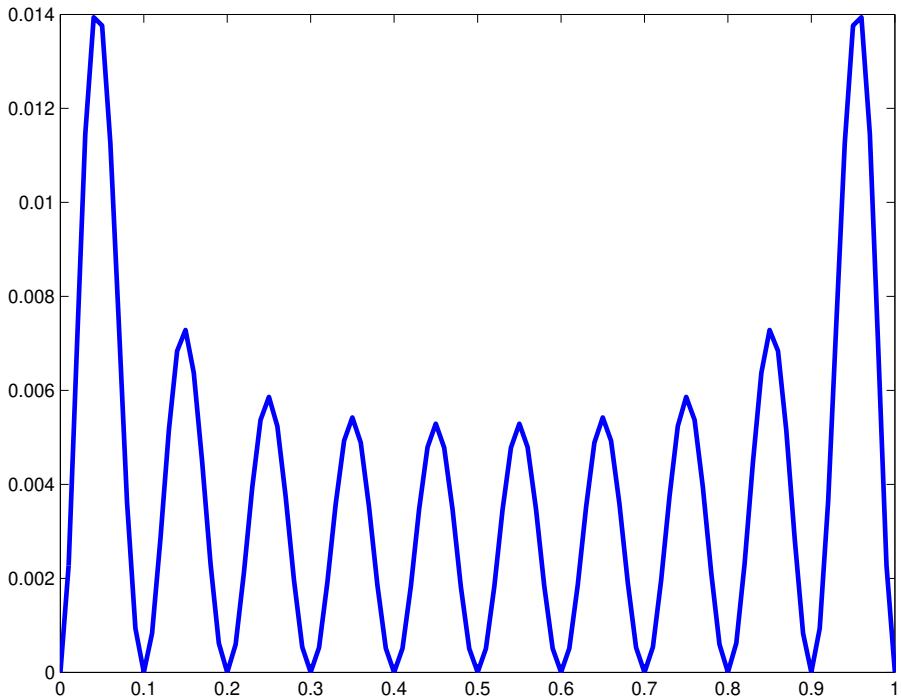
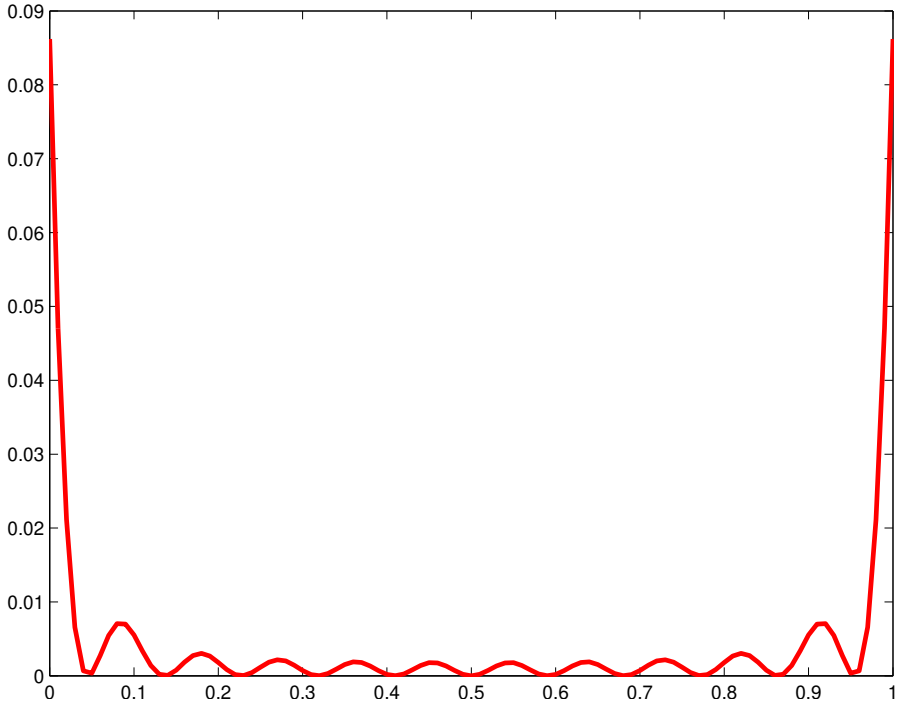
$\mathbf{X}_n$ Maximin



$\mathbf{X}_n$ miniMax



Uniform distribution of design points

$\Rightarrow$ prediction near boundaries relies on less points

$\Rightarrow$ precision is worse close to boundaries

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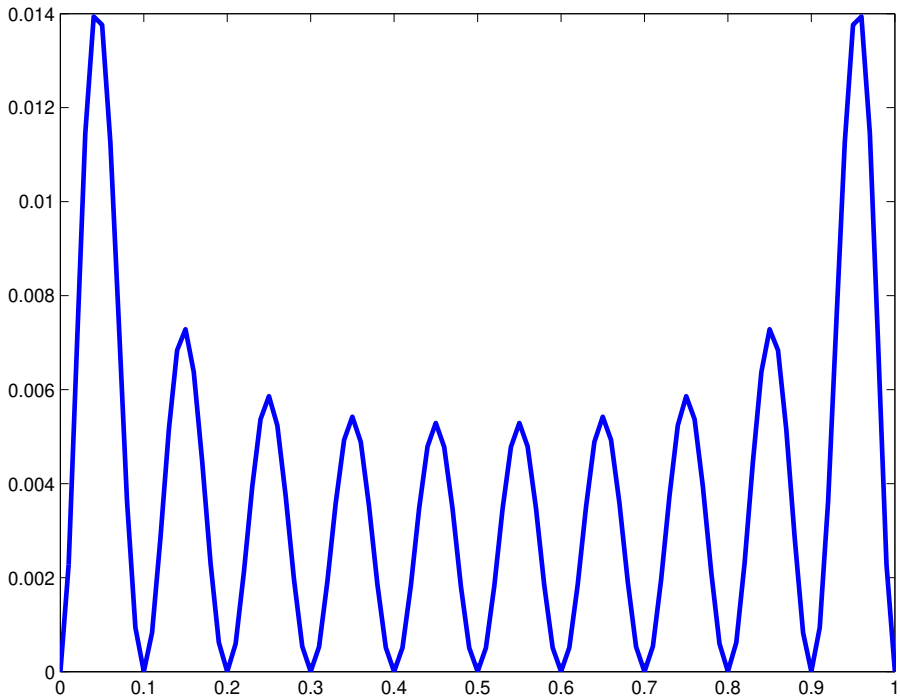
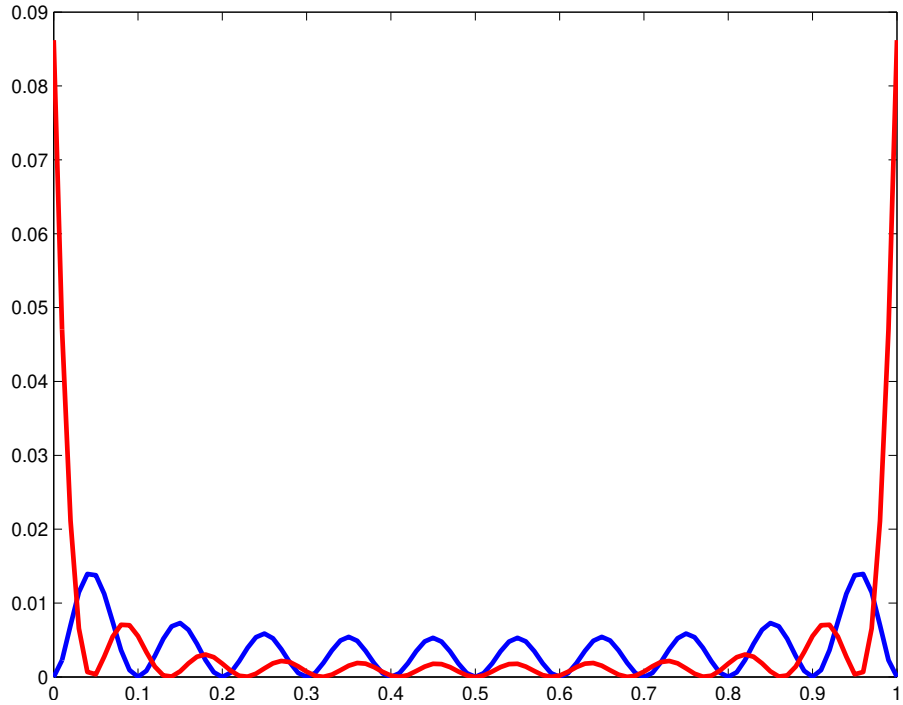


Maximin and miniMax



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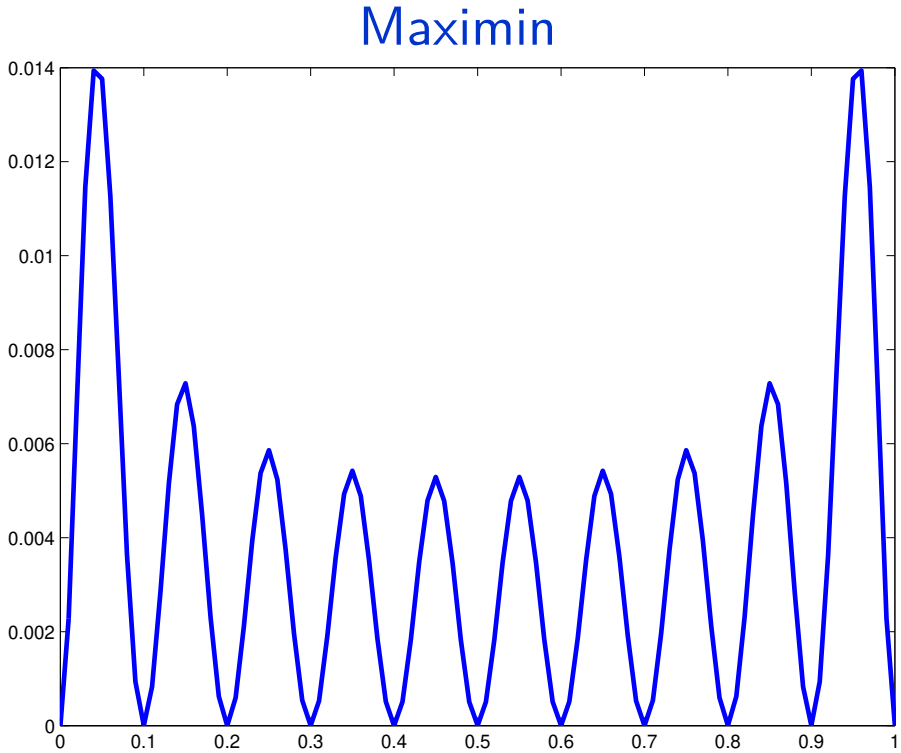
... But transformation $T : x \mapsto z = T(x) = \frac{1+\cos(\pi\, x)}{2}$ may be too "strong"



