

Planification d'expériences numériques : quelques tendances et questions ouvertes

Luc Pronzato

Laboratoire I3S, CNRS-Univ. Nice Sophia Antipolis,
France



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

1 Space-filling design: miniMax & Maximin

2 Regularized Maximin

3 Beyond space filling

4 Conclusions

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Computer experiment = simulations

$x \in \mathbb{R}^d \rightarrow$ observation $\mathcal{Y}(x)$ (real phenomenon, physical system)

Numerical simulation: $x \rightarrow Y(x) = f(x)$

Pairs $(X_i, f(X_i)), i = 1, 2, \dots, n \rightarrow$ approximation $\eta_n(\cdot)$ of $f(\cdot)$ (\rightarrow epistemic uncertainty – due to simulator, model $\eta_n(\cdot)$, finite data set...)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Computer experiment = simulations

$x \in \mathbb{R}^d \rightarrow$ observation $\mathcal{Y}(x)$ (real phenomenon, physical system)

Numerical simulation: $x \rightarrow Y(x) = f(x)$

Pairs $(X_i, f(X_i))$, $i = 1, 2, \dots, n \rightarrow$ approximation $\eta_n(\cdot)$ of $f(\cdot)$ (\rightarrow epistemic uncertainty – due to simulator, model $\eta_n(\cdot)$, finite data set...)

- optimization: find $x^* = \arg \max_{x \in \mathcal{X}} f(x)$ (hopefully close to $\arg \max_{x \in \mathcal{X}} \mathcal{Y}(x)$)
- inversion: reconstruct $\{x \in \mathcal{X} : f(x) = T\}$
- estimation of failure prob. $\text{Prob}\{f(x) > C\}$ when $x \sim \phi(\cdot)$ (intrinsic uncertainty due to input variability)
- sensitivity analysis (functional variance analysis)
- approximation/interpolation

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Objective = approximation/interpolation

$f(x)$ some unknown function defined for $x \in \mathcal{X} \subset \mathbb{R}^d$
 construct a 'good' approximation $\eta_n(\cdot)$ of $f(\cdot)$ over \mathcal{X} from
 pairs $(X_i, f(X_i))$, $i = 1, 2, \dots, n$ (n not necessarily fixed
 beforehand)

Since $f(\cdot)$ is unknown \rightarrow put n points $\mathbf{X}_n = (X_1, \dots, X_n)$ in
 \mathcal{X} as dispersed as possible (can be justified precisely
 [Biedermann & Dette, 2001])

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Classical measures of dispersion (often $\mathcal{X} = [0, 1]^d$)

① miniMax distance: minimize

$$\Phi_{mM}(\mathbf{X}_n) = \max_{x \in \mathcal{X}} \min_i \|x - X_i\|$$

$$d = 1 \Leftrightarrow X_i = (2i - 1)/(2n), \quad i = 1, \dots, n$$

$$\Rightarrow \Phi_{mM}^* = 1/(2n)$$

$$d > 1 \Leftrightarrow \text{sphere-covering}$$

Classical measures of dispersion (often $\mathcal{X} = [0, 1]^d$)

- ① miniMax distance: minimize

$$\Phi_{mM}(\mathbf{X}_n) = \max_{x \in \mathcal{X}} \min_i \|x - X_i\|$$

$$d = 1 \Leftrightarrow X_i = (2i - 1)/(2n), \quad i = 1, \dots, n$$

$$\Rightarrow \Phi_{mM}^* = 1/(2n)$$

$$d > 1 \Leftrightarrow \text{sphere-covering}$$

- ② Maximin distance: maximize

$$\Phi_{Mm}(\mathbf{X}_n) = \min_{i \neq j} d_{ij} = \min_{i \neq j} \|X_i - X_j\|$$

$$d = 1 \Leftrightarrow X_i = (i - 1)/(n - 1), \quad i = 1, \dots, n$$

$$\Rightarrow \Phi_{Mm}^* = 1/(n - 1)$$

$$d > 1 \Leftrightarrow \text{sphere-packing}$$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

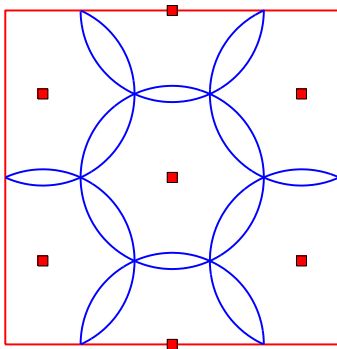
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

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



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

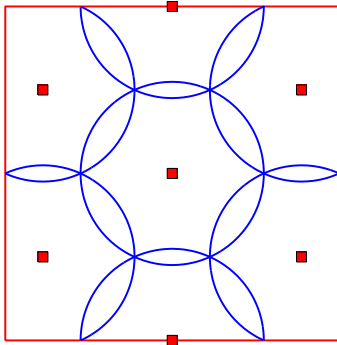
1 Space-filling

2 Regularized
Maximin

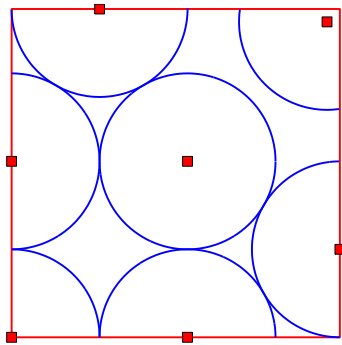
3 Beyond
space filling

4 Conclusions

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



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



① miniMax criterion Φ_{mM}

⇒ Φ_{mM} has nice properties in terms of approximation theory,
but is difficult to compute

Possible evaluation via Delaunay triangulation (tessellation)

① miniMax criterion Φ_{mM}

⇒ Φ_{mM} has nice properties in terms of approximation theory, but is difficult to compute

Possible evaluation via Delaunay triangulation (tessellation)

- \mathbf{X}_n ($= n$ points in $\mathcal{X} = [0, 1]^d$) → take all symmetric points w.r.t. $2d$ faces of \mathcal{X}
- Compute the Delaunay triangulation (tessellation)
- candidates for $\arg \max_{x \in \mathcal{X}} \min_i \|x - X_i\|$ are centers of a circumscribed spheres

Luc Pronzato

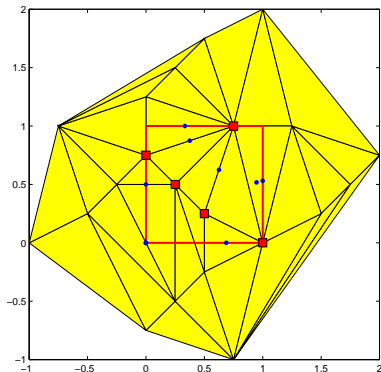
Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions



Luc Pronzato

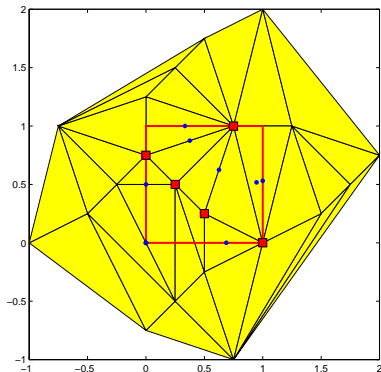
Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions



$\Phi_{Mm}(\mathbf{X})$ can be calculated... but remains computationally costly: up to $M^{\lceil d/2 \rceil}$ simplices (and circumscribed spheres) with $M = (2d + 1)n \rightarrow$ **computing time** $\mathcal{O}(M \log M + M^{\lceil d/2 \rceil})$

