Maximum Mean Discrepancy, Bayesian integration and kernel herding for space-filling design

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1 Space-filling design

Objective: approximate $f(\cdot)$ over $\mathscr{X}$ (a compact subset of $\mathbb{R}^d$)
using pairs $(\mathbf{x}_i, f(\mathbf{x}_i))$, $i = 1, 2, \ldots, n$ $\rightarrow$ observe "everywhere"

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

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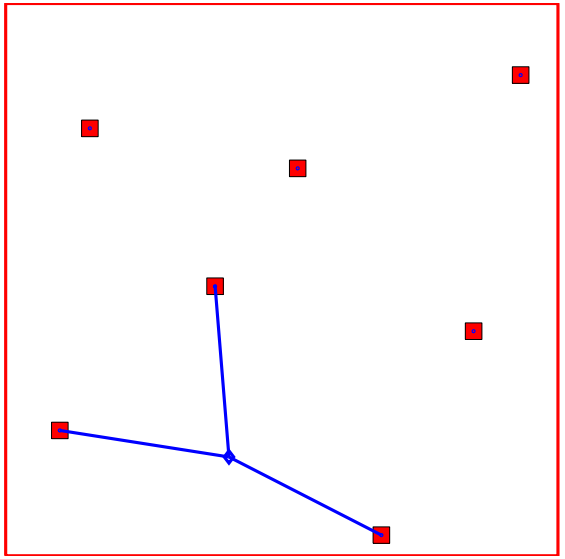
Design $\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$

Covering radius $\mathrm{CR}(\mathbf{X}_n) \triangleq \max_{\mathbf{x} \in \mathscr{X}} \min_{\mathbf{x}_i} \|\mathbf{x} - \mathbf{x}_i\|$

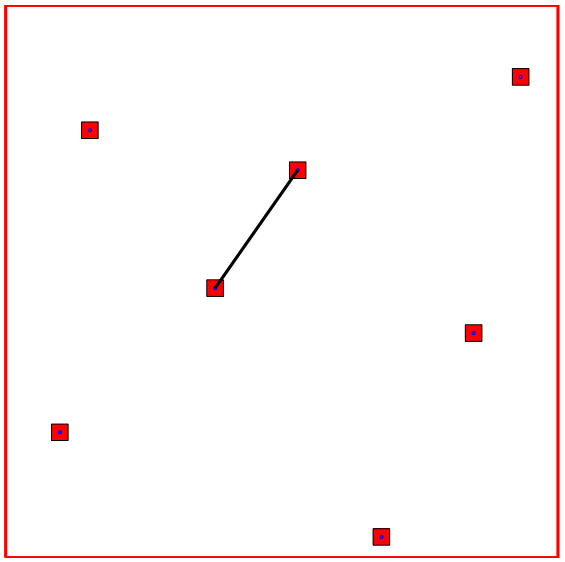
$\mathrm{CR}(\mathbf{X}_n)$ = fill distance = dispersion = miniMax distance criterion



⟶ we are never far from a design point

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

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

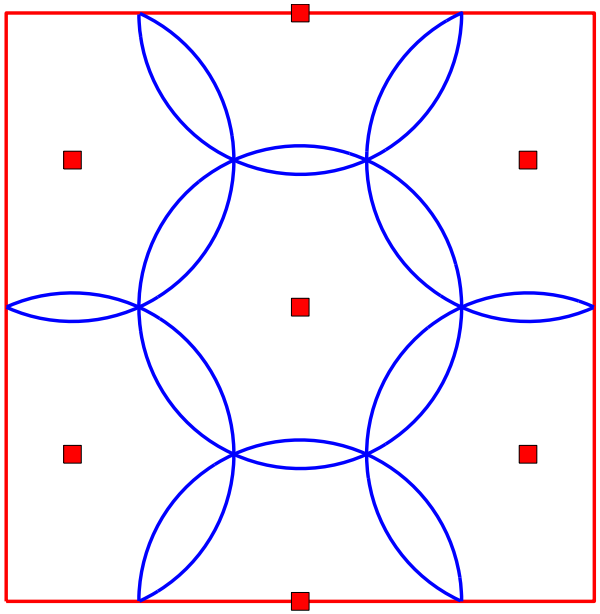


→ easier to compute, but pushes points to the boundary of $\mathscr{X}$

Examples:

① Covering, miniMax

$d = 2, n = 7$ (radius=CR($\mathbf{X}_n$))



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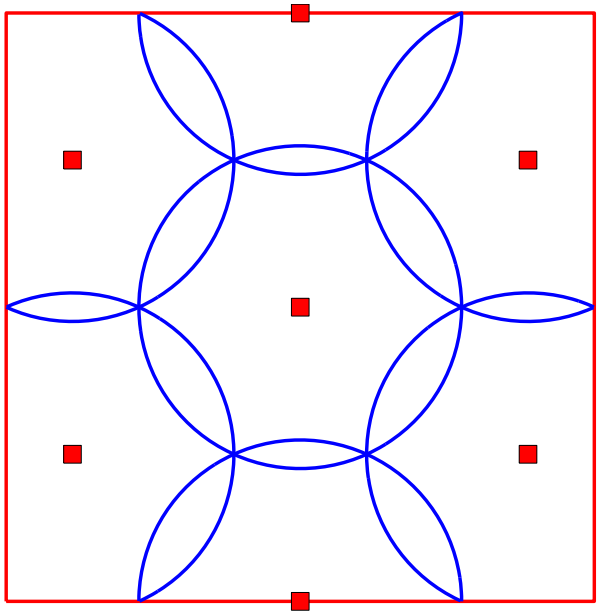
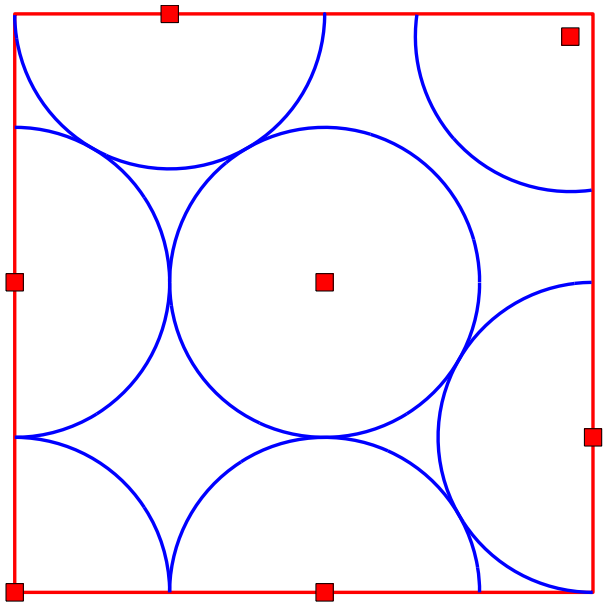


② Packing, Maximin

$d = 2, n = 7$ (radius=P($\mathbf{X}_n$))



→ Minimising CR is preferable to maximising PR; both are difficult

Bounds on approximation error are related to CR:

$$\|\text{error}\|_{L_\infty(\mathscr{X})} \leq \text{CR}(\mathbf{X}_n)^{\alpha - d/2} \text{ when } f \in \text{Sobolev space } W_2^\alpha(\mathscr{X})$$

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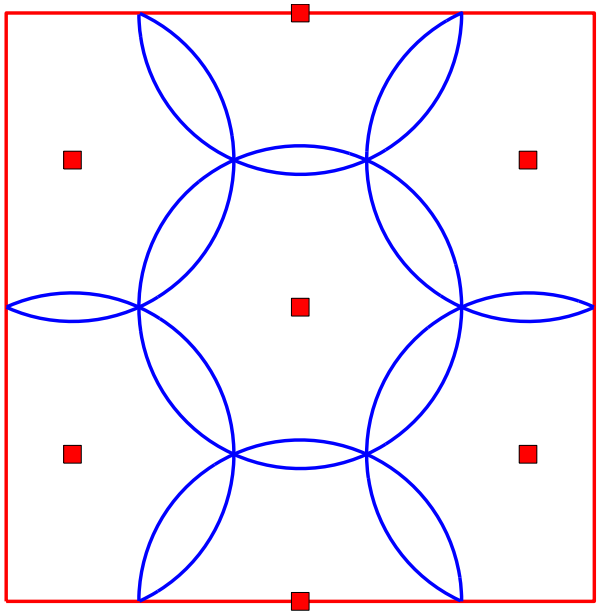

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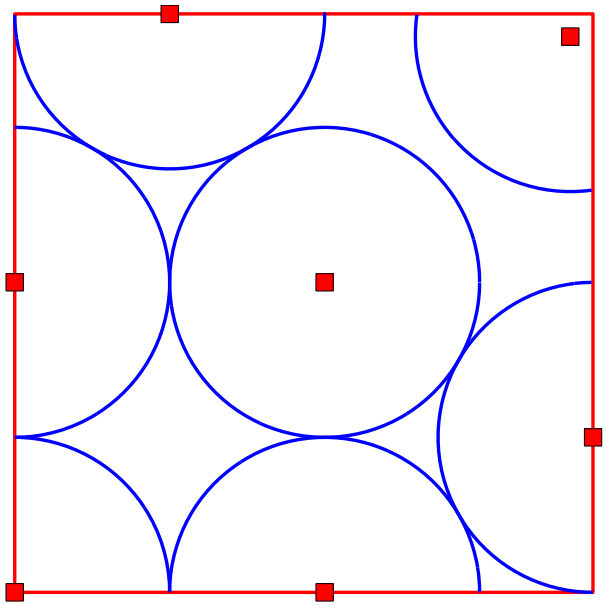

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Any-time design: good-space-filling properties for $\mathbf{X}_k \subset \mathbf{X}_{k+1} \subset \mathbf{X}_{k+3} \subset \ldots$?