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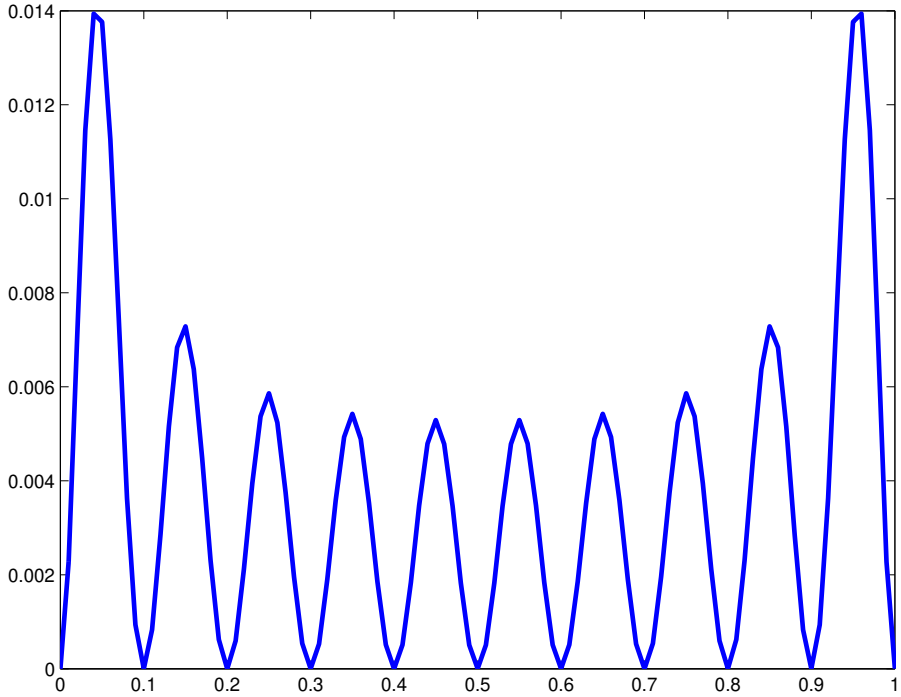
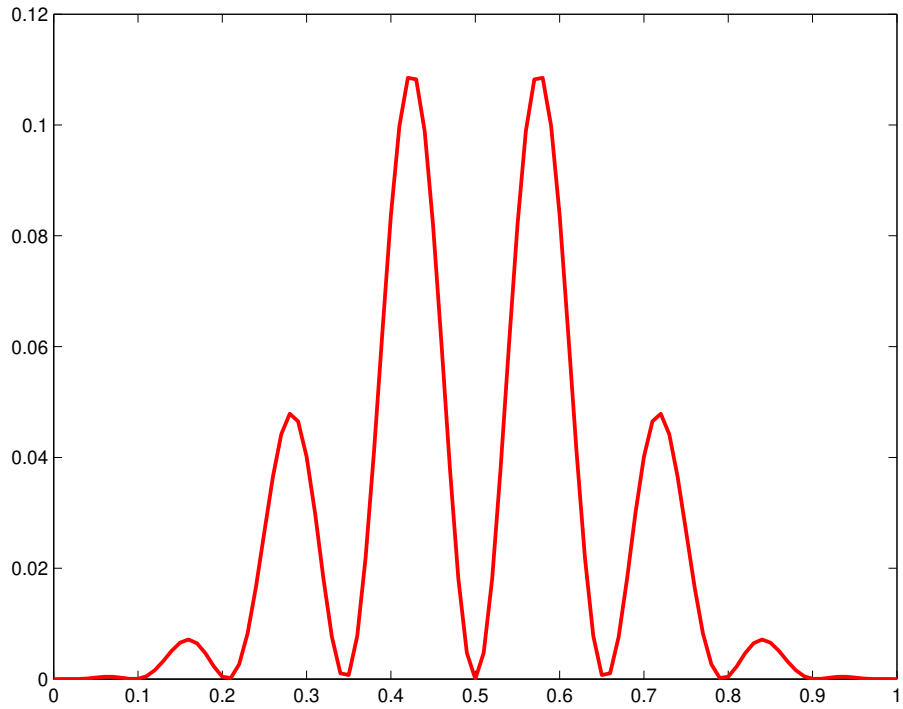


Transformed (arcsine) Maximin



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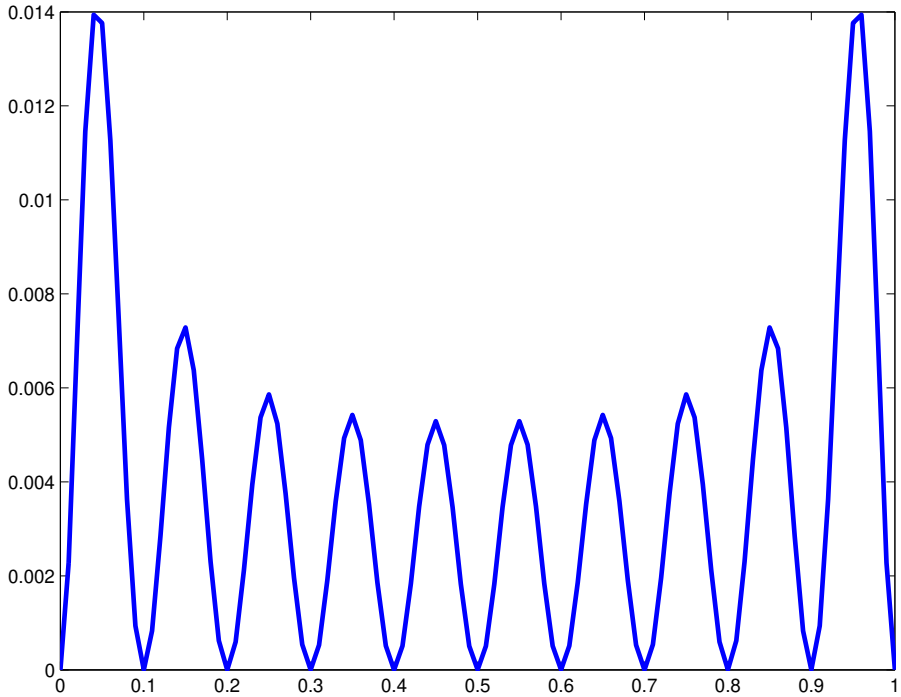
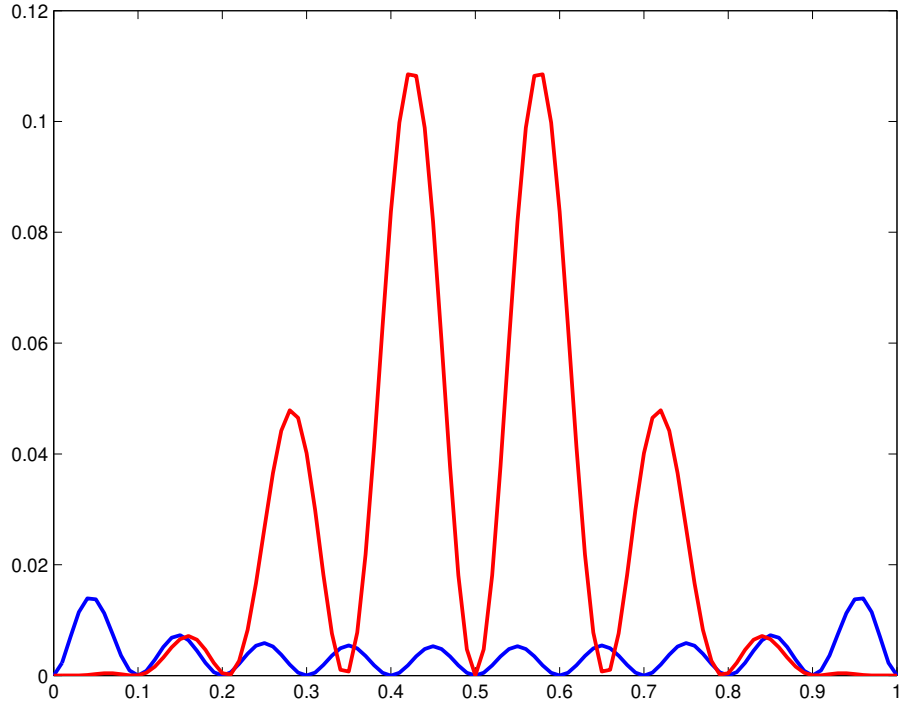


Maximin + transformed Maximin



Arcsine distribution: maximizes $\tilde{\Phi}_{[0]}(\xi) = \exp\left[\int_0^1 \int_0^1 \log\|x-y\|\,\xi(dx)\,\xi(dy)\right]$

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➤ Maximization of

$$\tilde{\Phi}_{[q]}(\xi) = \left[\int_0^1 \int_0^1 \|x-y\|^{-q}\,\xi(dx)\,\xi(dy)\right]^{-1/q}, \quad 0 < q < 1$$