② Maximin criterion Φ_{Mm}

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

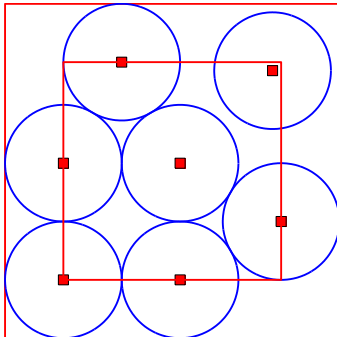
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Relation between Maximin-optimal design and sphere packing:

$$d = 2, n = 7$$



② Maximin criterion Φ_{Mm}

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

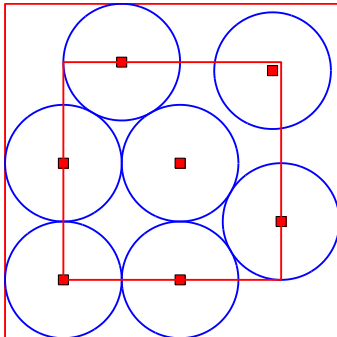
2 Regularized
Maximin

3 Beyond
space filling

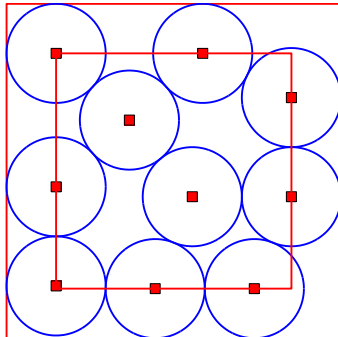
4 Conclusions

Relation between Maximin-optimal design and sphere packing:

$d = 2, n = 7$

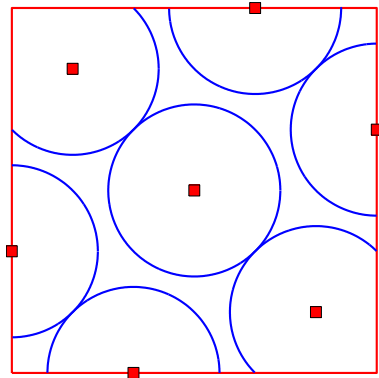


$d = 2, n = 10$



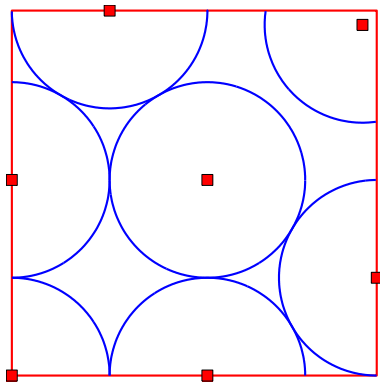
To ensure good projective properties along all axes: make each one-dimensional projection Maximin-optimal ($X_i = \frac{i-1}{n-1}$) (\rightarrow finite set, with $(n!)^{d-1}$ elements)

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



To ensure good projective properties along all axes: make each one-dimensional projection Maximin-optimal ($X_i = \frac{i-1}{n-1}$) (\rightarrow finite set, with $(n!)^{d-1}$ elements)

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



Define $d_{ij} = \|X_i - X_j\|$, so that $\Phi_{Mm}(\mathbf{X}) = \min_{i \neq j} d_{ij}$

$$\underline{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} d_{ij}^{-q} \right]^{-1/q} \quad \text{and} \quad \bar{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} \mu_{ij} d_{ij}^{-q} \right]^{-1/q}$$

with $\mu_{ij} > 0$ and $\sum_{i < j} \mu_{ij} = 1$

Define $d_{ij} = \|X_i - X_j\|$, so that $\Phi_{Mm}(\mathbf{X}) = \min_{i \neq j} d_{ij}$

$$\underline{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} d_{ij}^{-q} \right]^{-1/q} \quad \text{and} \quad \bar{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} \mu_{ij} d_{ij}^{-q} \right]^{-1/q}$$

with $\mu_{ij} > 0$ and $\sum_{i < j} \mu_{ij} = 1$

Then

$$\underline{\phi}_{[q]}(\mathbf{X}) \leq \phi_{Mm}(\mathbf{X}) \leq \bar{\phi}_{[q]}(\mathbf{X}) \leq \underline{\mu}^{-1/q} \underline{\phi}_{[q]}(\mathbf{X}), \quad q > 0,$$

with $\underline{\mu} = \min_{i < j} \mu_{ij}$ (convergence monotonic in q from both sides as $q \rightarrow \infty$)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Define $d_{ij} = \|X_i - X_j\|$, so that $\Phi_{Mm}(\mathbf{X}) = \min_{i \neq j} d_{ij}$

$$\underline{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} d_{ij}^{-q} \right]^{-1/q} \quad \text{and} \quad \bar{\phi}_{[q]}(\mathbf{X}) = \left[\sum_{i < j} \mu_{ij} d_{ij}^{-q} \right]^{-1/q}$$

with $\mu_{ij} > 0$ and $\sum_{i < j} \mu_{ij} = 1$

Then

$$\underline{\phi}_{[q]}(\mathbf{X}) \leq \phi_{Mm}(\mathbf{X}) \leq \bar{\phi}_{[q]}(\mathbf{X}) \leq \underline{\mu}^{-1/q} \underline{\phi}_{[q]}(\mathbf{X}), \quad q > 0,$$

with $\underline{\mu} = \min_{i < j} \mu_{ij}$ (convergence monotonic in q from both sides as $q \rightarrow \infty$)

By continuity: $\bar{\phi}_{[0]}(\mathbf{X}) = \exp \left[\sum_{i < j} \mu_{ij} \log(d_{ij}) \right]$

$\mu =$ uniform measure ($\mu_{ij} = \underline{\mu} = \binom{n}{2}^{-1}$ for all $i < j$) \Rightarrow

$$\frac{\phi_{Mm}(\underline{\mathbf{X}}_{[q]}^*)}{\phi_{Mm}^*} \geq \binom{n}{2}^{-1/q},$$

with $\underline{\mathbf{X}}_{[q]}^*$ optimal for $\underline{\phi}_{[q]}$

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

$\mu =$ uniform measure ($\mu_{ij} = \underline{\mu} = \binom{n}{2}^{-1}$ for all $i < j$) \Rightarrow

$$\frac{\phi_{Mm}(\underline{\mathbf{X}}_{[q]}^*)}{\phi_{Mm}^*} \geq \binom{n}{2}^{-1/q},$$

with $\underline{\mathbf{X}}_{[q]}^*$ optimal for $\underline{\phi}_{[q]}$

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

$q = 2 \rightarrow$ "Energy criterion" of [Audze & Eglaiss, 1977]

for $q \lesssim 5$ easier optimization (Lh designs) than for ϕ_{Mm}
[Morris & Mitchell, 1995]

\Rightarrow use the smallest q such that the optimum designs coincide

$\mu =$ uniform measure ($\mu_{ij} = \underline{\mu} = \binom{n}{2}^{-1}$ for all $i < j$) \Rightarrow

$$\frac{\phi_{Mm}(\underline{\mathbf{X}}_{[q]}^*)}{\phi_{Mm}^*} \geq \binom{n}{2}^{-1/q},$$

with $\underline{\mathbf{X}}_{[q]}^*$ optimal for $\underline{\phi}_{[q]}$

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

$q = 2 \rightarrow$ "Energy criterion" of [Audze & Eglais, 1977]

for $q \lesssim 5$ easier optimization (Lh designs) than for ϕ_{Mm}
[Morris & Mitchell, 1995]

\Rightarrow use the smallest q such that the optimum designs coincide

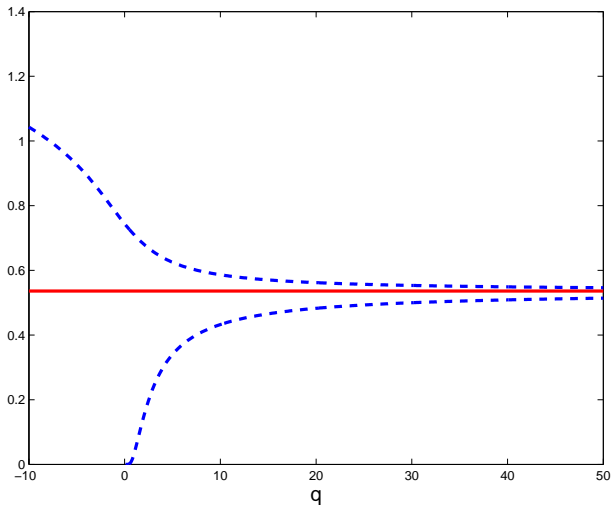
Continuous versions: ξ a probability measure on \mathcal{X} ,

$$\tilde{\phi}_{[q]}(\xi) = \left[\int_{\mathcal{X}} \int_{\mathcal{X}} \|x - y\|^{-q} \xi(dx) \xi(dy) \right]^{-1/q}$$

$$\tilde{\phi}_{[0]}(\xi) = \exp \int_{\mathcal{X}} \int_{\mathcal{X}} \log \|x - y\| \xi(dx) \xi(dy)$$