Can we apply a greedy gradient-type descent algorithm to a suitable criterion?

2 Bayesian integration

Notation:

- $\mathscr{M} = \mathscr{M}[\mathscr{X}]$ set of finite signed Borel measures on $\mathscr{X}$
- $\mathscr{M}(\alpha) = \{\mu \in \mathscr{M} : \mu(\mathscr{X}) = \alpha\}$ (signed measures with total mass $\alpha \in \mathbb{R}$)
- $\mathscr{M}^+$ positive measures in $\mathscr{M}$
- $\mathscr{M}^+(1)$ probability measures on $\mathscr{X}$

Objective: integrate f with respect to $\mu \in \mathscr{M}^+(1)$

$\rightarrow$ estimate $\boxed{I_\mu(f) = \mathsf{E}_\mu\{f(\mathbf{X})\} \triangleq \int_{\mathscr{X}} f(\mathbf{x})\,\mathrm{d}\mu(\mathbf{x})}$

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Suppose $\boxed{f(\mathbf{x}) = \beta + Z_x}$, with Z_x a Gaussian RF,
$\mathbb{E}\{Z_x\} = 0$ and $\mathbb{E}\{Z_x Z_{x'}\} = \sigma^2\, K(\mathbf{x}, \mathbf{x}')$
and a vague prior on β ($\sim \mathcal{N}(0, \sigma^2\, A)$ with $A \to +\infty$)

(K symmetric positive definite $\rightarrow$ defines a RKHS $\mathcal{H}_K$)

$\rightarrow$ observe f at $\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$

Bayesian integration of f:

Denote $\mathbf{1}_n = (1, \ldots, 1)^T$, $\mathbf{y}_n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))^T$, $\{\mathbf{K}_n\}_{i,j} = K(\mathbf{x}_i, \mathbf{x}_j)$,

$$P_\mu(\mathbf{x}) \triangleq \int_{\mathscr{X}} K(\mathbf{x}, \mathbf{x}')\, \mathrm{d}\mu(\mathbf{x}') \text{ (= kernel imbedding of } \mu \text{ into } \mathcal{H}_K)$$

$$\mathscr{E}_K(\mu) \triangleq \int_{\mathscr{X}^2} K(\mathbf{x}, \mathbf{x}')\, \mathrm{d}\mu(\mathbf{x}) \mathrm{d}\mu(\mathbf{x}') \text{ (= energy of } \mu)$$

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$I_\mu(f)$ has the normal posterior $\mathcal{N}(\widehat{I}_n, \sigma^2 s_n^2)$ (O'Hagan, 1991)

$$\begin{aligned} \widehat{I}_n &= \hat{\beta}^n + \mathbf{p}_n(\mu)^T \mathbf{K}_n^{-1}(\mathbf{y}_n - \hat{\beta}^n \mathbf{1}_n) \\ &= \hat{\mathbf{w}}_n^T \mathbf{y}_n \quad \text{(the estimation is linear)} \\ s_n^2 &= \mathscr{E}_K(\mu) - \mathbf{p}_n^T(\mu) \mathbf{K}_n^{-1} \mathbf{p}_n(\mu) + \frac{(1 - \mathbf{p}_n^T(\mu) \mathbf{K}_n^{-1} \mathbf{1}_n)^2}{\mathbf{1}_n^T \mathbf{K}_n^{-1} \mathbf{1}_n} \end{aligned}$$

where $\hat{\beta}^n = \dfrac{\mathbf{1}_n^T \mathbf{K}_n^{-1} \mathbf{y}_n}{\mathbf{1}_n^T \mathbf{K}_n^{-1} \mathbf{1}_n}$ (= BLUE) and $\mathbf{p}_n(\mu) = (P_\mu(\mathbf{x}_1), \ldots, P_\mu(\mathbf{x}_n))^T$

The approximation of $f(\mathbf{x}_0)$ is a particular case!

Take $\mu = \delta_{\mathbf{x}_0}$ → $\boxed{P_\mu(\mathbf{x}) = K(\mathbf{x}, \mathbf{x}_0),\ \mathscr{E}_K(\mu) = K(\mathbf{x}_0, \mathbf{x}_0)}$

and $f(\mathbf{x}_0)$ has the normal posterior $\mathcal{N}(\hat{\eta}_n(\mathbf{x}_0), \sigma^2\, \rho_n^2(\mathbf{x}_0))$ with

$$\begin{aligned}
\hat{\eta}_n(\mathbf{x}_0) &= \hat{\beta}^n + \mathbf{k}_n^T(\mathbf{x}_0)\mathbf{K}_n^{-1}(\mathbf{y}_n - \hat{\beta}^n \mathbf{1}_n) \\
\rho_n^2(\mathbf{x}_0) &= K(\mathbf{x}_0, \mathbf{x}_0) - \mathbf{k}_n^T(\mathbf{x}_0)\mathbf{K}_n^{-1}\mathbf{k}_n(\mathbf{x}_0) + \frac{(1 - \mathbf{k}_n^T(\mathbf{x}_0)\mathbf{K}_n^{-1}\mathbf{1}_n)^2}{\mathbf{1}_n^T\mathbf{K}_n^{-1}\mathbf{1}_n}
\end{aligned}$$

where $\{\mathbf{k}_n(\mathbf{x})\}_i = K(\mathbf{x}, \mathbf{x}_i)$

$\equiv$ ordinary kriging

→ minimise $\boxed{\mathrm{IMSPE}(\mathbf{X}_n) = \sigma^2 \int_{\mathscr{X}} \rho_n^2(\mathbf{x})\, \mathrm{d}\mu(\mathbf{x})}$

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➞ minimise $\boxed{\mathrm{IMSPE}(\mathbf{X}_n) = \sigma^2 \int_{\mathscr{X}} \rho_n^2(\mathbf{x})\, \mathrm{d}\mu(\mathbf{x})}$

➠ For $\underline{\mu \text{ uniform on } \mathscr{X}}$, a design minimising s_n^2 should be well spread

➠ Minimise $s_n^2 = \mathscr{E}_K(\mu) - \mathbf{p}_n^T(\mu)\mathbf{K}_n^{-1}\mathbf{p}_n(\mu) + \frac{(1-\mathbf{p}_n^T(\mu)\mathbf{K}_n^{-1}\mathbf{1}_n)^2}{\mathbf{1}_n^T\mathbf{K}_n^{-1}\mathbf{1}_n}$

instead of $\int_{\mathscr{X}} \rho_n^2(\mathbf{x})\, \mathrm{d}\mu(\mathbf{x})$ for space-filling design?

3 Kernel discrepancy, energy & potentials

Very much based on:

Damelin, S., Hickernell, F., Ragozin, D., Zeng, X., 2010. On energy, discrepancy and group invariant measures on measurable subsets of Euclidean space. *J. Fourier Anal. Appl.* 16, 813–839.

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For ν a signed measure,

$$\mathscr{E}_K(\nu) \triangleq \int_{\mathscr{X}^2} K(\mathbf{x},\mathbf{x}')\,\mathrm{d}\nu(\mathbf{x})\mathrm{d}\nu(\mathbf{x}') = \text{energy of } \nu$$

$$P_\nu(\mathbf{x}) \triangleq \int_{\mathscr{X}} K(\mathbf{x},\mathbf{x}')\,\mathrm{d}\nu(\mathbf{x}') = \text{potential of } \nu \text{ at } \mathbf{x}$$

$$[P_\nu(\cdot) = \text{kernel imbedding of } \nu \text{ into } \mathcal{H}_K]$$

Suppose $\underline{f \in \mathcal{H}_K}$, μ, ν prob. measures with finite energy

$K_{\mathbf{x}}(\cdot) = K(\mathbf{x}, \cdot)$, reproducing property $f(\mathbf{x}) = \langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}_K} \quad \Rightarrow$

$$|I_\mu(f) - I_\nu(f)| = \left| \int_{\mathscr{X}} \langle f, K_{\mathbf{x}} \rangle_{\mathcal{H}_K} \, \mathrm{d}(\mu - \nu)(\mathbf{x}) \right| = |\langle f, P_\mu - P_\nu \rangle_{\mathcal{H}_K}|$$

CS inequality ➞ a Koksma-Hlawka type inequality:

$$\left| \int_{\mathscr{X}} f(\mathbf{x}) \, \mathrm{d}\nu(\mathbf{x}) - \int_{\mathscr{X}} f(\mathbf{x}) \, \mathrm{d}\mu(\mathbf{x}) \right| \leq \|f\|_{\mathcal{H}_K} \gamma_K(\mu, \nu)$$

where $\boxed{\gamma_K^2(\mu, \nu) \triangleq \|P_\mu - P_\nu\|_{\mathcal{H}_K}^2 = \mathscr{E}_K(\nu - \mu)}$

$\gamma_K(\mu, \nu) = \sup_{\|f\|_{\mathcal{H}_K} = 1} |\int_{\mathscr{X}} f(\mathbf{x}) \, \mathrm{d}\nu(\mathbf{x}) - \int_{\mathscr{X}} f(\mathbf{x}) \, \mathrm{d}\mu(\mathbf{x})|$

$=$ **Maximum Mean Discrepancy** between (MMD) μ and ν

(Sriperumbudur et al., 2010; Sejdinovic et al., 2013)

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Space-filling design: take μ uniform on $\mathscr{X}$