(continuous version of $\overline{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i<j} \mu_{ij}\,d_{ij}^{-q}\right]^{-1/q}$, see § I-1.6) yields a measure ξ with density $\varphi_q(x) = \frac{x^{(q-1)/2}(1-x)^{(q-1)/2}}{B(\frac{q+1}{2},\frac{q+1}{2})}$ (Beta distribution) (Zhigljavsky et al., 2010)

(tends to arcsine when $q \to 0$, to uniform when $q \to 1$)

In order to counter the boundary effect (Dette and Pepelyshev, 2010) :

- Take a "standard" space-filling design (e.g., Maximin, Lh Maximin, LDS),
- for each $j = 1, \ldots, d$, transform j-th coordinates $\{\mathbf{x}_i\}_j$ with $T : x \mapsto z = T(x)$ such that $x = \int_0^z \varphi_q(t)\,\mathrm{d}t$ ($x \sim$ uniform $\rightarrow$ $z \sim \varphi_q$),
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dimension 2, 5-degree polynomials

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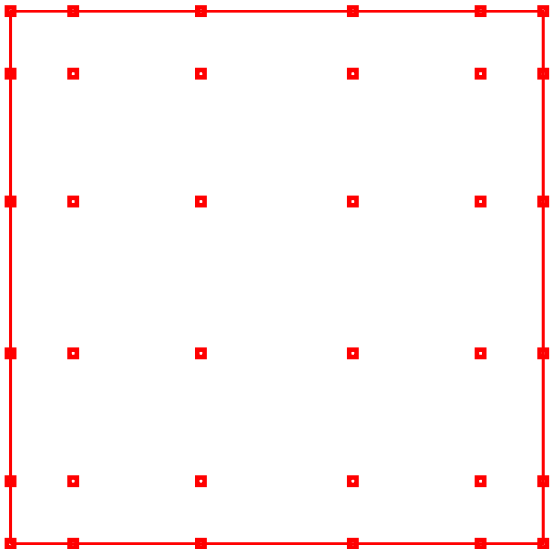

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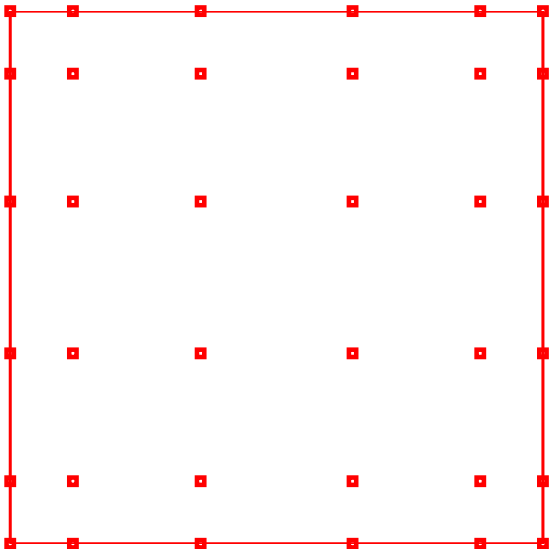
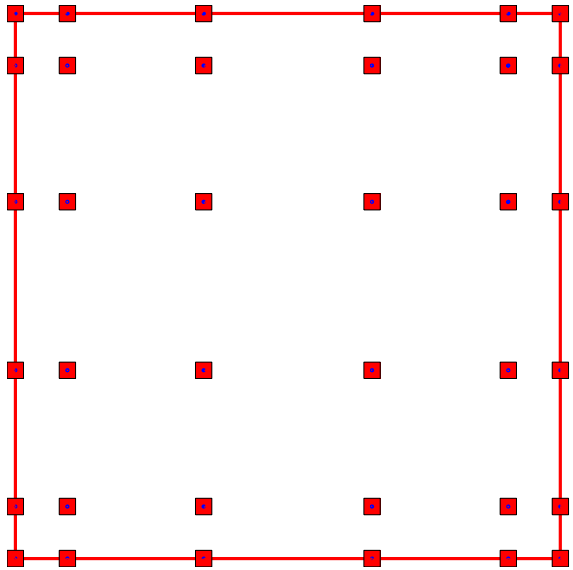


dimension 2, $n = 36$
Transformed (arcsine)
Maximin-optimal design



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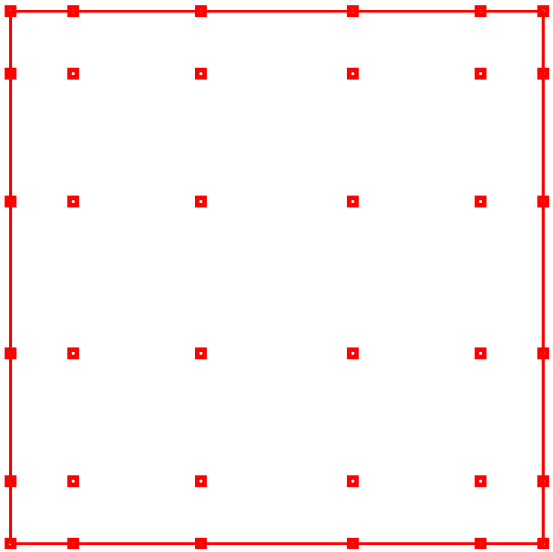
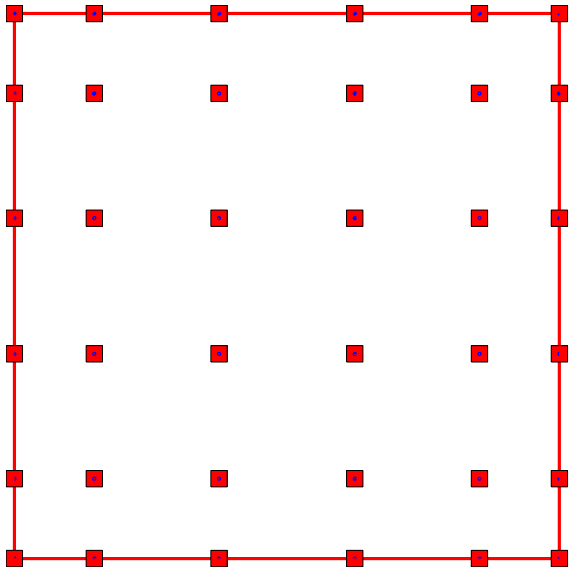
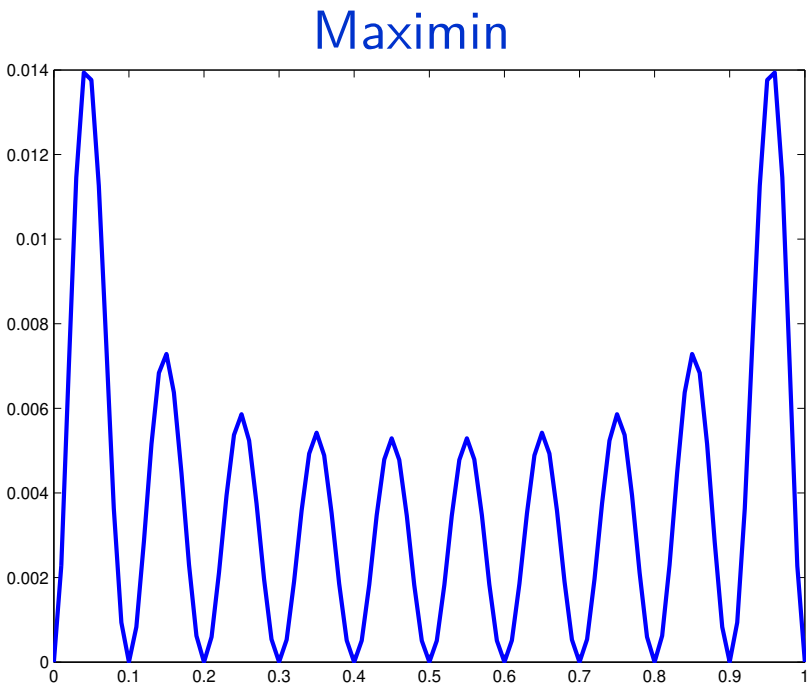


dimension 2, $n = 36$
Transformed (Beta, $q = 0.4$)
Maximin-optimal design



. . . For a suitably chosen Beta-transformation ($q = 0.84$)



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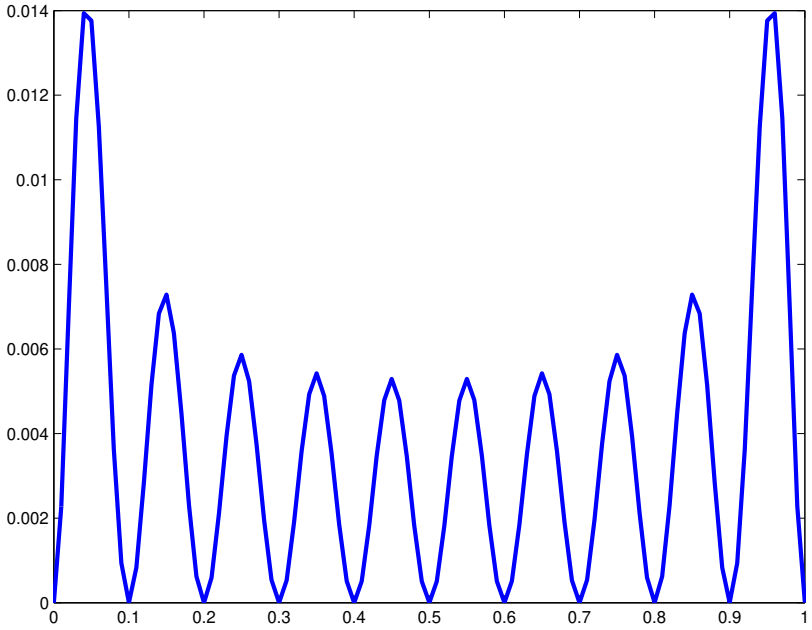
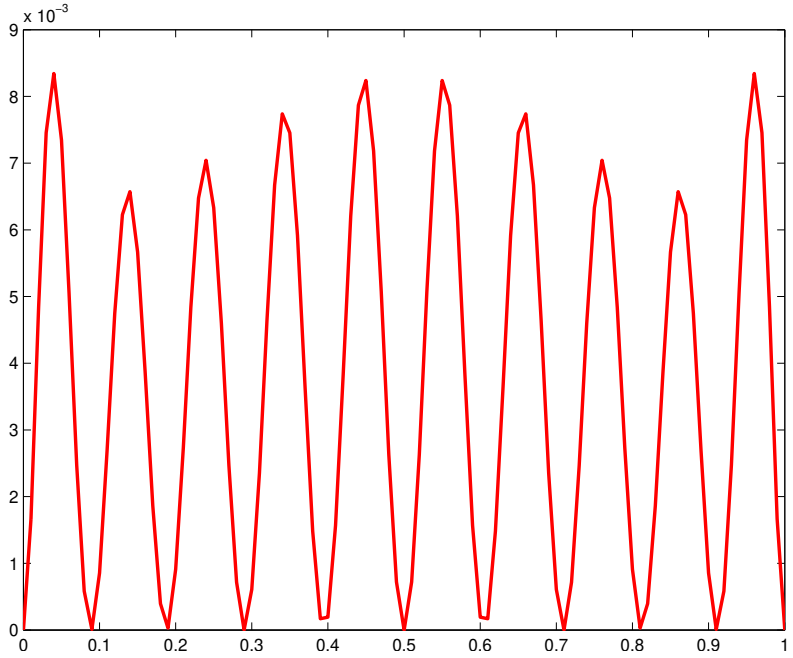
Maximin