7-point maximin-distance design ($d = 2$):

Φ_{Mm} and bounds $\underline{\phi}_{[q]}$ and $\overline{\phi}_{[q]}$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Write $\Phi_{Mm}(\mathbf{X}) = \min_i d_i^*$ with $d_i^* = \min_{j \neq i} \|X_i - X_j\|$
 (= Nearest Neighbor distance to X_i)

Define

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

Write $\Phi_{Mm}(\mathbf{X}) = \min_i d_i^*$ with $d_i^* = \min_{j \neq i} \|X_i - X_j\|$
 (= Nearest Neighbor distance to X_i)

Define

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

Then $\underline{\phi}_{[NN,q]}(\mathbf{X}) \leq \phi_{Mm}(\mathbf{X}) \leq n^{1/q} \underline{\phi}_{[NN,q]}(\mathbf{X})$, $q > 0$,
 (convergence monotonic in q from both sides as $q \rightarrow \infty$)

Write $\Phi_{Mm}(\mathbf{X}) = \min_i d_i^*$ with $d_i^* = \min_{j \neq i} \|X_i - X_j\|$
 (= Nearest Neighbor distance to X_i)

Define

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

Then $\underline{\phi}_{[NN,q]}(\mathbf{X}) \leq \phi_{Mm}(\mathbf{X}) \leq n^{1/q} \underline{\phi}_{[NN,q]}(\mathbf{X})$, $q > 0$,
 (convergence monotonic in q from both sides as $q \rightarrow \infty$)

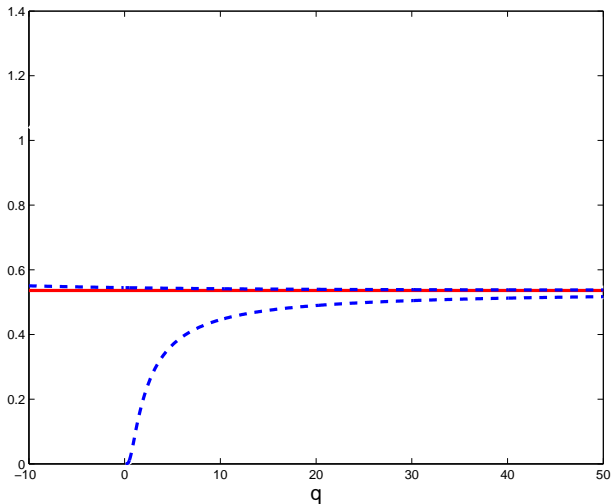
$$\frac{\phi_{Mm}(\underline{\mathbf{X}}_{[NN,q]}^*)}{\phi_{Mm}^*} \geq n^{-1/q},$$

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

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

7-point maximin-distance design ($d = 2$):

Φ_{Mm} and regularization via $\underline{\phi}_{[NN,q]}$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

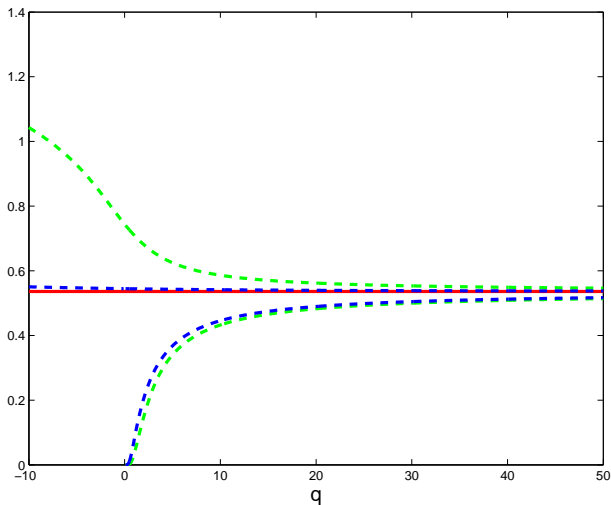
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

7-point maximin-distance design ($d = 2$):

Φ_{Mm} and regularization via $\underline{\phi}_{[NN,q]}$ and $\underline{\phi}_{[q]}$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

[Beardwood, Halton, Hammersley 1959]: X_i i.i.d., p.d.f. φ ,
TSP graph $\mathcal{G}_{TSP}(\mathbf{X})$

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

then [Steele, 1981] for other Euclidean functionals on \mathbf{X} ,
[Redmond & Yukich, 1994] using quasi-additivity

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

[Beardwood, Halton, Hammersley 1959]: X_i i.i.d., p.d.f. φ ,
TSP graph $\mathcal{G}_{TSP}(\mathbf{X})$

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

then [Steele, 1981] for other Euclidean functionals on \mathbf{X} ,
[Redmond & Yukich, 1994] using quasi-additivity

[Redmond & Yukich, 1996], [Yukich, 1998], [Penrose &
Yukich 2003...2011], [Wade, 2011]:

$$\frac{\sum_{e_i \in \mathcal{G}(\mathbf{X})} |e_i|^\beta}{n^{(d-\beta)/d}} \rightarrow C(\beta, d) \int \varphi^{(d-\beta)/d}(x) dx, n \rightarrow \infty$$

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

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

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

- \Rightarrow estimation of Rényi entropy

$$H_\alpha^*(\varphi) = \frac{1}{1-\alpha} \log \int \varphi^\alpha(t) dt \quad \text{with } \alpha = (d-\beta)/d$$

$1 \leq \beta < d \Rightarrow 0 < \alpha \leq 1 - 1/d$, RHS max for $\varphi = \text{ct.}$
(uniform)

\rightarrow maximize the LHS

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

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

- \Rightarrow estimation of Rényi entropy

$$H_\alpha^*(\varphi) = \frac{1}{1-\alpha} \log \int \varphi^\alpha(t) dt \quad \text{with } \alpha = (d-\beta)/d$$

$1 \leq \beta < d \Rightarrow 0 < \alpha \leq 1 - 1/d$, RHS max for $\varphi = \text{ct.}$
(uniform)

\rightarrow maximize the LHS

- NN graph: $|e_i| = d_i^* \rightarrow$ maximize $\underline{\phi}_{[NN,q]}$ with $q = -\beta$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

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

- \Rightarrow estimation of Rényi entropy

$$H_\alpha^*(\varphi) = \frac{1}{1-\alpha} \log \int \varphi^\alpha(t) dt \quad \text{with } \alpha = (d-\beta)/d$$

$1 \leq \beta < d \Rightarrow 0 < \alpha \leq 1 - 1/d$, RHS max for $\varphi = \text{ct.}$
(uniform)

\rightarrow maximize the LHS

- NN graph: $|e_i| = d_i^* \rightarrow$ maximize $\phi_{[NN,q]}$ with $q = -\beta$
- $(1/n) \sum_{e_i \in \mathcal{G}_{MST}(\mathbf{X})} |e_i|$ used in [Franco, Ph.D., 2008] to classify designs (also considers $\text{Var}_{\mathcal{G}_{MST}(\mathbf{X})} \{|e_i|\}$)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

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

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- \Rightarrow estimation of Rényi entropy

$$H_\alpha^*(\varphi) = \frac{1}{1-\alpha} \log \int \varphi^\alpha(t) dt \quad \text{with } \alpha = (d-\beta)/d$$

$1 \leq \beta < d \Rightarrow 0 < \alpha \leq 1 - 1/d$, RHS max for $\varphi = \text{ct.}$
(uniform)

\rightarrow maximize the LHS

- NN graph: $|e_i| = d_i^* \rightarrow$ maximize $\phi_{[NN,q]}$ with $q = -\beta$
- $(1/n) \sum_{e_i \in \mathcal{G}_{MST}(\mathbf{X})} |e_i|$ used in [Franco, Ph.D., 2008] to classify designs (also considers $\text{Var}_{\mathcal{G}_{MST}(\mathbf{X})}\{|e_i|\}$)
- Shannon entropy with kernel estimator in [Jourdan & Franco, 2009, 2010]

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Maximin optimal design is model-free,
→ model-specific design?