➞ find ξ_n (with n support points) minimising $\mathscr{E}_K(\xi_n - \mu) = \mathrm{MMD}^2(\xi_n, \mu)$

$\gamma_K(\cdot,\cdot)$ defines a pseudo-metric on $\mathscr{M}^+(1)$
Does it define a metric? ($\Leftrightarrow$ K is **characteristic**)

Definition

K is Integrally Strictly Positive Definite (ISPD) on $\mathscr{M}$ when $\mathscr{E}_K(\nu) > 0$ for any nonzero $\nu \in \mathscr{M}$

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Sriperumbudur et al. (2010):

- K bounded & ISPD $\Rightarrow$ K is strictly positive definite
  ($\rightarrow$ defines a RKHS $\mathcal{H}_K$)
- if K uniformly bounded: characteristic $\Leftrightarrow$ CISPD

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- Spectral interpretation (Sriperumbudur et al., 2010):
  if K translation invariant, $K(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x} - \mathbf{x}')$, with ψ bounded, continuous, pos. def., $\psi(\mathbf{x}) = \int_{\mathbb{R}^d} e^{-i\mathbf{x}^T\boldsymbol{\omega}} \, \mathrm{d}\Lambda(\boldsymbol{\omega})$ (Bochner)

  $\gamma_K(\mu, \nu) = L_2$ distance between characteristic functions of μ and ν:

$$\gamma_K(\mu, \nu) = \left[\int_{\mathbb{R}^d} |\Phi_\mu(\boldsymbol{\omega}) - \Phi_\nu(\boldsymbol{\omega})|^2 \, \mathrm{d}\Lambda(\boldsymbol{\omega}) \right]^{1/2}$$

  K characteristic $\Leftrightarrow$ Λ supported on $\mathbb{R}^d$
  (for example, Matérn kernels)

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Examples:

- Matérn kernels, e.g., $K_{1/2,\theta}(\mathbf{x},\mathbf{x}') = \exp(-\theta\,\|\mathbf{x}-\mathbf{x}'\|)$,

$$\begin{aligned} K_{3/2,\theta}(\mathbf{x},\mathbf{x}') &= (1+\sqrt{3}\theta\,\|\mathbf{x}-\mathbf{x}'\|)\,\exp(-\sqrt{3}\theta\,\|\mathbf{x}-\mathbf{x}'\|) \\ K_{5/2,\theta}(\mathbf{x},\mathbf{x}') &= [1+\sqrt{5}\theta\,\|\mathbf{x}-\mathbf{x}'\|+5\theta^2\,\|\mathbf{x}-\mathbf{x}'\|^2/3]\,\exp(-\sqrt{5}\theta\,\|\mathbf{x}-\mathbf{x}'\|) \\ &\ldots \end{aligned}$$

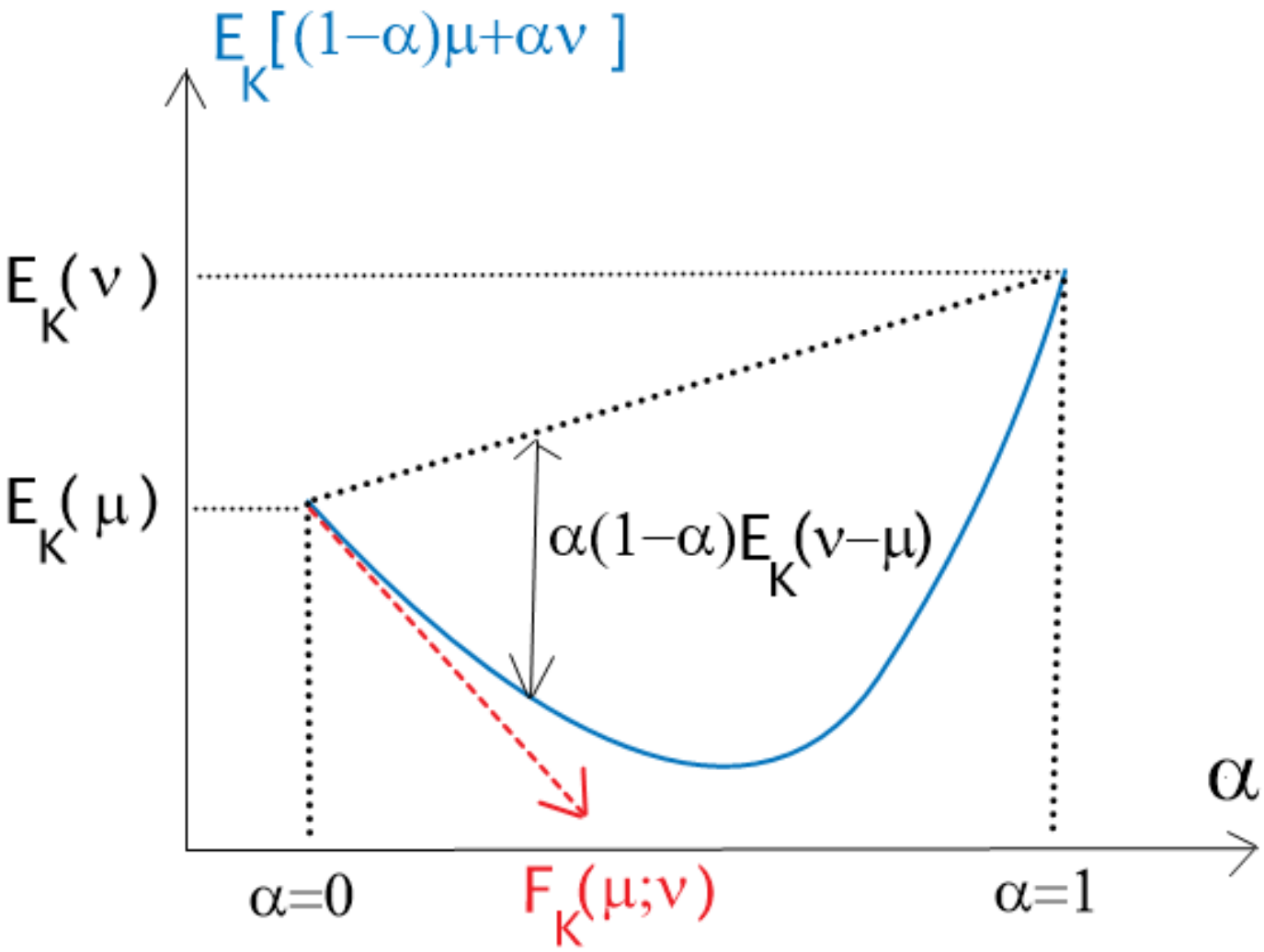
- distance-induced kernels (→ energy distance of Székely and Rizzo (2013)):

$$K'_{(s)}(\mathbf{x},\mathbf{x}') = \|\mathbf{x}\|^s + \|\mathbf{x}'\|^s - \|\mathbf{x}-\mathbf{x}'\|^s\,,\ 0<s<2$$

- Riesz kernels (unbounded):

$$K_{(s)}(\mathbf{x},\mathbf{x}') = \|\mathbf{x}-\mathbf{x}'\|^{-s}\,,\ s\in(0,d),\ K_{(0)}(\mathbf{x},\mathbf{x}') = -\log\|\mathbf{x}-\mathbf{x}'\|$$

- ...


$E_K[(1-\alpha)\mu+\alpha\nu]$
$E_K(\nu)$
$E_K(\mu)$
$\alpha(1-\alpha)E_K(\nu-\mu)$
α
$\alpha=0$
$F_K(\mu;\nu)$
$\alpha=1$

For $\alpha \in (0,1)$, $\mu, \nu \in \mathscr{M}$:

$$\boxed{(1-\alpha)\,\mathscr{E}_K(\mu) + \alpha\,\mathscr{E}_K(\nu) - \mathscr{E}_K[(1-\alpha)\mu + \alpha\nu] = \alpha(1-\alpha)\,\mathscr{E}_K(\nu - \mu)}$$

- K ISPD $\Leftrightarrow$ $\mathscr{E}_K(\cdot)$ strictly convex on $\mathscr{M}$
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<u>Directional derivative</u> of $\mathscr{E}_K(\cdot)$ at μ in the direction ν:

$$\begin{aligned} F_K(\mu;\nu) &= \lim_{\alpha \to 0^+} \frac{\mathscr{E}_K[(1-\alpha)\mu + \alpha\nu] - \mathscr{E}_K(\mu)}{\alpha} \\ &= 2\left[\int_{\mathscr{X}^2} K(\mathbf{x},\mathbf{x}')\,\mathrm{d}\nu(\mathbf{x})\mathrm{d}\mu(\mathbf{x}') - \mathscr{E}_K(\mu)\right] \end{aligned}$$

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$\Rightarrow$ $F_K(\mu;\delta_{\mathbf{x}})$ is related to the potential $P_\mu(\mathbf{x})$:

$$\boxed{P_\mu(\mathbf{x}) = \tfrac{1}{2}\,F_K(\mu;\delta_{\mathbf{x}}) + \mathscr{E}_K(\mu)}$$

Suppose $\mathscr{X}$ compact

Theorem (Equivalence theorem in DOE)

If $\mathscr{E}_K(\cdot)$ strictly convex on $\mathscr{M}^+(1)$, $\mu_K^* \in \mathscr{M}^+(1)$ is the minimum-energy probability measure on $\mathscr{X}$ iff $\forall\, \mathbf{x} \in \mathscr{X}$, $P_{\mu_K^*}(\mathbf{x}) \geq \mathscr{E}_K(\mu_K^*)$; moreover, $P_{\mu_K^*}(\mathbf{x}) = \mathscr{E}_K(\mu_K^*)$ on the support of μ_K^*

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Potential theory (K singular, ISPD):

$$\mu_K^* \in \mathscr{M}^+(1) = \textit{equilibrium measure} \text{ of } \mathscr{X}$$
$$C_K = [\inf_{\mu \in \mathscr{M}^+(1)} \mathscr{E}_K(\mu)]^{-1} \geq 0 = \textit{capacity} \text{ of } \mathscr{X}$$

Consider now (signed) measures in $\mathscr{M}(1)$

Theorem

If $\mathscr{E}_K(\cdot)$ strictly convex on $\mathscr{M}(1)$, $\widetilde{\mu}_K^* \in \mathscr{M}(1)$ is the minimum-energy signed measure on $\mathscr{X}$ with total charge 1 iff $\forall\, \mathbf{x} \in \mathscr{X}$, $P_{\widetilde{\mu}_K^*}(\mathbf{x}) = \mathscr{E}_K(\widetilde{\mu}_K^*)$

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. . . but $\widetilde{\mu}_K^*$ does not always exist!