Transformed (Beta) Maximin



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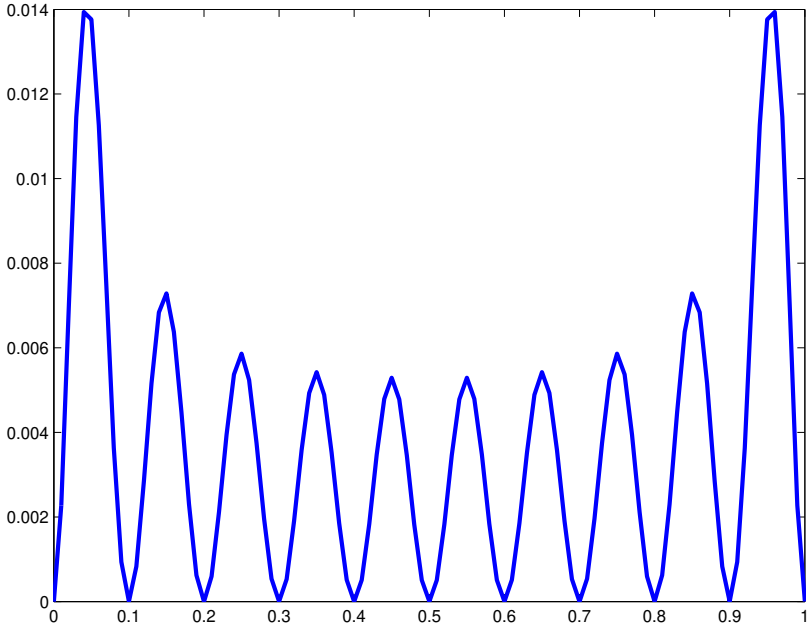
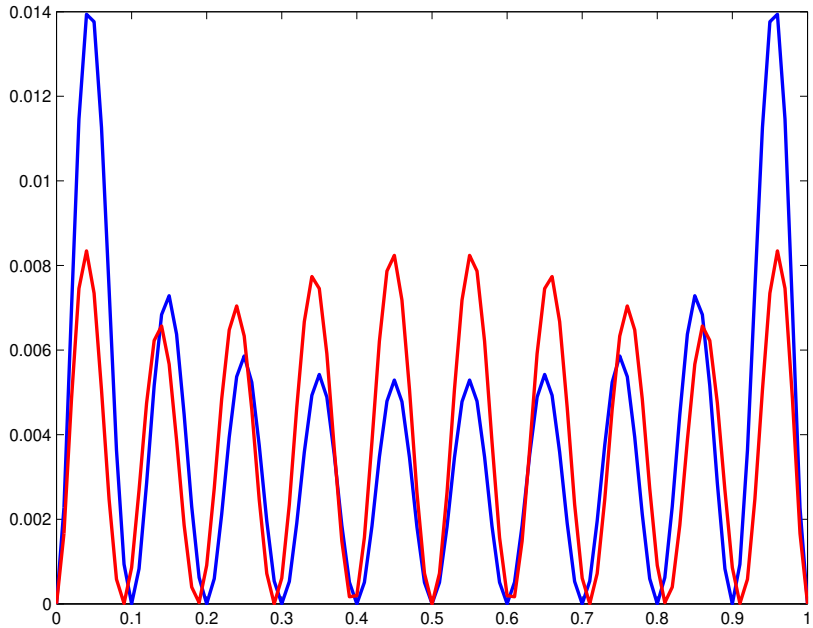


Maximin + transformed Maximin



Choice of a suitable q?

➠ Optimize a precision criterion based on $\rho_n(\mathbf{x})$
(depends on covariance $C(\cdot)$)

▲ requires $\mathscr{X}$ = hypercube ▲

▲ if d is big, many points are on the boundary (or at the vertices!) of $\mathscr{X}$ ▲

3 Optimal design for Bayesian prediction

3.1 Karhunen-Loève decomposition of a Gaussian process

Model without trend: $f(\mathbf{x}) = Z(\mathbf{x})$, Gaussian process

$\mathrm{E}\{Z(\mathbf{x})\} = 0$, $\mathrm{E}\{Z(\mathbf{x})Z(\mathbf{x}')\} = C(\mathbf{x}, \mathbf{x}')$ $(= C(\mathbf{x} - \mathbf{x}')$ if stationary)

$$\mathrm{IMSE}_\mu(\mathbf{X}_n) \triangleq \int_{\mathscr{X}} \mathrm{E}\left\{[Z(\mathbf{x}) - \mathrm{E}\{Z(\mathbf{x})|\mathbf{y}_n\}]^2\right\} \mathrm{d}\mu(\mathbf{x})$$

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The integral operator T_μ defined by
$\forall f \in L^2(\mathscr{X}, \mu),\ \forall \mathbf{x} \in \mathscr{X},\quad T_\mu[f](\mathbf{x}) = \int_{\mathscr{X}} f(\mathbf{x}')K(\mathbf{x}, \mathbf{x}')\mathrm{d}\mu(\mathbf{x}')$
is diagonalisable:

eigenvalues λ_i, $i = 1, 2, 3 \ldots$ (in $\searrow$ order)
associated eigenfunctions $\varphi_i(\cdot)$ (extended over $\mathscr{X}$), with
$\int_{\mathscr{X}} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x})\mathrm{d}\mu(\mathbf{x}) = \delta_{ij}$

$$\boxed{Z'(\mathbf{x}) \triangleq P_{\mathbb{H}_\mu}[Z_{\mathbf{x}}] = \sum_i \zeta_i \sqrt{\lambda_i} \varphi_i(\mathbf{x})}$$

with all ζ_i i.i.d. $\mathcal{N}(0,1)$

$P_{\mathbb{H}_\mu}$ = projection $\perp$ on the space "which contributes to IMSE$_\mu$"

$Z'(\mathbf{x}) = \sum_i \gamma_i \varphi_i(\mathbf{x})$ where the r.v. γ_i are independent $\mathcal{N}(0, \lambda_i)$

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For a given truncation level m,

$$\begin{aligned} Z'(\mathbf{x}) &= \sum_{i=1}^{m} \gamma_i \varphi_i(\mathbf{x}) + \sum_{i>m} \gamma_i \varphi_i(\mathbf{x}) \\ &\simeq \boxed{Z''(\mathbf{x}) = \sum_{i=1}^{m} \gamma_i \varphi_i(\mathbf{x}) + \varepsilon(\mathbf{x})} \end{aligned}$$

with $\mathsf{E}\{\varepsilon(\mathbf{x}_i)\} = 0$, $\mathsf{E}\{\varepsilon(\mathbf{x}_i)\varepsilon(\mathbf{x}_j)\} = \sigma^2 \delta_{ij}$ et $\sigma^2 = \sum_{i>m} \lambda_i$

$$\boxed{Z''(\mathbf{x}_i) = \phi^\top(\mathbf{x}_i)\gamma + \varepsilon_i}$$

= linear regression model (as in § 2.1)
(with eigenfunctions $\varphi_i(\cdot)$, $i = 1, \ldots, m$, instead of polynomials)

(Fedorov, 1996) ➠ construct an optimal design for this model

3.2 Bayesian prediction for $Z''(\mathbf{x}_i) = \phi^\top(\mathbf{x}_i)\gamma + \varepsilon_i$

LS estimation:

$$\hat{\gamma}_n = (\Phi_n^\top \Phi_n)^{-1}\Phi_n^\top \mathbf{y}_n, \text{ with } \mathbf{y}_n = (y_1, \ldots, y_n)^\top \text{ and } \Phi_n = \begin{pmatrix} \phi^\top(\mathbf{x}_1) \\ \vdots \\ \phi^\top(\mathbf{x}_n) \end{pmatrix}$$

$$\text{cov}(\hat{\gamma}_n) = \sigma^2(\Phi_n^\top \Phi_n)^{-1} = \frac{\sigma^2}{n}\left[\underbrace{\frac{1}{n}\sum_{i=1}^{n}\phi(\mathbf{x}_i)\phi^\top(\mathbf{x}_i)}_{\mathbf{M}_n}\right]^{-1}$$

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Prediction at $\mathbf{x}$: $\eta_n(\mathbf{x}) = \phi^\top(\mathbf{x})\hat{\gamma}_n$

$$\text{IMSE}(\mathbf{X}_n) = \int_{\mathscr{X}} \phi^\top(\mathbf{x})\text{cov}(\hat{\gamma}_n)\phi(\mathbf{x})\,\mathrm{d}\mu(\mathbf{x}) = \frac{\sigma^2}{n}\text{trace}[\mathbf{M}_n^{-1}]$$