Maximin optimal design is model-free,
→ model-specific design?

Model for $f(\cdot)$

$f(x) = \mathbf{r}^\top(x)\beta + Z(x, \omega)$ with

$\mathbf{r}(x)$ a known (vector of) functions(s) of x

$Z(x, \omega) =$ realization of a (second-order stationary)

Gaussian process (random field)

$\mathbb{E}\{Z(x, \omega)\} = 0, \mathbb{E}\{Z(x, \omega)Z(u, \omega)\} = \sigma^2 C((x - u); \theta)$

Maximin optimal design is model-free,
→ model-specific design?

Model for $f(\cdot)$

$f(x) = \mathbf{r}^\top(x)\beta + Z(x, \omega)$ with

$\mathbf{r}(x)$ a known (vector of) functions(s) of x

$Z(x, \omega) =$ realization of a (second-order stationary)

Gaussian process (random field)

$\mathbb{E}\{Z(x, \omega)\} = 0, \mathbb{E}\{Z(x, \omega)Z(u, \omega)\} = \sigma^2 C((x - u); \theta)$

Computer experiments

[Sacks, Welch, Mitchell, Wynn, 1989]: Take $C(\delta; \theta)$
continuous at $\delta = 0, C(0; \theta) = 1 \rightarrow$ two repetitions for the
same x give the same $f(x)$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Objective

Interpolate (or extrapolate): construct a prediction $\eta_n(x)$ for one particular realization of $Z(\cdot)$

\neq situation: prediction for future realizations
(\rightarrow simply estimate $\beta!$)

Objective

Interpolate (or extrapolate): construct a prediction $\eta_n(x)$ for one particular realization of $Z(\cdot)$

\neq situation: prediction for future realizations
(\rightarrow simply estimate β !)

Ordinary kriging:

$$\underline{f(x) = \beta + Z(x, \omega)} \rightarrow \eta_n(x) = \eta_n[f](x)$$

BLUP at x : $\eta_n(x) = \mathbf{v}_n^\top(x) \mathbf{y}_n$ where

- $\mathbf{y}_n = (f(X_1), \dots, f(X_n))^\top$
- $\mathbf{v}_n(x)$ minimizes $\mathbb{E}\{(\mathbf{v}_n^\top \mathbf{y}_n - [\beta + Z(x, \omega)])^2\}$

- under the constraint

$$\mathbb{E}\{\mathbf{v}_n^\top \mathbf{y}_n\} = \beta \sum_{i=1}^n \{\mathbf{v}_n\}_i = \mathbb{E}\{f(x)\} = \beta, \text{ i.e.,}$$

$$\sum_{i=1}^n \{\mathbf{v}_n\}_i = 1$$

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

MSPE: proportional to

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

[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 $\mathbf{1} = (1, \dots, 1)^\top$]

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

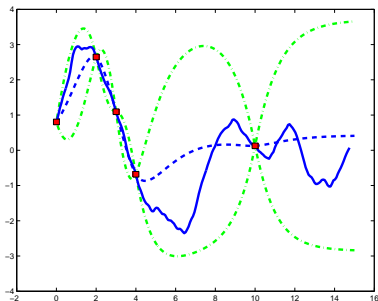
Prediction: $\eta_n(x) = \hat{\beta}^n + \mathbf{c}_n^\top(x) \mathbf{C}_n^{-1} (\mathbf{y}_n - \hat{\beta}^n \mathbf{1})$

MSPE: proportional to

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

[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 $\mathbf{1} = (1, \dots, 1)^\top$]



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Typical criteria: based on MSPE $\rho_n(x)$

E.g., minimize Max. MSPE: $\max_{x \in \mathcal{X}} \rho_n(x)$
with $\rho_k(X_i) = 0, i = 1, \dots, k$

Typical criteria: based on MSPE $\rho_n(x)$

E.g., minimize Max. MSPE: $\max_{x \in \mathcal{X}} \rho_n(x)$
with $\rho_k(X_i) = 0, i = 1, \dots, k$

The designs constructed are typically space-filling

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

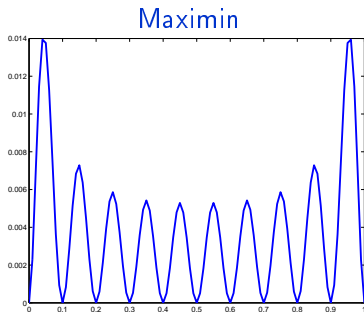
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$d = 1$ $n = 11$ observations in $[0, 1]$, $C(t) = \exp(-50t^2)$
plot of $\rho_n(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

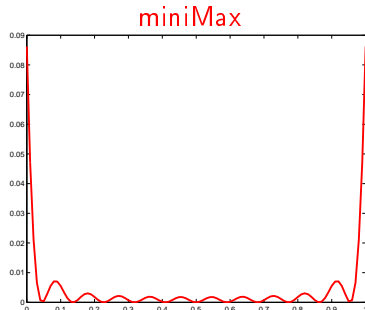
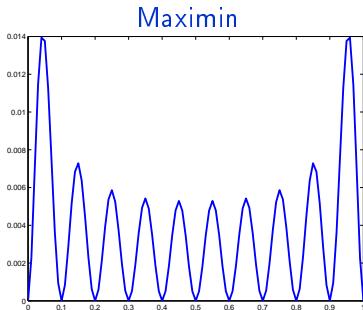
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$d = 1$ $n = 11$ observations in $[0, 1]$, $C(t) = \exp(-50t^2)$
plot of $\rho_n(x)$



Uniform distribution of points

- ⇒ less points available for prediction near the boundary
- ⇒ larger uncertainty near the boundary

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

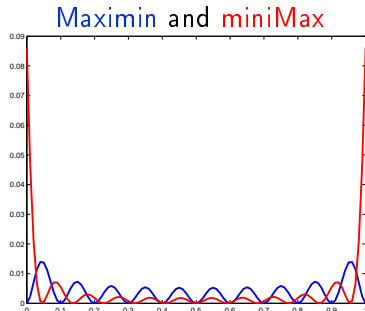
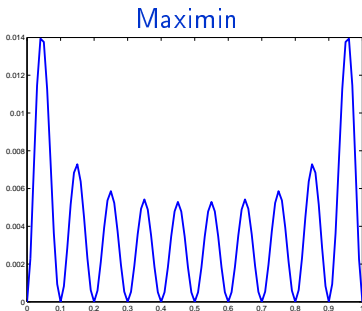
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$d = 1$ $n = 11$ observations in $[0, 1]$, $C(t) = \exp(-50t^2)$
plot of $\rho_n(x)$



Uniform distribution of points

- ⇒ less points available for prediction near the boundary
- ⇒ larger uncertainty near the boundary

Similar to polynomial regression (e.g. D-optimality):

- put design points at the roots of some orthogonal polynomials

(e.g., roots of $t(t-1)P'_{p-1}(2t-1)$ for D-optimal design on $[0, 1]$ with $P_n = n$ -th Legendre polynomial on $[-1, 1]$)

Similar to polynomial regression (e.g. D-optimality):

- put design points at the roots of some orthogonal polynomials
(e.g., roots of $t(t-1)P'_{p-1}(2t-1)$ for D-optimal design on $[0, 1]$ with $P_n = n$ -th Legendre polynomial on $[-1, 1]$)
- Erdős-Turan theorem: roots r of orthogonal polynomials on $[0, 1]$ are asymptotically distributed with the arcsine density $\varphi(r) = \frac{1}{\pi \sqrt{r(1-r)}}$

Similar to polynomial regression (e.g. D-optimality):