When minimum-energy signed measures are probability measures?

Theorem

Assume that K is ISPD and translation invariant, with $K(\mathbf{x}, \mathbf{x}') = \Psi(\mathbf{x} - \mathbf{x}')$ and Ψ continuous, twice differentiable except at the origin, with Laplacian $\Delta_\Psi(\mathbf{x}) = \sum_{i=1}^d \partial^2 \Psi(\mathbf{x}) / \partial x_i^2 \geq 0$, $\mathbf{x} \neq \mathbf{0}$. Then there exists a unique $\widetilde{\mu}_K^*$ in $\mathscr{M}(1)$, and $\widetilde{\mu}_K^* \in \mathscr{M}^+(1)$

(Generalises (Hájek, 1956) to $d > 1$, but $\Psi(\cdot)$ must have a singularity at zero.)

minimise $\mathscr{E}_K(\xi - \mu)$=MMD$^2(\xi, \mu)$

Relation with (continuous) BLUE of β in $\boxed{f(\mathbf{x}) = \beta + Z_x}$

with Z_x a Gaussian RF ($\mathbb{E}\{Z_x\} = 0$, $\mathbb{E}\{Z_x Z_{x'}\} = \sigma^2 K(\mathbf{x}, \mathbf{x}')$)
Näther (1985, Sect. 4.2):

- Any linear estimator of β: $\hat{\beta} = \hat{\beta}(\xi) = \int_{\mathscr{X}} f(\mathbf{x})\, \mathrm{d}\xi(\mathbf{x})$, $\xi \in \mathscr{M}$
- $\hat{\beta}(\xi)$ unbiased: $\xi \in \mathscr{M}(1)$
- Variance: $V_\xi = \mathbb{E}\{(\hat{\beta}(\xi) - \beta)^2\} = \sigma^2\, \mathscr{E}_K(\xi)$

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$\rightarrow$ Existence of a minimum-energy signed measure $\widetilde{\mu}_K^* \in \mathscr{M}(1)$
$\Leftrightarrow$ existence of the BLUE $\hat{\beta}^* = \hat{\beta}(\widetilde{\mu}_K^*)$, with variance $\sigma^2\, \mathscr{E}_K(\widetilde{\mu}_K^*)$

(The property $[\forall\, \mathbf{x} \in \mathscr{X}\ ,\ P_{\widetilde{\mu}_K^*}(\mathbf{x}) = \mathscr{E}_K(\widetilde{\mu}_K^*)]$ corresponds to Wiener-Hopf equation in Grenander's theorem (1950)).

We do not want to minimise $\mathscr{E}_K(\nu)$ but $\mathscr{E}_K(\xi-\mu)$=$\mathrm{MMD}^2(\xi,\mu)$
for a given μ

Kernel reduction

Damelin et al. (2010): for μ with total mass 1, consider the kernel

$$\boxed{\widetilde{K}_\mu(\mathbf{x},\mathbf{x}') \triangleq K(\mathbf{x},\mathbf{x}') - P_\mu(\mathbf{x}) - P_\mu(\mathbf{x}') + \mathscr{E}_K(\mu)}$$

- $\forall\,\xi$ with total mass 1 , $\boxed{\underbrace{\mathscr{E}_K(\xi-\mu)}_{\gamma_K^2(\xi,\mu)} = \mathscr{E}_{\widetilde{K}_\mu}(\xi-\mu) = \mathscr{E}_{\widetilde{K}_\mu}(\xi)}$

For μ,ξ having total mass 1,

minimising MMD $\gamma_K(\xi,\mu)$ w.r.t. ξ $\Leftrightarrow$ minimising MMD $\gamma_{\widetilde{K}_\mu}(\xi,\mu)$
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[For $\mu=\delta_{\mathbf{x}_0}$ (function approximation):
$\widetilde{K}_\mu(\mathbf{x},\mathbf{x}') \triangleq K(\mathbf{x},\mathbf{x}') - K(\mathbf{x},\mathbf{x}_0) - K(\mathbf{x}',\mathbf{x}_0) + K(\mathbf{x}_0,\mathbf{x}_0)$]

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compute $\widetilde{K}_\mu(\mathbf{x},\mathbf{x}')$

Back to the (continuous) BLUE of β

$\boxed{f(\mathbf{x}) = \beta + Z_x}$, Z_x a Gaussian RF, $\mathbb{E}\{Z_x\} = 0$, $\mathbb{E}\{Z_x Z_{x'}\} = \sigma^2 K(\mathbf{x}, \mathbf{x}')$

Denote $\mathfrak{p} \triangleq$ orthogonal projection of $L^2(\mathscr{X}, \mu)$ onto the linear space spanned by constant 1

$$a)\ f(\mathbf{x}) = \beta + \underbrace{Z_x}_{\mathfrak{p} Z_x + (\mathrm{Id}_{L^2} - \mathfrak{p}) Z_x} \quad \to \sigma^2 K$$

a) $\mathrm{var}\{BLUE(\beta)\} = \sigma^2 \mathscr{E}_K(\widetilde{\mu}_K^*)$ (if BLUE(β) exists...)

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$$b)\ f(\mathbf{x}) = \underbrace{\beta'}_{\beta + \mathfrak{p}Z_x} + \underbrace{\widetilde{Z}_x}_{(\mathrm{Id}_{L^2} - \mathfrak{p})Z_x} \quad \to \boxed{\sigma^2 \widetilde{K}_\mu}$$

a) $\mathrm{var}\{BLUE(\beta)\} = \sigma^2 \mathscr{E}_K(\widetilde{\mu}_K^*)$ (if BLUE(β) exists...)

b) $\mathrm{var}\{BLUE(\beta')\} = \sigma^2 \mathscr{E}_{\widetilde{K}_\mu}(\mu) = 0$ (with BLUE(β') $= I_\mu(f)$)

How to compute $\widetilde{K}_\mu(\mathbf{x},\mathbf{x}') \triangleq K(\mathbf{x},\mathbf{x}') - P_\mu(\mathbf{x}) - P_\mu(\mathbf{x}') + \mathscr{E}_K(\mu)$?

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Tensor product kernels:

Take K separable on $\mathscr{X} = \times_{i=1}^d \mathscr{X}_i$:

$$K(\mathbf{x},\mathbf{x}') = K^{(t)}(\mathbf{x},\mathbf{x}') = \prod_{i=1}^d K_i(x_i, x_i')$$

Szabó and Sriperumbudur (2018): each K_i continuous, bounded, translation invariant and CISPD on $\mathscr{M}^{(i)} = \mathscr{M}[\mathscr{X}_i] \Rightarrow K^{(t)}$ is CISPD on $\mathscr{M}[\mathscr{X}]$

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When $\mu = \otimes_{i=1}^d \mu^{(i)}$ is a product measure on $\mathscr{X} = \times_{i=1}^d \mathscr{X}_i$, then

$$\mathscr{E}_{K^{(t)}}(\mu) = \prod_{i=1}^d \mathscr{E}_{K_i}(\mu^{(i)}), \quad P_\mu(\mathbf{x}) = \prod_{i=1}^d P_{\mu^{(i)}}(x_i)$$

and $\mathscr{E}_{K_i}(\mu^{(i)})$ and $P_{\mu^{(i)}}(x)$ easily computed (analytical expressions available for some $\mu^{(i)}$ and K_i on $\mathscr{X}_i = [a,b]$ — Matérn, Riesz...)

4 Design of experiments

$\boxed{\mu \text{ is uniform on } \mathscr{X}}$

Minimise $\mathscr{E}_K(\xi - \mu) = \mathrm{MMD}^2(\xi, \mu)$ w.r.t. $\xi \rightarrow \xi = \mu$, not very useful...

4 Design of experiments

μ is uniform on $\mathscr{X}$

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We want a discrete measure !