$= A$-optimality criterion

(requires $n \geq m$ to have a full rank $\mathbf{M}_n$)

Bayesian estimation: prior distribution $\mathcal{N}(\mathbf{0}, \Lambda_m)$ for γ,
with $\Lambda_m = \mathrm{diag}\{\lambda_1, \ldots, \lambda_m\}$

$$\hat{\gamma}_n = [\Phi_n^\top \Phi_n/\sigma^2 + \Lambda_m^{-1}]^{-1}[\Phi_n^\top \mathbf{y}_n/\sigma^2]$$

$$\mathrm{cov}(\hat{\gamma}_n) = [\Phi_n^\top \Phi_n/\sigma^2 + \Lambda_m^{-1}]^{-1} = \frac{\sigma^2}{n} \underbrace{\left[\underbrace{\frac{1}{n}\sum_{i=1}^{n} \phi(\mathbf{x}_i)\phi^\top(\mathbf{x}_i)}_{\mathbf{M}_n} + \frac{\sigma^2}{n}\Lambda_m^{-1} \right]^{-1}}_{\mathbf{M}_B(\mathbf{x}_n)}$$

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Prediction at $\mathbf{x}$: $\eta_n(\mathbf{x}) = \phi^\top(\mathbf{x})\hat{\gamma}_n$

$$\mathrm{IMSE}(\mathbf{X}_n) = \int_{\mathcal{X}} \phi^\top(\mathbf{x})\mathrm{cov}(\hat{\gamma}_n)\phi(\mathbf{x})\,\mathrm{d}\mu(\mathbf{x}) = \frac{\sigma^2}{n}\mathrm{trace}[\mathbf{M}_B^{-1}(\mathbf{X}_n)]$$

$= A$-optimality criterion applied to $\mathbf{M}_B(\mathbf{X}_n)$

($\mathbf{M}_B(\mathbf{X}_n)$ has full rank for any m!)

3.3 IMSE-optimal design

All the machinery of optimal design for parametric models is available (Pilz, 1983)

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Approximate design: minimize $\Psi(\xi) = \text{trace}[\mathbf{M}_B^{-1}(\xi)]$, with ξ a probability measure over $\mathscr{X}$ and

$$\mathbf{M}_B(\xi) = \int \phi(\mathbf{x})\phi^\top(\mathbf{x})\,\xi(\mathrm{d}\mathbf{x}) + \frac{\sigma^2}{n}\Lambda_m^{-1}$$

➤ guaranteed convergence towards an optimal ξ^*, with N^* support points

In practice: eigen-decomposition

- use a finite Q-point set $\mathscr{X}_Q = \{\mathbf{x}^{(k)}, \ldots, \mathbf{x}^{(Q)}\}$
- diagonalize $\mathbf{QW}$ where

$$\{\mathbf{Q}\}_{k\ell} = C(\mathbf{x}^{(k)}, \mathbf{x}^{(\ell)}),\ \mathbf{W} = \mathrm{diag}\{w_1, \ldots, w_Q\}$$

($w_k = 1/Q$ when μ uniform)

$$\rightarrow \mathbf{QW} = \mathbf{P}\Lambda\mathbf{P}^{-1} \text{ with } \mathbf{P}^\top\mathbf{WP} = \mathbf{I}_Q \text{ and}$$

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$$\mathbf{M}_B(\xi) = \sum_{k=1}^{m} p_k \phi(\mathbf{x}_k)\phi^\top(\mathbf{x}_k) + \frac{\sum_{i=m+1}^{Q} \lambda_i}{n} \text{diag}\{\lambda_1^{-1}, \ldots, \lambda_m^{-1}\},\ m < Q$$

where $p_k = \xi\{\mathbf{x}_k\}$ and $\{\phi(\mathbf{x}_k)\}_j = \varphi_j(\mathbf{x}_k) = \mathbf{P}_{kj}$, $k = 1, \ldots, m$, $j = 1, \ldots, m$

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➤ minimization of $\mathrm{trace}[\mathbf{M}_B^{-1}(\xi)]$ ➔ ξ^*

$p_k^* = 0$ for many k, but some $p_k^* > 0$ are very small,

there may exist clusters of points, etc.

➔ aggregate support points of ξ^*

➔ remove some points (transfer their weights on others, optimally)

(Gauthier & P., 2016)

The number N of points is not totally controlled, but 2 tuning parameters are available: m (truncation level) and n (take $m \approx n \approx N$)

N points ➠ initialization for optimization of the true IMSE($\mathbf{X}_N$) by any standard algorithm (optimal points remain in the convex hull of $\mathscr{X}$)

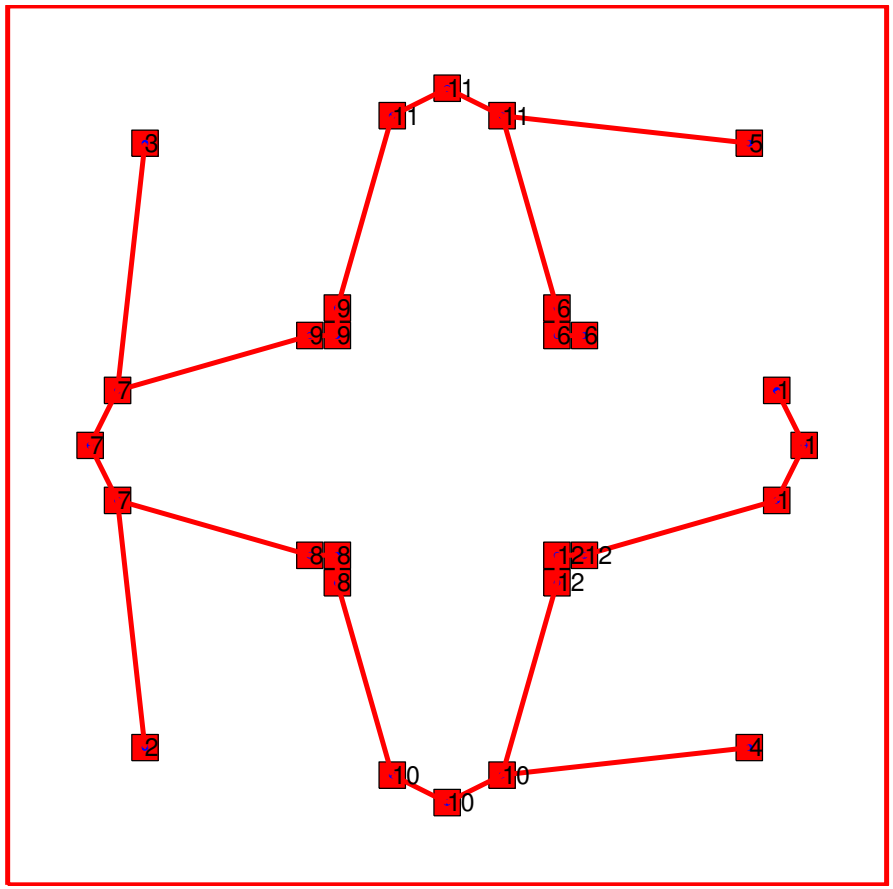
Example :

$d = 2$, $C(\mathbf{x}, \mathbf{x}') = (1 + 10\|\mathbf{x} - \mathbf{x}'\|)\exp(-10\|\mathbf{x} - \mathbf{x}'\|)$ (Matérn 3/2)

$\mathscr{X}_Q$ = regular grid with $Q = 33 \times 33 = 1\,089$ points, $\sigma^2 = \sum_{i>m} \lambda_i$