- put design points at the roots of some orthogonal polynomials
(e.g., roots of $t(t-1)P'_{p-1}(2t-1)$ for D-optimal design on $[0, 1]$ with $P_n = n$ -th Legendre polynomial on $[-1, 1]$)
- Erdős-Turan theorem: roots r of orthogonal polynomials on $[0, 1]$ are asymptotically distributed with the arcsine density $\varphi(r) = \frac{1}{\pi \sqrt{r(1-r)}}$
- [Dette & Pepelyshev, 2010]:
 - use a space filling-design (e.g., Maximin Lh),
 - for all $j = 1, \dots, d$, transform the j -th coordinates $\{X_i\}_j$ by $T : x \mapsto z = T(x) = \frac{1+\cos(\pi x)}{2}$
($x \sim \text{uniformly} \rightarrow z \sim \text{arcsine}$),
 - use the transformed design points Z_i

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

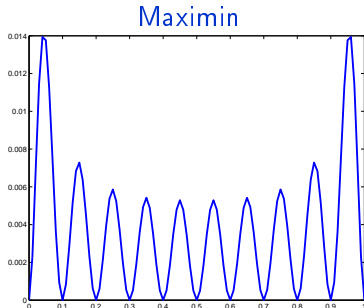
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

... The arcsine transformation can be too severe for small n
Back to the example, plot of $\rho_n(x)$:



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

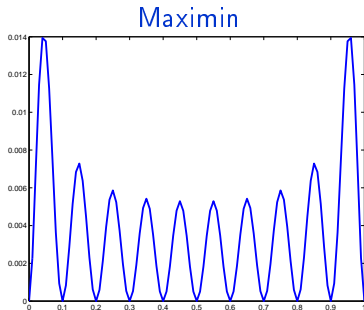
1 Space-filling

2 Regularized
Maximin

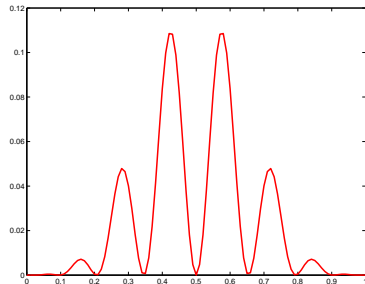
3 Beyond
space filling

4 Conclusions

... The arcsine transformation can be too severe for small n
Back to the example, plot of $\rho_n(x)$:



transformed Maximin (arcsine)



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

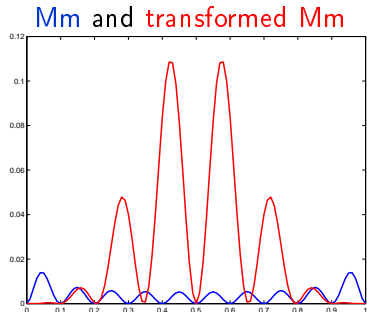
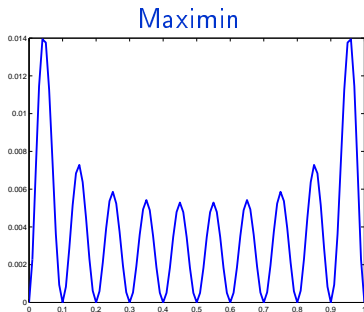
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

... The arcsine transformation can be too severe for small n
Back to the example, plot of $\rho_n(x)$:



Arcsine distribution: maximizes

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

(continuous version of $\bar{\phi}_{[0]}(\mathbf{X}) = \exp \left[\sum_{i < j} \mu_{ij} \log(d_{ij}) \right]$)

Arcsine distribution: maximizes

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

(continuous version of $\bar{\phi}_{[0]}(\mathbf{X}) = \exp \left[\sum_{i < j} \mu_{ij} \log(d_{ij}) \right]$)

Maximization of

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

is obtained for ξ having the density $\varphi(x) = \frac{x^{(q-1)/2}(1-x)^{(q-1)/2}}{B(\frac{q+1}{2}, \frac{q+1}{2})}$

(Beta distribution) [Dette, Pepelyshev, Zhigljavsky, 2009]

(tends to arcsine for $q \rightarrow 0$ and to uniform for $q \rightarrow 1$)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

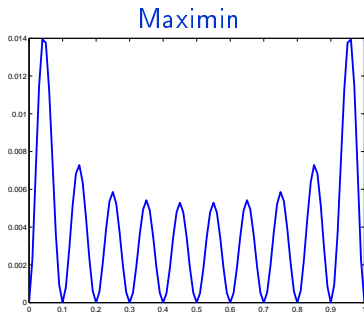
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

... For a suitable Beta transformation ($q = 0.84$)



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

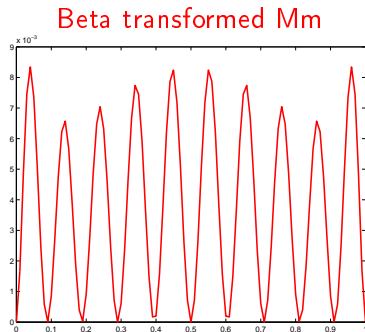
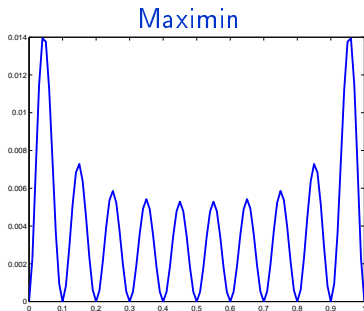
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

... For a suitable Beta transformation ($q = 0.84$)



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

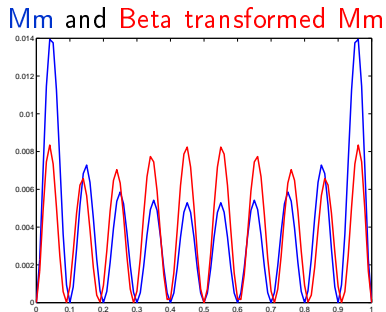
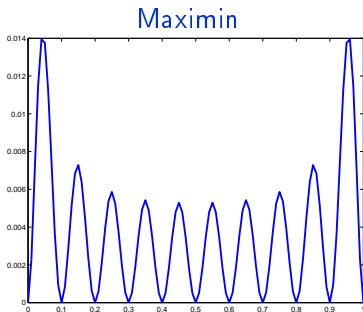
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

... For a suitable Beta transformation ($q = 0.84$)

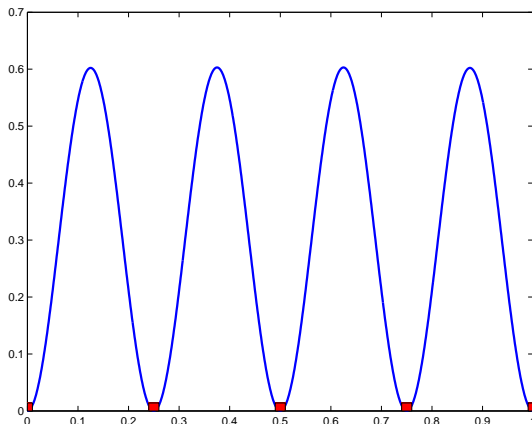


Choice of a suitable q ?