- $\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ a n-point design ($\mathbf{x}_i \in \mathscr{X}$ for all i)
- $\xi_n = \sum_{i=1}^n w_i \, \delta_{\mathbf{x}_i}$ a finite signed measure supported on $\mathbf{X}_n$, $\mathbf{w}_n = (w_1, \ldots, w_n)^\top$

$\rightarrow$ $\boxed{\mathscr{E}_K(\xi_n - \mu) = \mathscr{E}_K(\mu) - 2\mathbf{w}_n^\top \mathbf{p}_n(\mu) + \mathbf{w}_n^\top \mathbf{K}_n \mathbf{w}_n}$

where $\mathbf{p}_n(\mu) = (P_\mu(\mathbf{x}_1), \ldots, P_\mu(\mathbf{x}_n))^\top$ and $\{\mathbf{K}_n\}_{i,j} = K(\mathbf{x}_i, \mathbf{x}_j)$

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➞ $\boxed{\mathscr{E}_K(\xi_n - \mu) = \mathscr{E}_{\widetilde{K}_\mu}(\xi_n) = \mathbf{w}_n^\top \widetilde{\mathbf{K}}_n \mathbf{w}_n}$

$\mathbf{X}_n$ fixed, optimal weights $\hat{\mathbf{w}}_n$ summing to 1: Bayesian integration

$$\hat{\mathbf{w}}_n = \frac{\widetilde{\mathbf{K}}_n^{-1}\mathbf{1}_n}{\mathbf{1}_n^\top \widetilde{\mathbf{K}}_n^{-1}\mathbf{1}_n}$$

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$$\begin{cases} \hat{\mathbf{w}}_n & = \text{weights} \\ \sigma^2 \mathscr{E}_K(\hat{\xi}_n - \mu) & = \text{variance} \end{cases}$$ for **Bayesian integration w.r.t.** μ

in the model

$\boxed{f(\mathbf{x}) = \beta + Z_x}$ with $\mathrm{E}\{Z_x\} = 0$ and $\mathrm{E}\{Z_x Z_{x'}\} = \sigma^2 K(\mathbf{x}, \mathbf{x}')$

→ Posterior mean: $\widehat{I}_n = \hat{\mathbf{w}}_n{}^\top \mathbf{y}_n$, with $\mathbf{y}_n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))^\top$

→ Posterior variance $\sigma^2 s_n^2 = \sigma^2 \mathscr{E}_K(\hat{\xi}_n - \mu) = \sigma^2 \mathscr{E}_{\widetilde{K}_\mu}(\hat{\xi}_n) = \dfrac{\sigma^2}{\mathbf{1}_n^\top \widetilde{\mathbf{K}}_n^{-1}\mathbf{1}_n}$

▸▸ all weights $= 1/n$

. . . ?!? initially we had

$$\begin{aligned}
\hat{\mathbf{w}}_n &= \left(\mathbf{K}_n^{-1} - \frac{\mathbf{K}_n^{-1}\mathbf{1}_n\mathbf{1}_n^T\mathbf{K}_n^{-1}}{\mathbf{1}_n^T\mathbf{K}_n^{-1}\mathbf{1}_n}\right)\mathbf{p}_n(\mu) + \frac{\mathbf{K}_n^{-1}\mathbf{1}_n}{\mathbf{1}_n^T\mathbf{K}_n^{-1}\mathbf{1}_n} \\
s_n^2 &= \mathscr{E}_K(\mu) - \mathbf{p}_n^T(\mu)\mathbf{K}_n^{-1}\mathbf{p}_n(\mu) + \frac{(1-\mathbf{p}_n^T(\mu)\mathbf{K}_n^{-1}\mathbf{1}_n)^2}{\mathbf{1}_n^T\mathbf{K}_n^{-1}\mathbf{1}_n}
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$\mathfrak{p} \triangleq$ orthogonal projection of $L^2(\mathscr{X},\mu)$ onto the linear space spanned by 1

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New trend β', but the predictions are not modified when $K \to \widetilde{K}_\mu$

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$$s_n^2 = \frac{1}{\mathbf{1}_n^T\widetilde{\mathbf{K}}_n^{-1}\mathbf{1}_n}$$

Equivalence with estimation in a location model

$$\begin{cases} \hat{\mathbf{w}}_n & = \text{ weights} \\ \sigma^2 \mathscr{E}_K(\hat{\xi}_n - \mu) & = \text{ variance} \end{cases}$$ for **(discrete) BLUE** of β' in the model

$$\boxed{f(\mathbf{x}) = \beta' + \widetilde{Z}_x}$$ with $\mathrm{E}\{\widetilde{Z}_x\} = 0$, $\mathrm{E}\{\widetilde{Z}_x \widetilde{Z}_{x'}\} = \sigma^2 \widetilde{K}_\mu(\mathbf{x}, \mathbf{x}')$

→ $\widehat{I}_n = \hat{\beta'}^n$ = (discrete) BLUE of β'
→ $\sigma^2 s_n^2 = \mathrm{var}[\hat{\beta'}^n]$

(design for) Bayesian integration ⇔ (design for) parameter estimation in a model with errors having a modified covariance

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(design for) Bayesian integration ⇔ (design for) parameter estimation in a model with errors having a modified covariance

[$\mu = \delta_{\mathbf{x}_0}$ yields a similar equivalence between function approximation (at $\mathbf{x}_0$) and parameter estimation]

1/ Fix the weights to $1/n$, optimise w.r.t. $\mathbf{X}_n$

→ choose $\mathbf{X}_n$ that minimises $\mathscr{E}_K(\xi_n - \mu) = \mathbf{1}_n^\top \widetilde{\mathbf{K}}_n \mathbf{1}_n / n^2$

→ *Projection kernel* of Mak and Joseph (2017);
Support points of Mak and Joseph (2018) based on energy distance;
L_2 *discrepancy* of QMC (symmetric, centred, wrap-around...) based on tensorised kernels related to variants of Brownian-motion covariance (Hickernell, 1998)

2/ **Nested designs (extensible point sequences)**

Choose n points sequentially among a finite set $\mathscr{X}_Q = \{\mathbf{s}_1, \ldots, \mathbf{s}_Q\} \subset \mathscr{X}$
A measure ξ on $\mathscr{X}_Q \Leftrightarrow$ a vector $\boldsymbol{\omega} \in \mathbb{R}^Q$

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A measure ξ on $\mathscr{X}_Q \Leftrightarrow$ a vector $\boldsymbol{\omega} \in \mathbb{R}^Q$

<u>Vertex Direction</u> (="kernel herding" in machine learning):
$\rightarrow$ minimise $\mathscr{E}_K(\xi - \mu)$, quadratic in $\boldsymbol{\omega}$,
using Frank-Wolfe conditional gradient (Wynn's algorithm):

$$\xi^{(n+1)} = \frac{n}{n+1}\,\xi^{(n)} + \frac{1}{n+1}\,\delta_{\mathbf{x}_{n+1}}$$

with $\mathbf{x}_{n+1} \in \operatorname{Arg\,min}_{\mathbf{x}\in\mathscr{X}_Q} \left[\sum_{i=1}^n w_i^{(n)} K(\mathbf{x}, \mathbf{x}_i) - P_\mu(\mathbf{x})\right]$
(well defined also for singular kernels, e.g., Riesz kernels)

2/ **Nested designs (extensible point sequences)**

Choose n points sequentially among a finite set $\mathscr{X}_Q = \{\mathbf{s}_1, \ldots, \mathbf{s}_Q\} \subset \mathscr{X}$
A measure ξ on $\mathscr{X}_Q \Leftrightarrow$ a vector $\boldsymbol{\omega} \in \mathbb{R}^Q$

<u>Vertex Direction</u> (="kernel herding" in machine learning):
$\rightarrow$ minimise $\mathscr{E}_K(\xi - \mu)$, quadratic in $\boldsymbol{\omega}$,
using Frank-Wolfe conditional gradient (Wynn's algorithm):

$$\xi^{(n+1)} = \frac{n}{n+1}\,\xi^{(n)} + \frac{1}{n+1}\,\delta_{\mathbf{x}_{n+1}}$$

with $\mathbf{x}_{n+1} \in \operatorname{Arg\,min}_{\mathbf{x}\in\mathscr{X}_Q} \left[\sum_{i=1}^n w_i^{(n)} K(\mathbf{x}, \mathbf{x}_i) - P_\mu(\mathbf{x})\right]$
(well defined also for singular kernels, e.g., Riesz kernels)

- $\xi^{(1)} = \delta_{\mathbf{x}_1} \rightarrow$ all weights $w_i^{(n)}$ in $\xi^{(n)}$ equal $1/n$
- Rate of decrease of $\mathscr{E}_K(\xi^{(n)} - \mu) = \mathcal{O}(1/n)$
  Cost $\mathcal{O}(Q)$ at each iteration ($\mathcal{O}(nQ)$ for n iterations) $\boxed{\rightarrow \mathbf{X}_n^{VD}}$

Minimum-Norm-point algorithm of (Bach et al., 2012):

replace $\xi^{(n)}$ (uniform on its support) by $\hat{\xi}^{(n)}$ having the same support but optimal weights, positive with sum $= 1$

➠ We use $\hat{\mathbf{w}}_n$ from Bayesian quadrature

(extra comput. cost ➞ $\mathcal{O}(n^2 Q)$ for n iterations (P., 2021)) $\boxed{\rightarrow \mathbf{X}_n^{MN}}$

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Comparison with:

- (scrambled) Sobol' sequence $\boxed{\rightarrow \mathbf{X}_n^{sS}}$
- Extensible Lattice sequence $\mathbf{X}_n^{EL}$: $\mathbf{x}_k = \{k\mathbf{g}\}$ ($\mathbf{g}$ has irrational components independent over the rationals, $\{\cdot\}$ = fractional part) We use $\mathbf{g} = (1/\varphi_d, 1/\varphi_d^2, \ldots, 1/\varphi_d^d)^\top$, with φ_d the unique positive root of $x^{d+1} = x + 1$, see http://extremelearning.com.au/ $\boxed{\rightarrow \mathbf{X}_n^{EL}}$

  (but not competitive for large d)