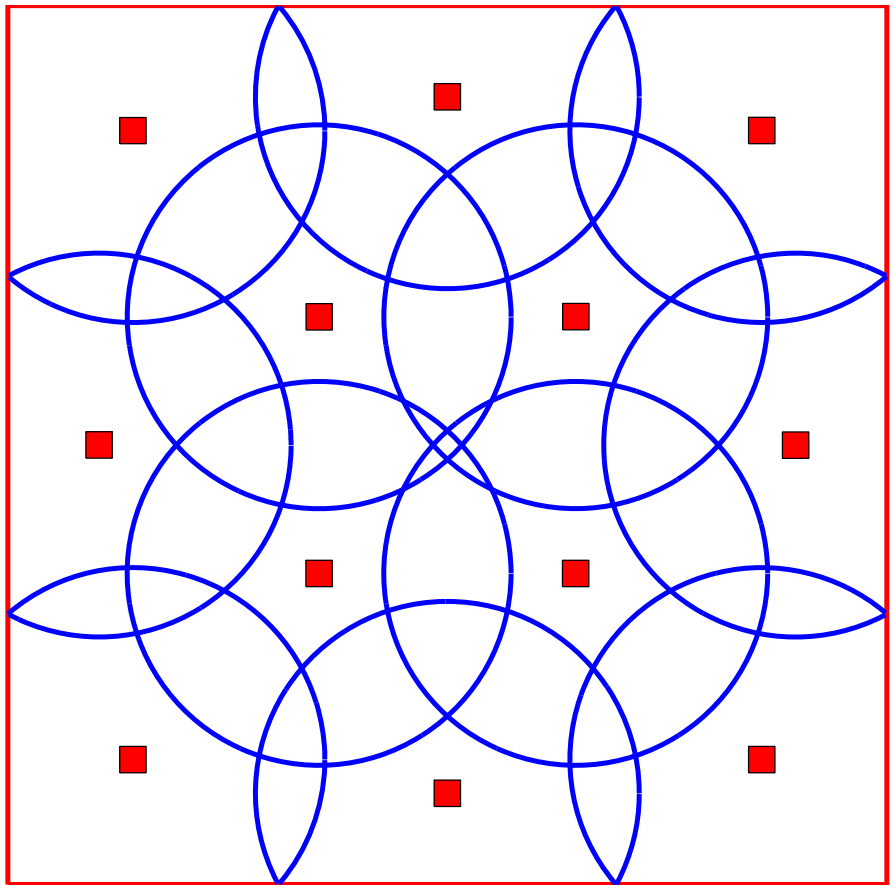
$m = n = 10$

aggregation of support of ξ^*



$m = n = 10$

➠ $N = 12$



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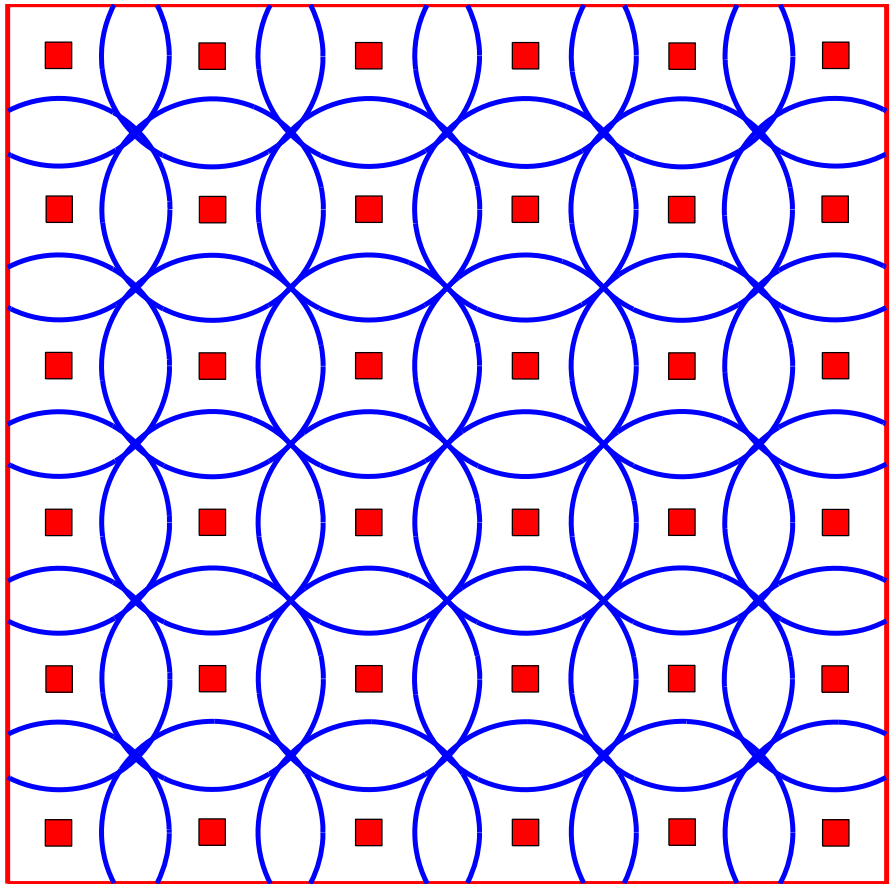
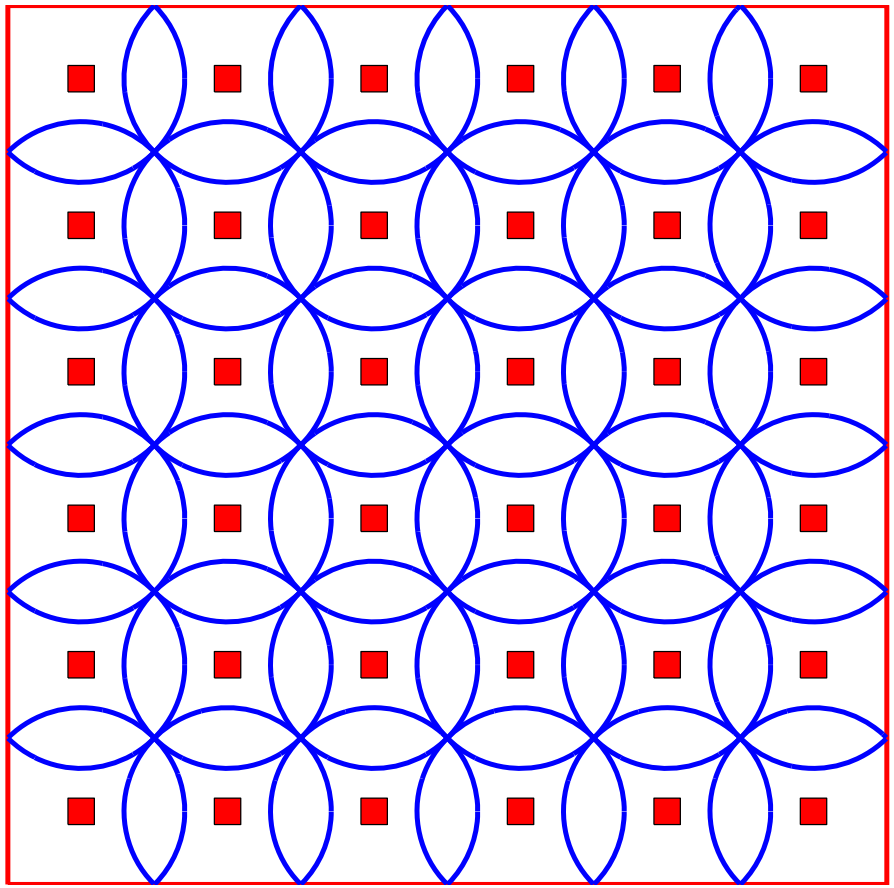
$m = 30$, $n = 10$ ➠ $N = 36$



$\mathbf{X}_{36}$ miniMax optimal



Can be used for any $\mathscr{X}$ if d not too big: use a finite $\mathscr{X}_Q$ given by first Q points of a LDS in $\mathscr{X}$

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Same thing (Spöck and Pilz, 2010), with slightly more complicated expressions

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Same thing (Spöck and Pilz, 2010), with slightly more complicated expressions

More advanced: avoid mixing eigenfunctions $\varphi_i(\cdot)$ with trend components $\{\mathbf{r}\}_j(\cdot)$ (Gauthier & P., 2016)

⏩ Conclusions part (2)

4 Beyond space filling

Optimal design for kriging: there is a hidden difficulty
the value of θ in covariance $C(\cdot;\theta)$ is unknown

➠ use the same observations to estimate θ and then construct $\eta_n(x)$ with $\hat{\theta}^n$ estimated (plug-in method)

4 Beyond space filling

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➠ use the same observations to estimate θ and then construct $\eta_n(x)$ with $\hat{\theta}^n$ estimated (plug-in method)

➠ In particular, we may use $\hat{\theta}^n$ = Maximum Likelihood Estimator (MLE) ($Z(\mathbf{x})$ is supposed to be Gaussian)

➠ there is a corrective term (Harville and Jeske, 1992; Abt, 1999) :

$$\hat{\rho}_n(\mathbf{x};\theta) = \rho_n(\mathbf{x};\theta) + \mathrm{trace}\{\mathbf{M}_\theta^{-1} \frac{\partial \mathbf{v}_n(\mathbf{x};\theta)}{\partial \theta} \mathbf{C}_n \frac{\partial \mathbf{v}_n(\mathbf{x};\theta)}{\partial \theta^\top}\}$$

(= Empirical Kriging (EK) variance)

avec :

$\mathbf{v}_n(\mathbf{x};\theta)$ such that $\eta_n(\mathbf{x}) = \mathbf{v}_n^\top(\mathbf{x};\theta)\mathbf{y}_n$

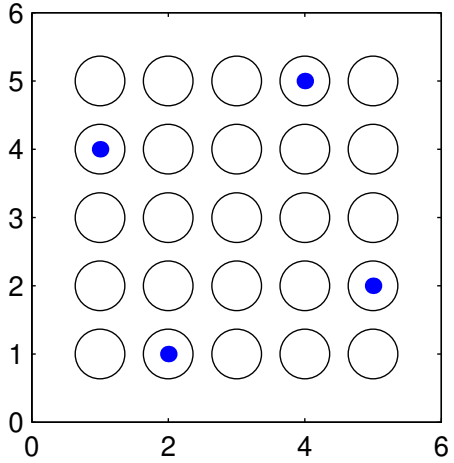
$\mathbf{M}_\theta$ = Fisher Information Matrix (FIM) for θ

Example (Zimmerman, 2006):

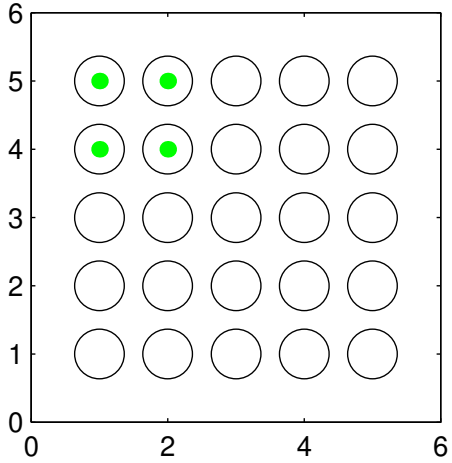
$\mathrm{E}\{Z(\mathbf{x})Z(\mathbf{x}')\} = \theta^{\|\mathbf{x}-\mathbf{x}'\|}$, $\theta = 0.3$