(depends on the correlation function $C(\cdot, \theta)$)

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_5(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

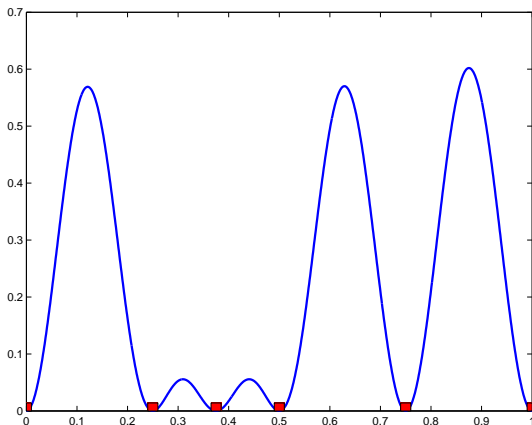
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_6(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

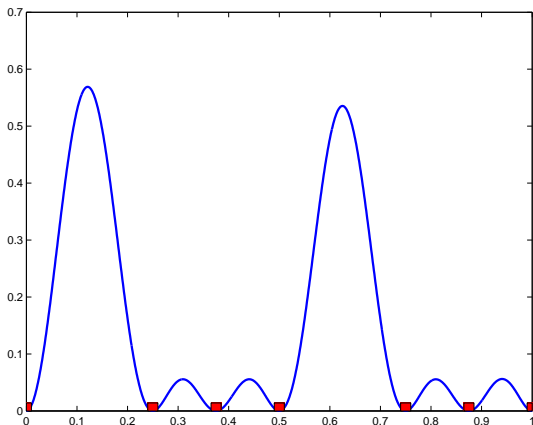
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_7(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

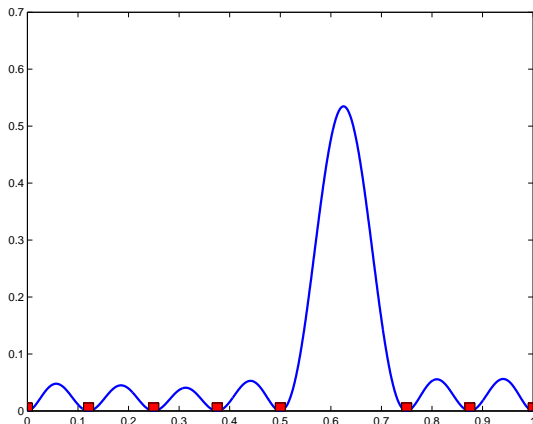
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_8(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

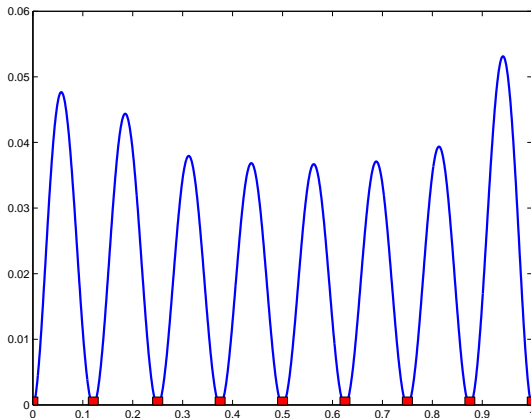
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_9(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

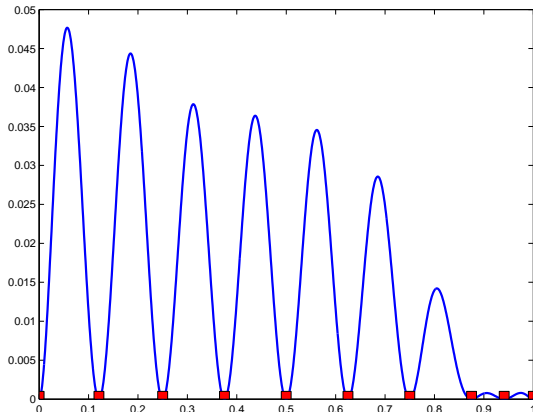
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_{10}(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

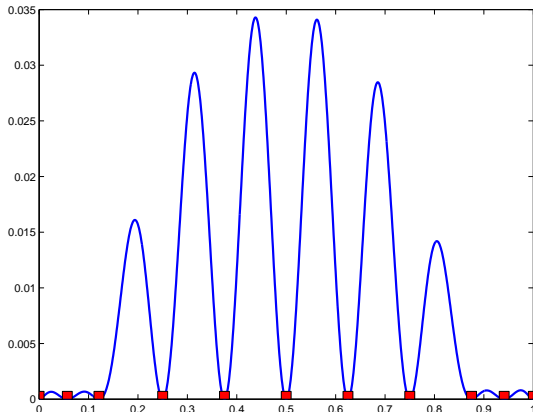
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_{11}(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

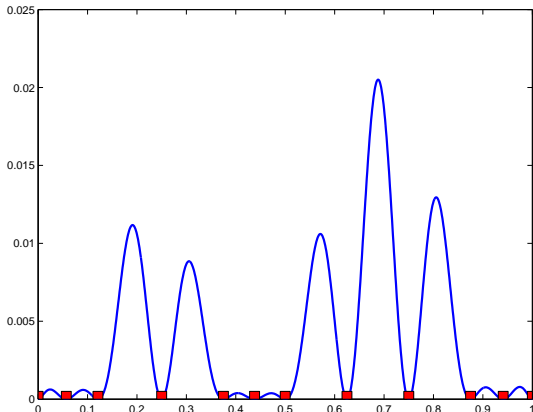
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_{12}(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

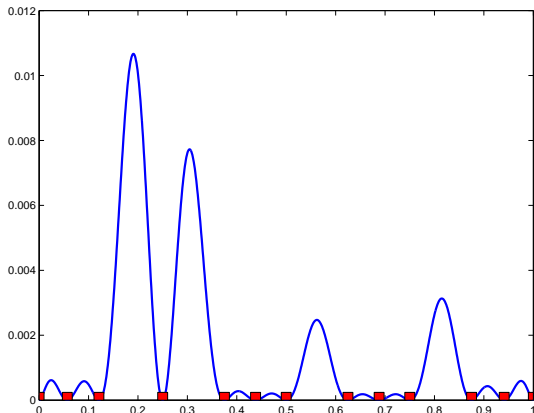
2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_{13}(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

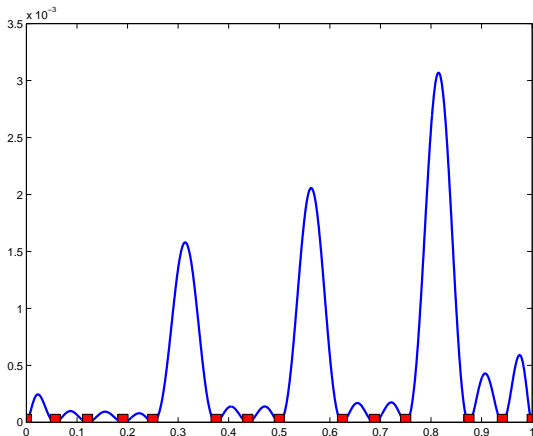
1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

$\rho_{14}(x)$



$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

Luc Pronzato

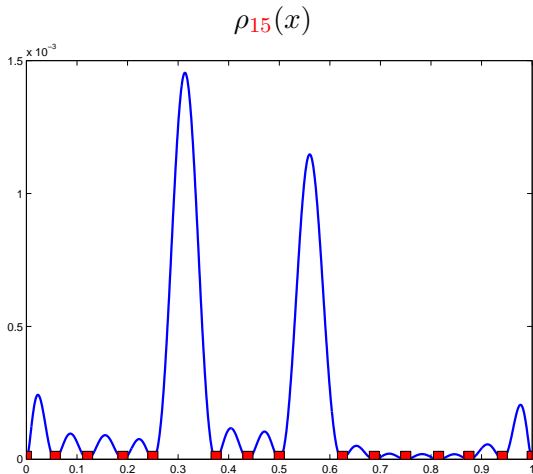
Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions



$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

Luc Pronzato

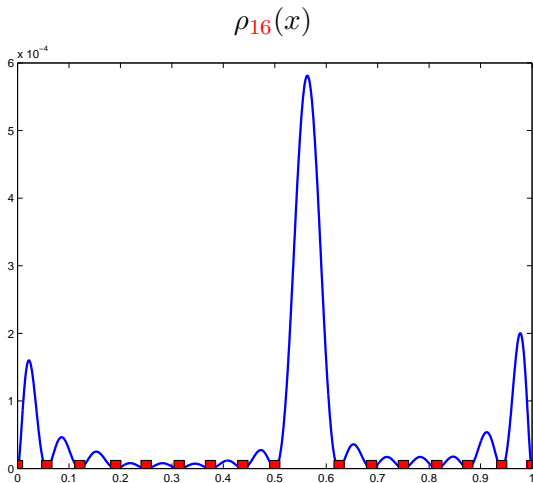
Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