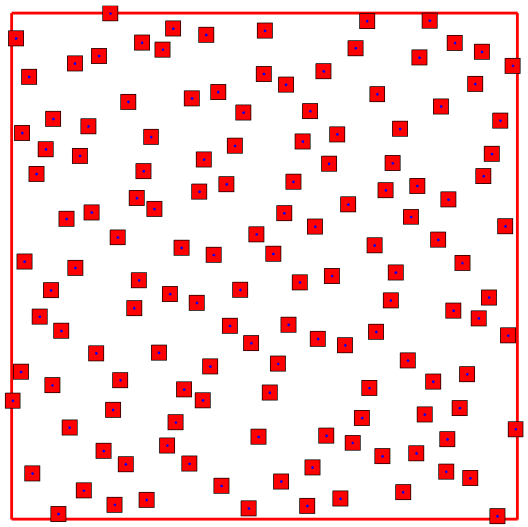
Example: $d = 2$, $\mathscr{X} = [0,1]^2$, $\mathscr{X}_Q =$ regular grid 64×64

$n_{\max} = 140$, $\mathbf{X}_1 = (0.5, 0.5)$, $\xi_{(1)} = \delta_{\mathbf{x}_1}$

$K =$ tensor product of Matérn 3/2:

$K_{3/2,\theta}(x, x') = (1 + \sqrt{3}\theta|x - x'|)\exp(-\sqrt{3}\theta|x - x'|)$, $\theta = 10$ $(n_{\max}^{1/d} \simeq 11.8)$

scrambled Sobol' LDS $\mathbf{X}_{140}^{sS}$



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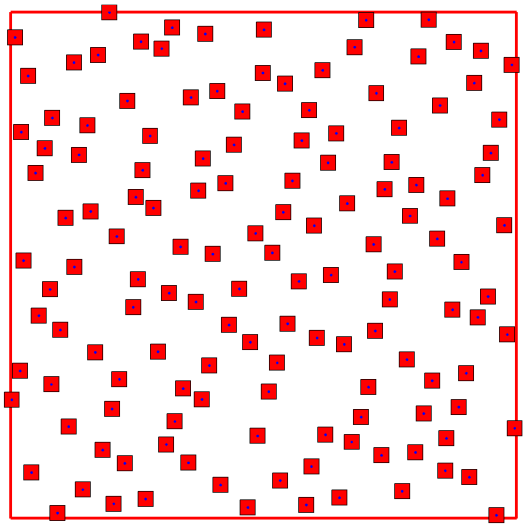
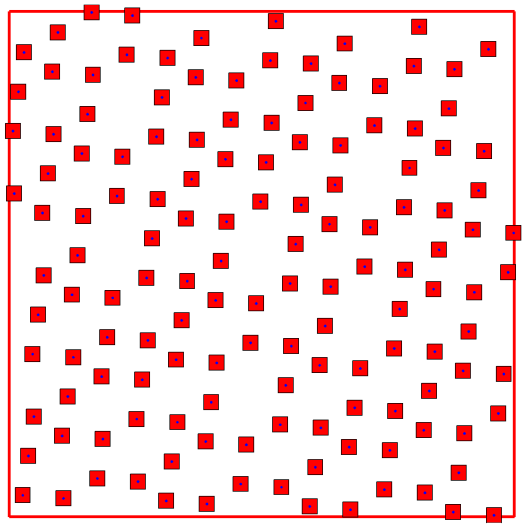


Extensible Lattice sequence $\mathbf{X}_{140}^{EL}$



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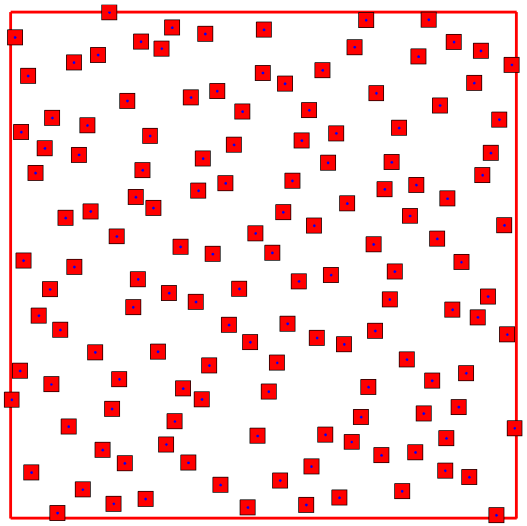
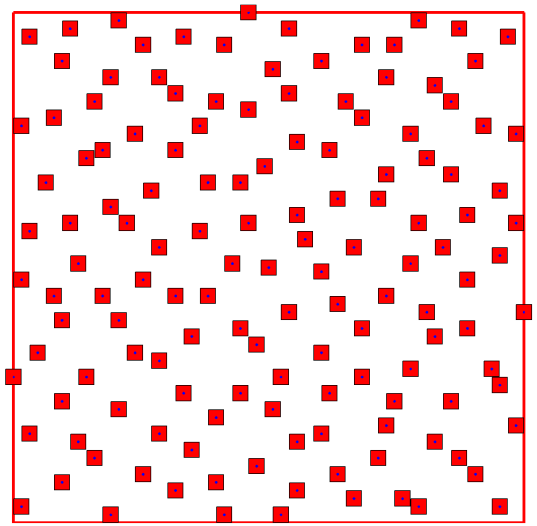


Vertex Direction $\mathbf{X}_{140}^{VD}$



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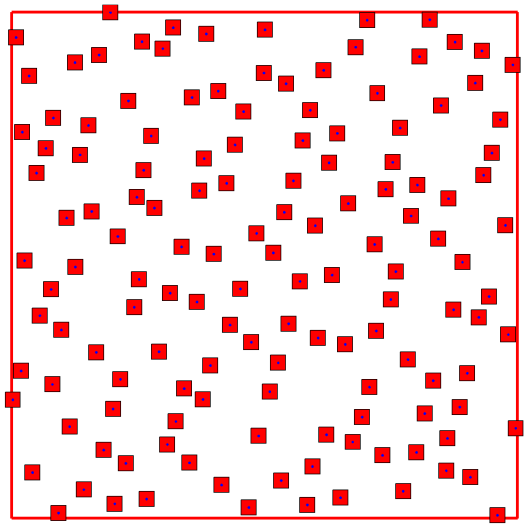
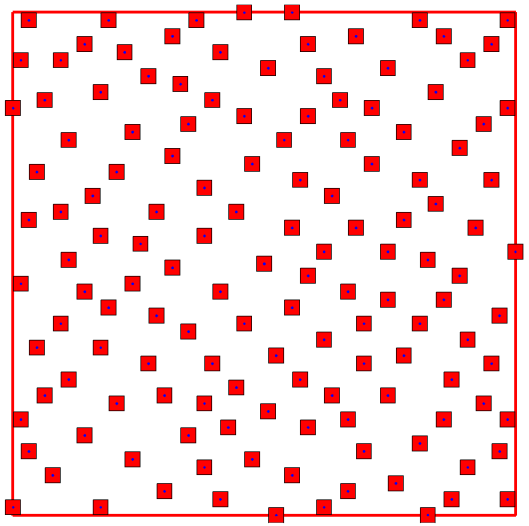


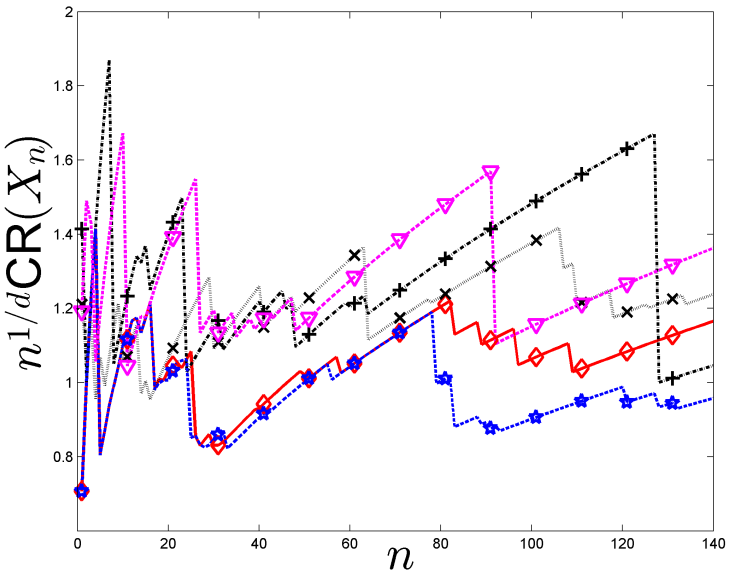
Minimum-Norm $\mathbf{X}_{140}^{MN}$



Space-filling performance

$$n^{1/d}\,\mathrm{CR}(\mathbf{X}_n)$$

(smaller is better)



$\mathbf{X}_n^{S}$, $\mathbf{X}_n^{sS}$, $\mathbf{X}_n^{EL}$, $\mathbf{X}_n^{VD}$, $\mathbf{X}_n^{MN}$