$\mathscr{X}$ = regular grid 5×5, optimal designs for:

prediction for θ known



estimation of θ



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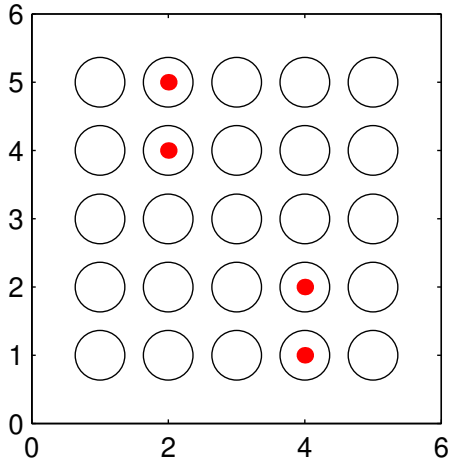
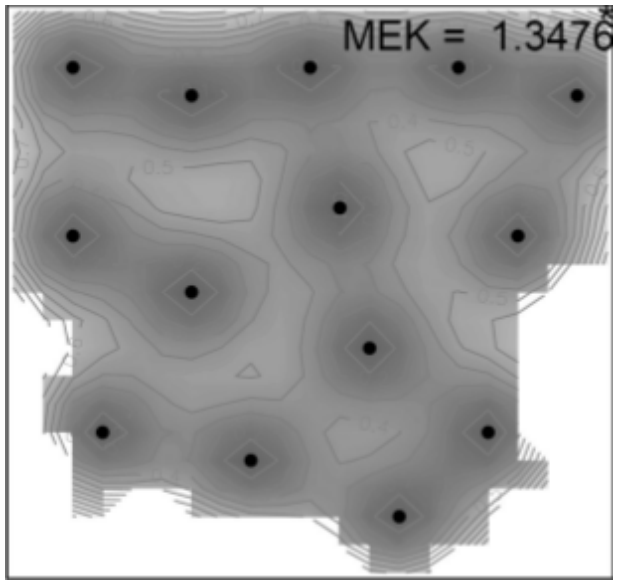


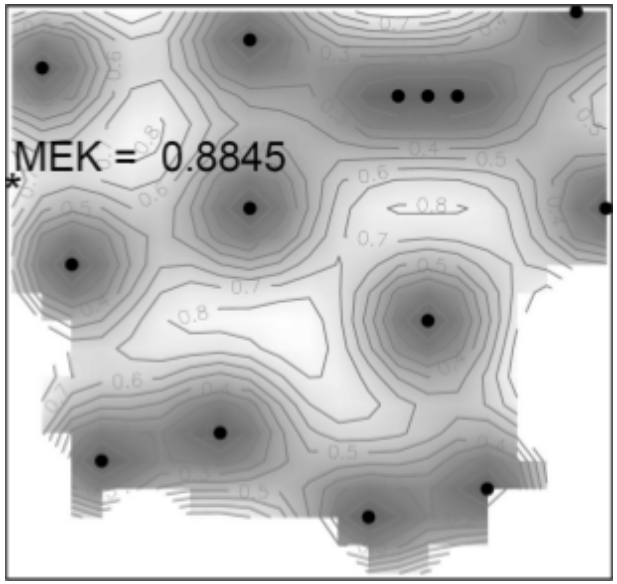
prediction with known θ:
$\mathbf{X}_4$ minimizes $\max_{\mathbf{x}\in\mathscr{X}} \rho_4(\mathbf{x})$
estimation of θ:
$\mathbf{X}_4$ maximizes $\det \mathbf{M}_\theta$
prediction with θ estimated:
$\mathbf{X}_4$ minimizes MEK=$\max_{\mathbf{x}\in\mathscr{X}} \hat{\rho}_4(\mathbf{x};\theta)$

Example (Müller et al., 2015):
NH4 concentration in north sea (collaboration with MUMM, Belgium) — simulated data, kriging with Matérn 3/2 kernel

$\hat{\rho}_{14}(\mathbf{x};\theta)$ for miniMax-optimal design $\mathbf{X}^*_{mM,n=14}$



$\hat{\rho}_{14}(\mathbf{x};\theta)$ for $\mathbf{X}^*_{14}$ minimizing MEK$=\max_{\mathbf{x}\in\mathscr{X}} \hat{\rho}_{14}(\mathbf{x};\theta)$



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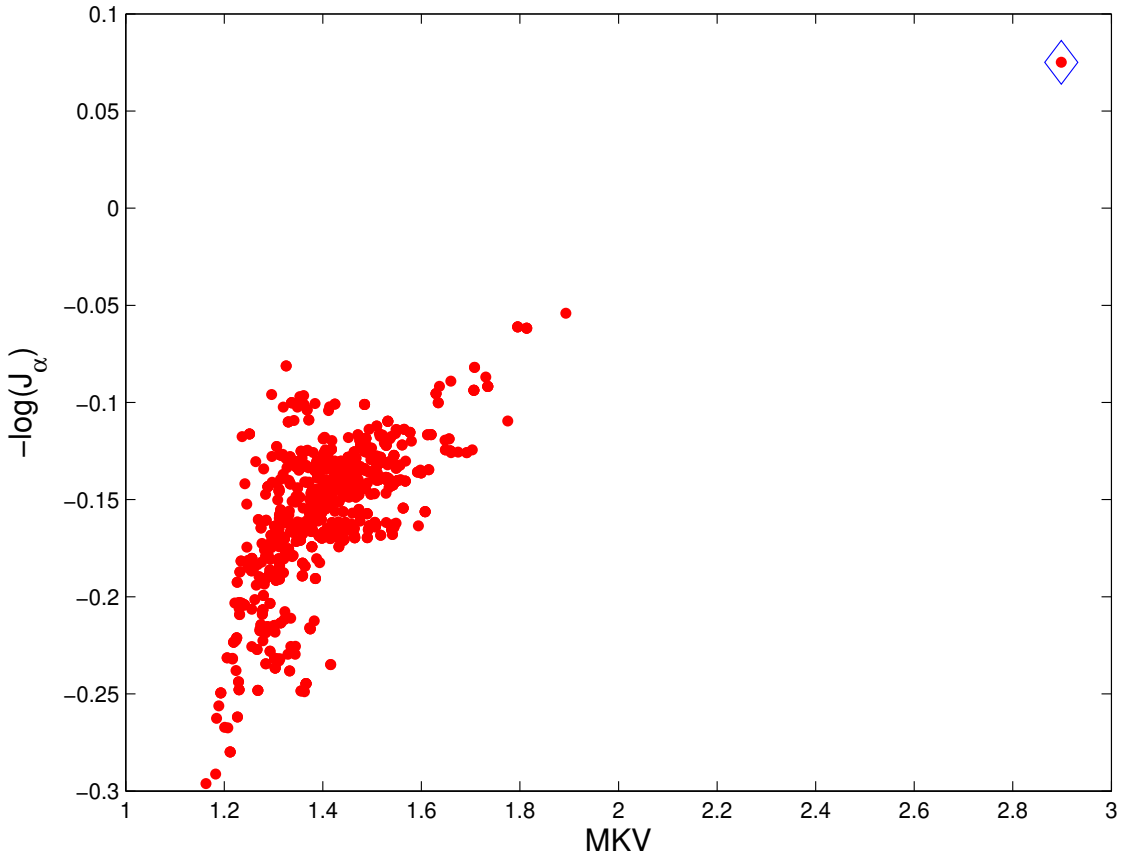
➠ Use a compromise criterion between space filling and "aggregation of points"

for instance, take $\mathbf{X}_n$ that maximizes $\gamma \log\det(\mathbf{M}_\beta) + (1-\gamma)\log\det(\mathbf{M}_\theta)$ (Müller et al., 2011, 2015), with

- $\mathbf{M}_\beta$= FIM for trend parameters β (maximization $\rightarrow$ space filling design)
- $\mathbf{M}_\theta$= FIM for correlation parameters θ (maximization $\rightarrow$ aggregation)

Example: $n = 7$, $d = 2$, $C(\mathbf{x} - \mathbf{x}'; \theta) = \exp(-\theta \|\mathbf{x} - \mathbf{x}'\|)$, $\theta = 0.7$,
1000 Lh (999 random + $\diamondsuit$ for a Maximin optimal design)
MKV=$\max_{\mathbf{x} \in \mathscr{X}} \hat{\rho}_n(\mathbf{x}; \theta)$, $J_\alpha = \det^\alpha(\mathbf{M}_\beta) + \det^{1-\alpha}(\mathbf{M}_\theta)$ ($\alpha = 0.8$)



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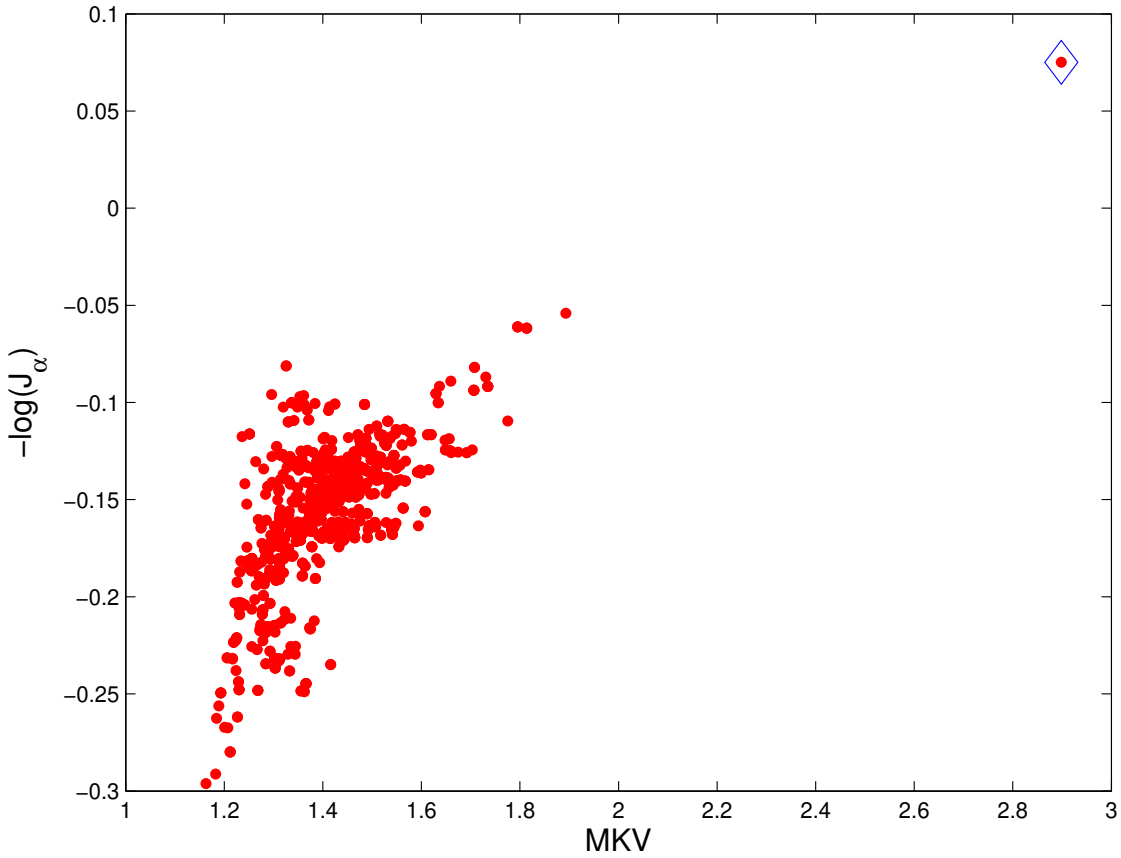