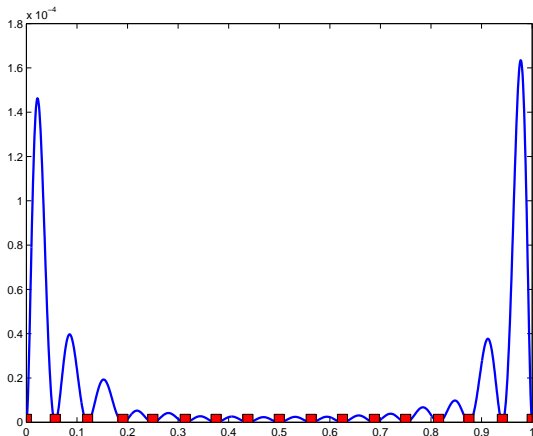
3 Beyond
space filling

4 Conclusions



$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \quad (\text{initialized with } \mathbf{X}_n, n \text{ small})$$

$\rho_{17}(x)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Irregularities in $\rho_k(x)$ are difficult to avoid \rightarrow related to a property of low discrepancy sequences:

\mathbf{X}_{mM}^* miniMax optimal ($x_i = (2i - 1)/(2n)$) minimizes
 $\mathcal{D}(\mathbf{X}) = \max_{x \in \mathbf{X}} |F_n(x) - U(x)|$ ($U(\cdot)$ = cdf of the
 uniform distribution, $F_n(\cdot)$ empirical cdf for \mathbf{X}) and
 $\mathcal{D}(\mathbf{X}_{mM}^*) = 1/(2n)$

but $\mathcal{D}(x_1, x_2, \dots, x_n) \geq 0.06 \log(n)/n$ for any *sequence*
 of n points

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- [Vazquez & Bect, 2011]

$\rho_n(x) = \sup_{f \in \mathcal{H}_1} |f(x) - \eta_n[f](x)|^2$, with \mathcal{H}_1 the unit ball of the RKHS \mathcal{H} of functions generated by

$$k(u, v) = C((u - v); \theta)$$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- [Vazquez & Bect, 2011]
 $\rho_n(x) = \sup_{f \in \mathcal{H}_1} |f(x) - \eta_n[f](x)|^2$, with \mathcal{H}_1 the unit ball of the RKHS \mathcal{H} of functions generated by
 $k(u, v) = C((u - v); \theta)$
- [Vazquez & Bect, 2011] If $t \mapsto C(t; \theta)$ has a Fourier transform $\tilde{C}(u) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} C(t; \theta) e^{i(t, u)} dt$ satisfying
 $c_1(1 + \|u\|_2^2)^{-s} \leq \tilde{C}(u) \leq c_2(1 + \|u\|_2^2)^{-s}$, $u \in \mathbb{R}^d$
 with $s > d/2$, $0 < c_1 \leq c_2$, then,

$$x_{k+1} = \arg \max_{x \in \mathcal{X}} \rho_k(x) \Rightarrow \sup_{x \in \mathcal{X}} \rho_n(x) = \mathcal{O}(n^{1-2s/d})$$

— same rate as for non-sequential construction —

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Comparison with non-parametric estimation with i.i.d. additive errors [Tsybakov, 2004]:
 - $\sup_{f \in \Sigma(L, \alpha)} \mathbb{E} \|f - \eta_n[f]\|_2^2 = \mathcal{O}(n^{-2\alpha/(2\alpha+d)})$
 ($\Sigma(L, \alpha)$ = Hölder smooth, $\mathbb{E} \leftrightarrow$ presence of random errors)
 = best achievable rate for passive (non-sequential) or active (sequential) constructions [Castro, Willett, Nowak, 2005]

- Comparison with non-parametric estimation with i.i.d. additive errors [Tsybakov, 2004]:
 - $\sup_{f \in \Sigma(L, \alpha)} \mathbb{E} \|f - \eta_n[f]\|_2^2 = \mathcal{O}(n^{-2\alpha/(2\alpha+d)})$
 ($\Sigma(L, \alpha)$ = Hölder smooth, $\mathbb{E} \leftrightarrow$ presence of random errors)
 = best achievable rate for passive (non-sequential) or active (sequential) constructions [Castro, Willett, Nowak, 2005]
 - [different for piecewise smooth functions: [Castro, Willett, Nowak, 2005]
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/d}\})$ for passive construction
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/(d-1)}\})$ for active construction
 — not important for α small, some effect when f is regular enough]

- Comparison with non-parametric estimation with i.i.d. additive errors [Tsybakov, 2004]:
 - $\sup_{f \in \Sigma(L, \alpha)} \mathbb{E} \|f - \eta_n[f]\|_2^2 = \mathcal{O}(n^{-2\alpha/(2\alpha+d)})$
 ($\Sigma(L, \alpha)$ = Hölder smooth, $\mathbb{E} \leftrightarrow$ presence of random errors)
 = best achievable rate for passive (non-sequential) or active (sequential) constructions [Castro, Willett, Nowak, 2005]
 - [different for piecewise smooth functions: [Castro, Willett, Nowak, 2005]
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/d}\})$ for passive construction
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/(d-1)}\})$ for active construction
 — not important for α small, some effect when f is regular enough]
- But sequential construction is useful when objective = optimization, inversion, estimation of failure prob.

- Comparison with non-parametric estimation with i.i.d. additive errors [Tsybakov, 2004]:
 - $\sup_{f \in \Sigma(L, \alpha)} \mathbb{E} \|f - \eta_n[f]\|_2^2 = \mathcal{O}(n^{-2\alpha/(2\alpha+d)})$
 ($\Sigma(L, \alpha)$ = Hölder smooth, $\mathbb{E} \leftrightarrow$ presence of random errors)
 = best achievable rate for passive (non-sequential) or active (sequential) constructions [Castro, Willett, Nowak, 2005]
 - [different for piecewise smooth functions: [Castro, Willett, Nowak, 2005]
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/d}\})$ for passive construction
 $\mathcal{O}(\max\{n^{-2\alpha/(2\alpha+d)}, n^{-1/(d-1)}\})$ for active construction
 — not important for α small, some effect when f is regular enough]
- But sequential construction is useful when objective = optimization, inversion, estimation of failure prob.
- Importance of asymptotic statements? (how large n should be?)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin3 Beyond
space filling

4 Conclusions

→ We must estimate θ from the same data as those use to construct $\eta_n(x)$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

→ We must estimate θ from the same data as those use to construct $\eta_n(x)$

→ Maximum likelihood estimator $\hat{\theta}^n$
($Z(x, \omega)$ is Gaussian)

→ corrective term [Harville & Jeske, 1992; Abt 1999]:

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

where:

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

$\mathbf{M}_\theta =$ Fisher information matrix for θ

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

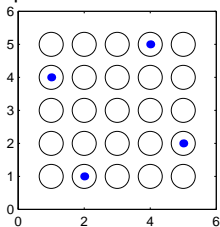
2 Regularized
Maximin

3 Beyond
space filling

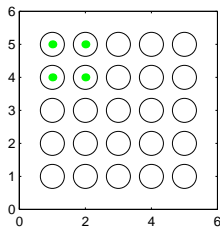
4 Conclusions

$\mathbb{E}\{Z(x, \omega)Z(u, \omega)\} = \sigma^2\theta^{\|x-u\|}$, $\theta = 0.3$ (σ^2 known),
 \mathcal{X} = regular grid 5×5

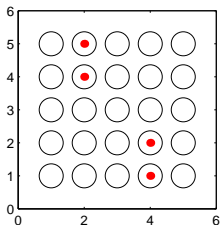
prediction for θ known



estimation of θ



prediction with θ estimated



prediction for θ known:

\mathbf{X}_4 minimizes $\max_{x \in \mathcal{X}} \rho_4(x)$

estimation of θ :

\mathbf{X}_4 maximizes $\det \mathbf{M}_\theta$

prediction with θ estimated:

\mathbf{X}_4 minimizes $\max_{x \in \mathcal{X}} \hat{\rho}_4(x; \theta)$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