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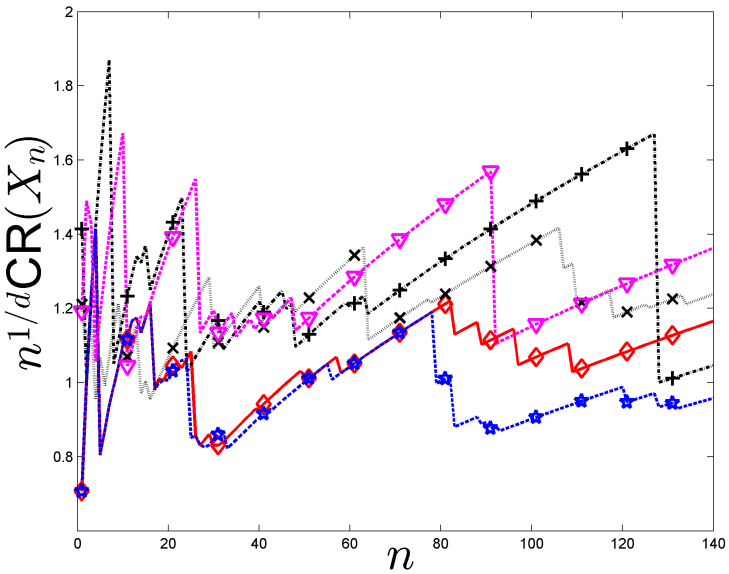
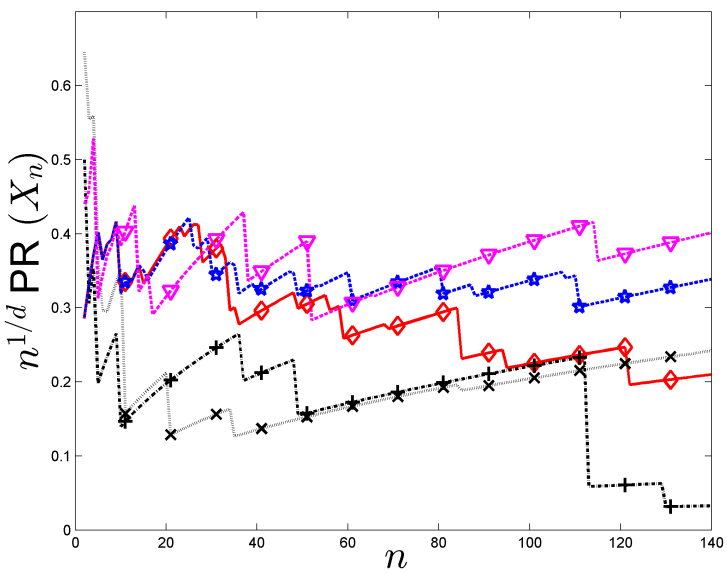


$\mathbf{X}_n^{S}$, $\mathbf{X}_n^{sS}$, $\mathbf{X}_n^{EL}$, $\mathbf{X}_n^{VD}$, $\mathbf{X}_n^{MN}$

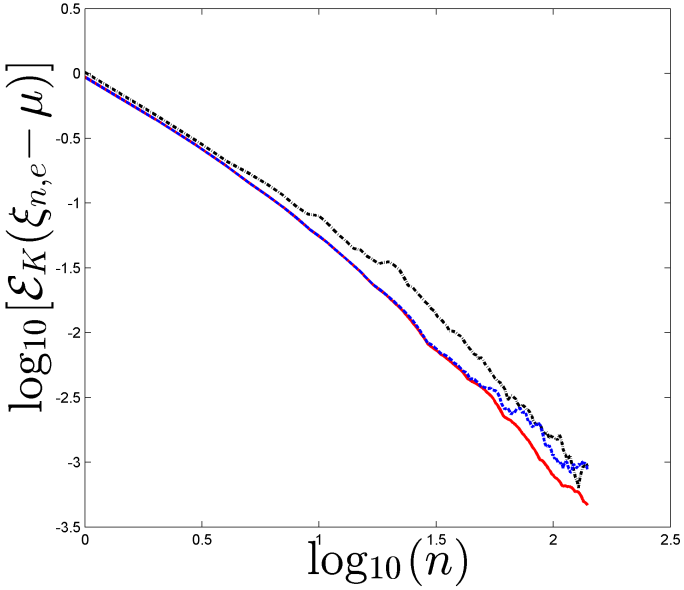
$n^{1/d}\,\mathrm{PR}(\mathbf{X}_n)$

(larger is better)



$\mathbf{X}_n^{S}$, $\mathbf{X}_n^{sS}$, $\mathbf{X}_n^{EL}$, $\mathbf{X}_n^{VD}$, $\mathbf{X}_n^{MN}$

Decrease of $\mathscr{E}_{K_{3/2,10}}(\xi_n - \mu)$
$(\mathbf{X}_n^S, \mathbf{X}_n^{VD}, \mathbf{X}_n^{MN})$



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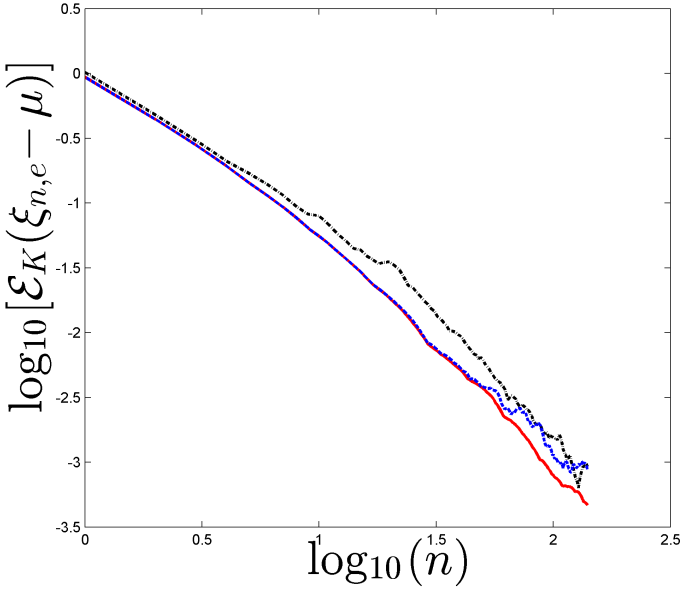
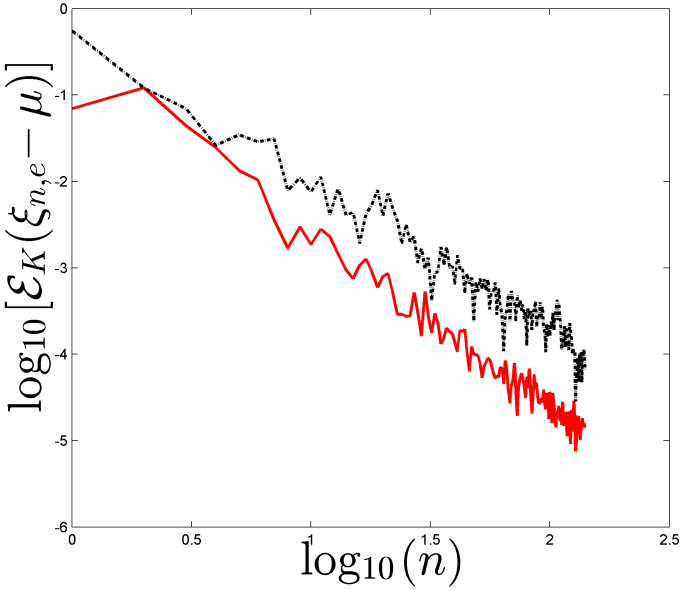


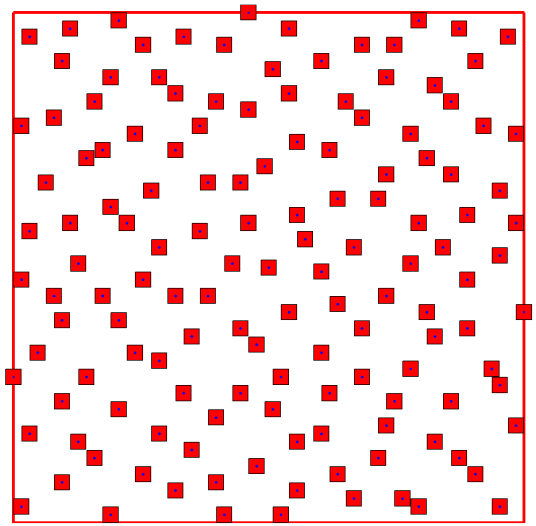
Decrease of $\mathscr{E}_{K_{3/2,1}}(\xi_n - \mu)$
$(\mathbf{x}_n^S, \mathbf{x}_n^{VD})$



For a large enough correlation length the rate of decrease can reach $\mathcal{O}(1/n^2)$ (no proof available)

How meaningful is the rate of convergence?

"kernel herding" with $K_{3/2,10}$
$\mathbf{X}_{140}^{VD}$ (rate $\lesssim 1/k$)



"kernel herding" with $K_{3/2,1}$
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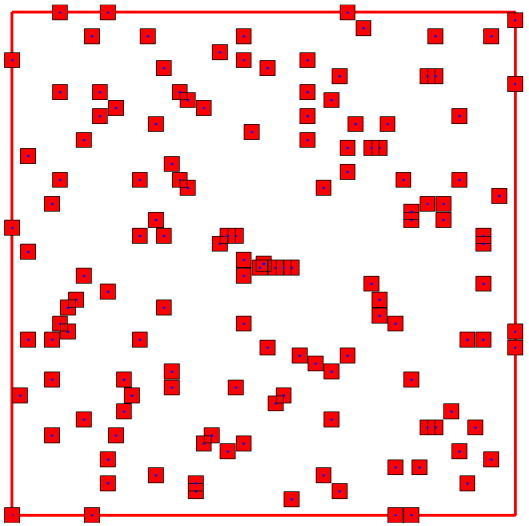

A faster rate does not mean that points are more evenly distributed!