However, the effet of corrective term in
$\hat{\rho}_n(\mathbf{x}; \theta) = \rho_n(\mathbf{x}; \theta) + \mathrm{trace}\{\mathbf{M}_\theta^{-1} \frac{\partial \mathbf{v}_n(\mathbf{x};\theta)}{\partial \theta} \mathbf{C}_n \frac{\partial \mathbf{v}_n(\mathbf{x};\theta)}{\partial \theta^\top}\}$
quickly vanishes as n increases

5 Conclusions part (2) — with model

➤ Design criteria relying on a Gaussian-process model (entropy, MMSE, IMSE) depend on the chosen covariance (and on θ in $C(\cdot, \theta)$)

- ➠ expectation w.r.t. θ (Joseph et al., 2015) $\rightarrow$ entropy
- ➠ worst case w.r.t. θ (Spöck and Pilz, 2010) $\rightarrow$ IMSE
- ➠ However, the model is often just a tool to generate a space-filling design: the value of θ is not critical (choose a small enough correlation length to spread the points in $\mathscr{X}$)

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➤ Put more points near the boundaries than in the central part of $\mathscr{X}$ (but be careful ➠ in high dimension almost all the volume is near the boundaries!)

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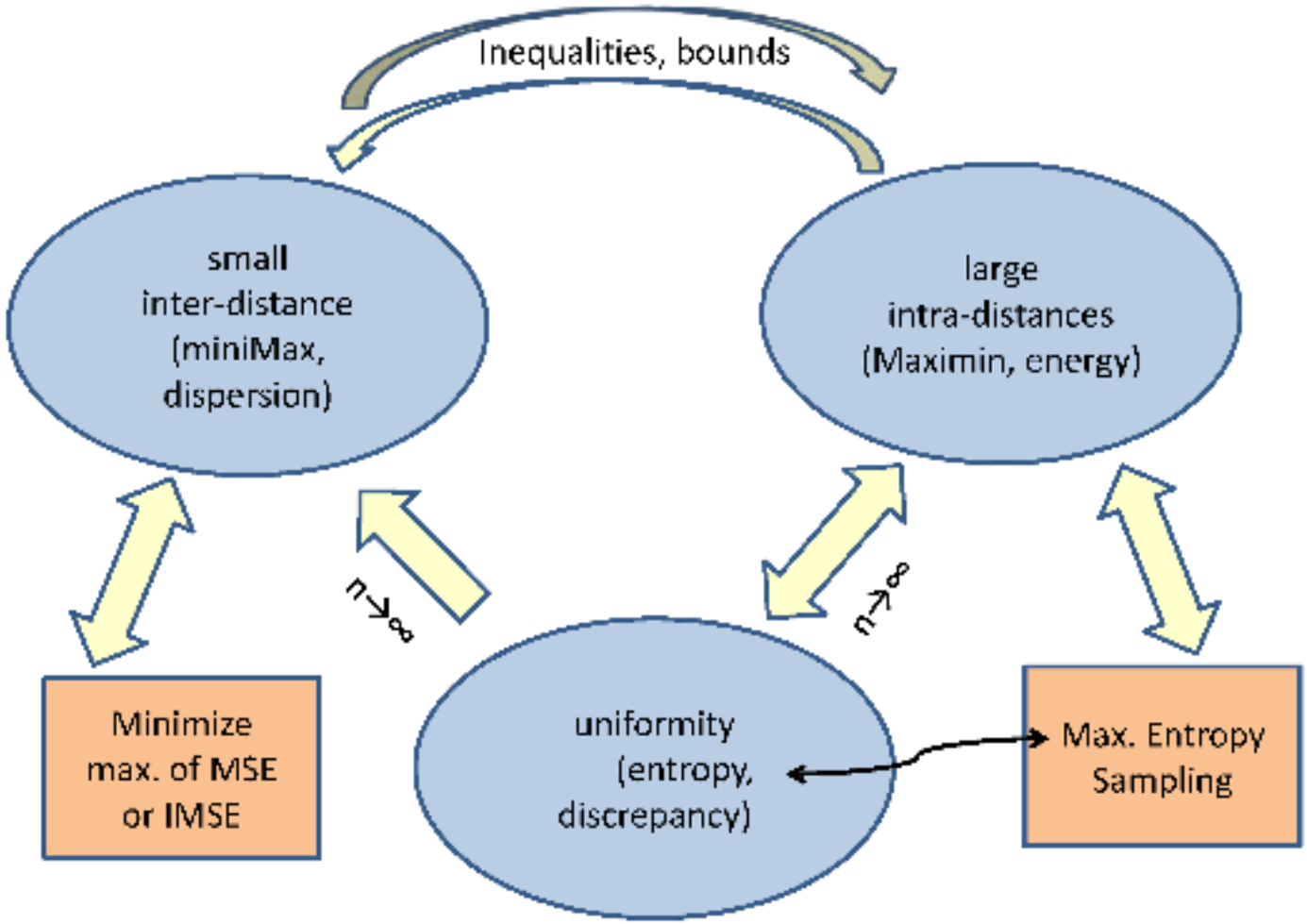
Test several methods (none is perfect) by comparing values of different criteria


Inequalities, bounds
small
inter-distance
(miniMax,
dispersion)
large
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$n \to \infty$
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Minimize
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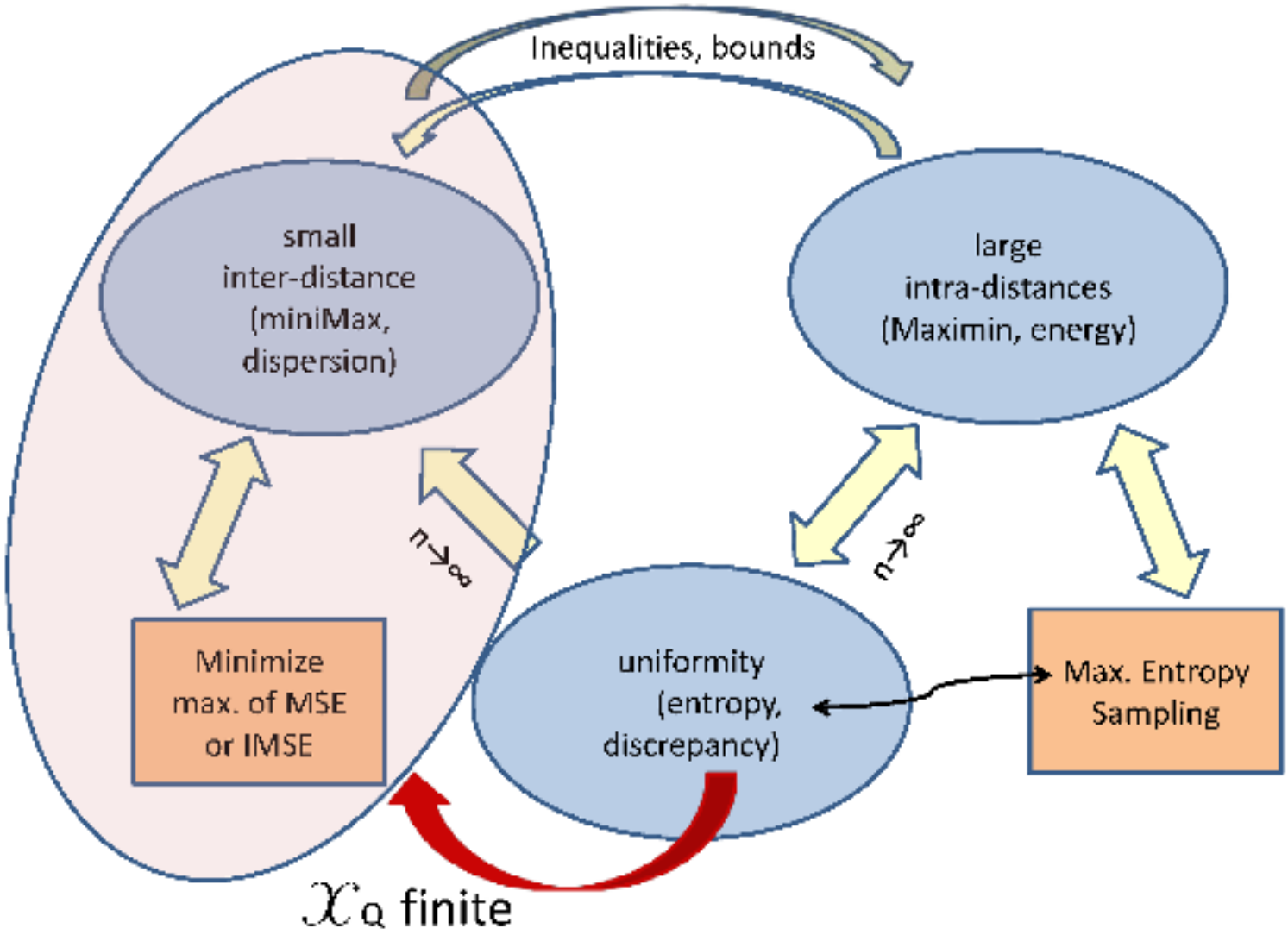
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