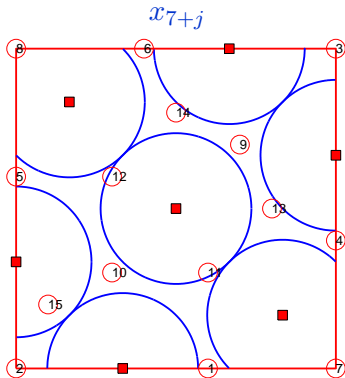
2 Regularized
Maximin

3 Beyond
space filling

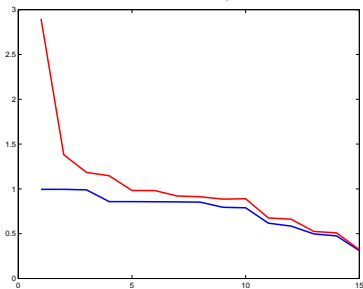
4 Conclusions

$d = 2$, $C(t; \theta) = \exp(-\theta \|t\|_2)$, $\theta = 0.7$, $\mathbf{X}_7 = \text{Mm Lh}$, then

$x_{7+j} = \arg \max_{x \in \mathcal{X}} \hat{\rho}_{7+j-1}(x; \theta)$, $j = 1, 2, \dots$



$\max_{x \in \mathcal{X}} \rho_{7+j}(x; \theta)$ and
 $\max_{x \in \mathcal{X}} \hat{\rho}_{7+j}(x; \theta)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

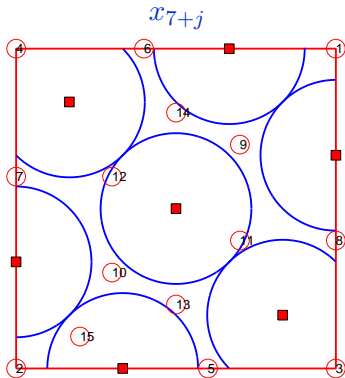
2 Regularized
Maximin

3 Beyond
space filling

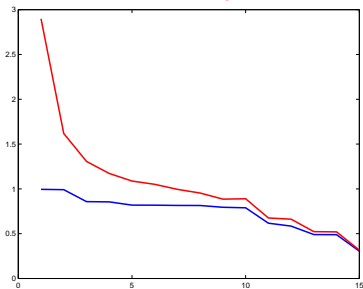
4 Conclusions

$d = 2$, $C(t; \theta) = \exp(-\theta \|t\|_2)$, $\theta = 0.7$, $\mathbf{X}_7 = \text{Mm Lh}$, then

$x_{7+j} = \arg \max_{x \in \mathcal{X}} \rho_{7+j-1}(x; \theta)$, $j = 1, 2, \dots$



$\max_{x \in \mathcal{X}} \rho_{7+j}(x; \theta)$ and
 $\max_{x \in \mathcal{X}} \hat{\rho}_{7+j}(x; \theta)$



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

Choosing \mathbf{X}_n that minimizes $\max_{x \in \mathcal{X}} \hat{\rho}_n(x; \theta)$ is difficult

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

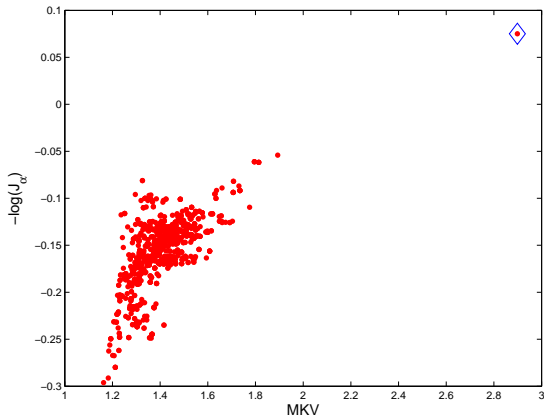
Choosing \mathbf{X}_n that minimizes $\max_{x \in \mathcal{X}} \hat{\rho}_n(x; \theta)$ is difficult

→ Use a criterion that makes compromise between space filling and clustering, e.g., choose \mathbf{X}_n that maximizes $\gamma \log \det(\mathbf{M}_\beta) + (1 - \gamma) \log \det(\mathbf{M}_\theta)$ [Müller et al., 2010, 2011], with

- \mathbf{M}_β = FIM for trend parameters (maximization → space filling)
- \mathbf{M}_θ = FIM for correlation parameters (maximization → clustering)

Example: $n = 7$, $d = 2$, $C(t; \theta) = \exp(-\theta \|t\|_2)$, $\theta = 0.7$,
 1000 Lh (999 random + \diamond for Mm optimal)

$MKV = \max_{x \in \mathcal{X}} \hat{\rho}_n(x; \theta)$, $J_\alpha = \det^\alpha(\mathbf{M}_\beta) + \det^{1-\alpha}(\mathbf{M}_\theta)$
 ($\alpha = 0.8$)



Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Only considered design for approximation/interpolation

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Only considered design for approximation/interpolation
- Nothing on algorithms (heuristics — genetic, taboo search, SA —, MCMC — spatial point process —, local search)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Only considered design for approximation/interpolation
- Nothing on algorithms (heuristics — genetic, taboo search, SA —, MCMC — spatial point process —, local search)
- Nothing on Bayesian methods:
 - Karhunen-Loève representation + Bayesian optimal design [Fedorov & Müller, 2007]
 - Maximum Entropy Sampling [Shewry & Wynn, 1987; Wynn & Youssef, 2011] (with substitution of INLA for MCMC to compute posterior means?)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Basic guidelines:
 - Precision of the construction (\leftrightarrow final objective) for a given horizon n ?
(IE or worst-case) — e.g., $\max_{x \in \mathcal{X}} \rho_n(x)$
 - \rightarrow design criterion

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Basic guidelines:
 - Precision of the construction (\leftrightarrow final objective) for a given horizon n ?
(\mathbb{E} or worst-case) — e.g., $\max_{x \in \mathcal{X}} \rho_n(x)$
 - \rightarrow design criterion
 - ... taking all sources of uncertainty into account
(estimation of parameters, simulations with variable precision...) — e.g., $\max_{x \in \mathcal{X}} \hat{\rho}_n(x)$

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Basic guidelines:
 - Precision of the construction (\leftrightarrow final objective) for a given horizon n ?
(\mathbb{E} or worst-case) — e.g., $\max_{x \in \mathcal{X}} \rho_n(x)$
 - \rightarrow design criterion
 - ... taking all sources of uncertainty into account
(estimation of parameters, simulations with variable precision...) — e.g., $\max_{x \in \mathcal{X}} \hat{\rho}_n(x)$
 - Some constraints may exist on real physical experiments
(e.g., dynamical constraints \rightarrow mobile sensors)

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Basic guidelines:
 - Precision of the construction (\leftrightarrow final objective) for a given horizon n ?
(\mathbb{E} or worst-case) — e.g., $\max_{x \in \mathcal{X}} \rho_n(x)$
 - \rightarrow design criterion
 - ... taking all sources of uncertainty into account
(estimation of parameters, simulations with variable precision...) — e.g., $\max_{x \in \mathcal{X}} \hat{\rho}_n(x)$
 - Some constraints may exist on real physical experiments
(e.g., dynamical constraints \rightarrow mobile sensors)
- Only simplest rules and constructions will be used!

Luc Pronzato

Workshop de
clôture ANR
OPUS
21/10/2011

1 Space-filling

2 Regularized
Maximin

3 Beyond
space filling

4 Conclusions

- Basic guidelines:
 - Precision of the construction (\leftrightarrow final objective) for a given horizon n ?
(\mathbb{E} or worst-case) — e.g., $\max_{x \in \mathcal{X}} \rho_n(x)$
 - \rightarrow design criterion
 - ... taking all sources of uncertainty into account
(estimation of parameters, simulations with variable precision...) — e.g., $\max_{x \in \mathcal{X}} \hat{\rho}_n(x)$
 - Some constraints may exist on real physical experiments
(e.g., dynamical constraints \rightarrow mobile sensors)
- Only simplest rules and constructions will be used!

Thank you for your attention!