Example: $d = 10$, $\mathscr{X}_Q = 2^{12}$ points of scrambled Sobol' in $\mathscr{X} = [0,1]^2$

$n_{\max} = 140$, $\mathbf{X}_1 = \mathbf{1}_d/2$, $\xi_{(1)} = \delta_{\mathbf{X}_1}$

K = tensor product of Matérn 3/2:

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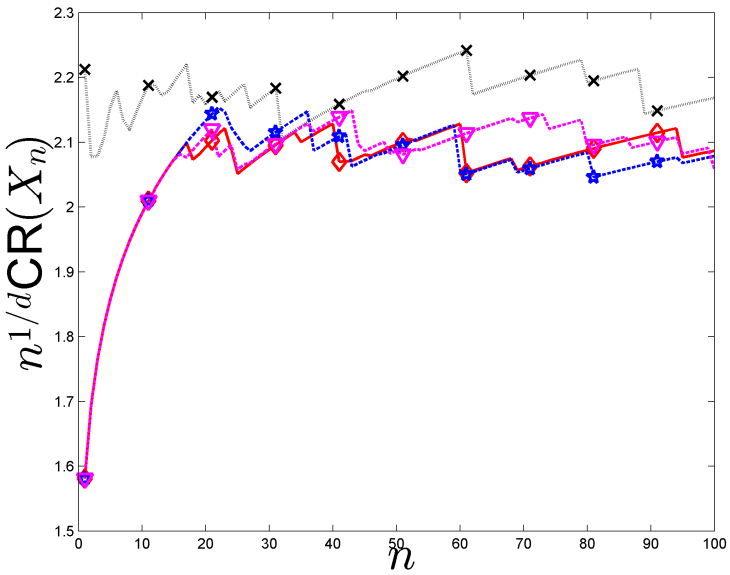
$\mathbf{X}_n^S$, $\mathbf{X}_n^{VD}$, $\mathbf{X}_n^{MN}$, $\mathbf{X}_n^{MN-\log}$



$[K_{\log}(x_i, x_i') = -\log|x_i - x_i'|]$

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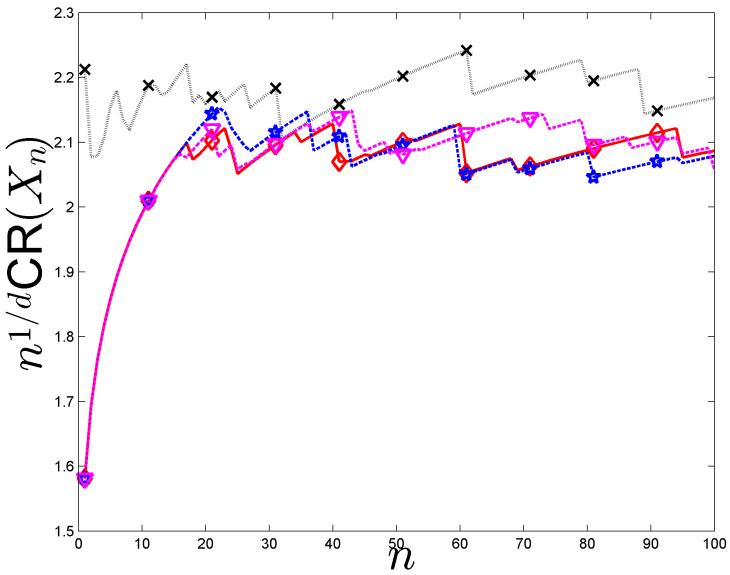

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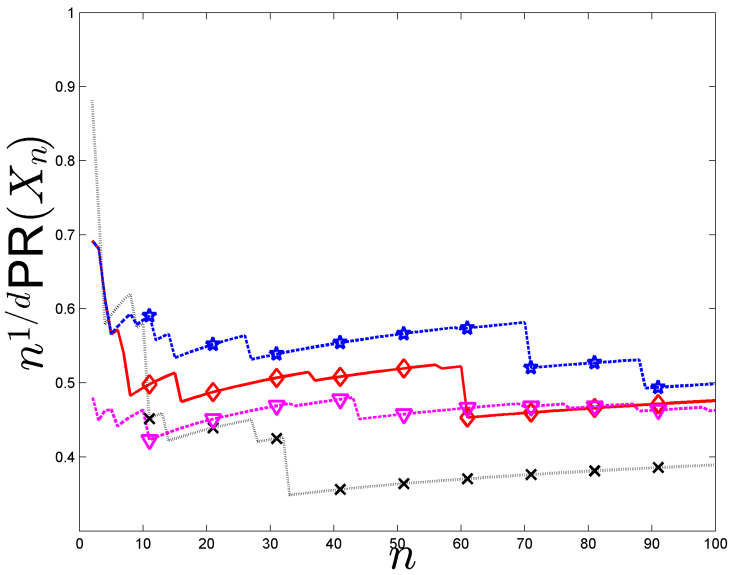


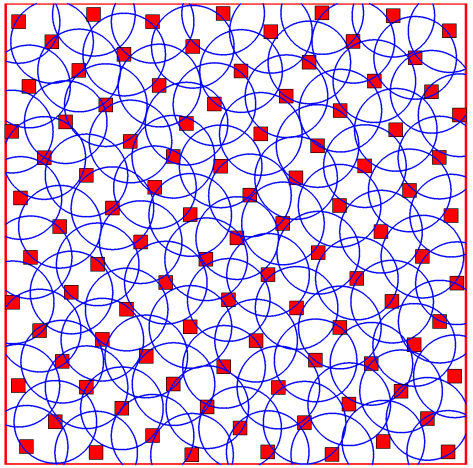
$[K_{\log}(x_i, x_i') = -\log|x_i - x_i'|]$

3/ n fixed: minimise $s_n^2 = \mathscr{E}_K(\hat{\xi}_n - \mu) = \frac{1}{\mathbf{1}_n^\top \widetilde{\mathbf{K}}_n^{-1} \mathbf{1}_n}$ w.r.t. $\mathbf{X}_n$

a) First (initialisation), use a greedy algorithm, stop at n $\boxed{\rightarrow \mathbf{X}_n^{VD}}$

b) Then, maximise $\mathbf{1}_n^\top \widetilde{\mathbf{K}}_n^{-1} \mathbf{1}_n$ viewed as a function of $\mathbf{X}_n$ $\boxed{\rightarrow \mathbf{X}_n^{VDopt}}$

a) Initialisation at $\mathbf{X}_{100}^{VD}$ generated by Vertex-Direction method with $\mathrm{CR}(\mathbf{X}_{100}^{VD}) \simeq 0.0925$, $2\,\mathrm{PR}(\mathbf{X}_{100}^{VD}) \simeq 0.0523$



$\rightarrow$ b) $\mathrm{CR}(\mathbf{X}_{100}^{VDopt}) \simeq 0.0897$, $2\,\mathrm{PR}(\mathbf{X}_{100}^{VDopt}) \simeq 0.0738$

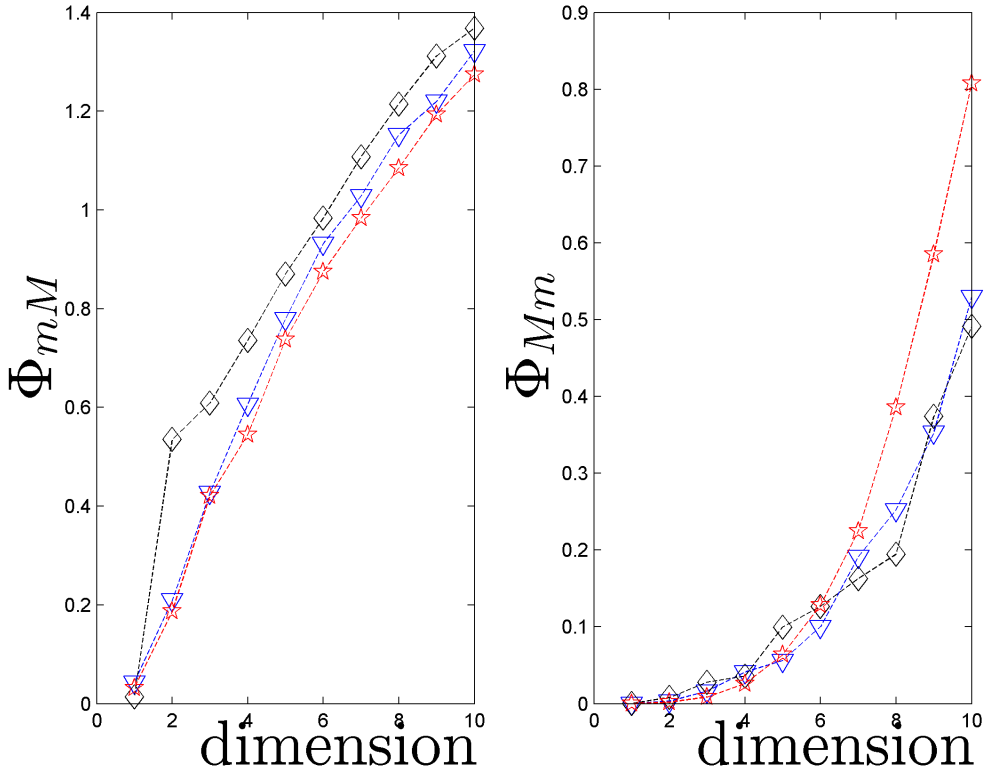
Example: $d = 10$, $\mathscr{X} = [0,1]^{10}$, $n_{\max} = 100$

$K = \bigotimes K_{3/2,\theta}(x,x')$, $\theta = \lfloor n_{\max}^{1/d} \rfloor = 1$

a) VD $\mathbf{X}_n^{VD}$, $n = 1, \ldots, 100$, then b) $\mathbf{X}_{100}^{VDopt}$

$\max \mathrm{CR} = \max \Phi_{mM}$ and $2 \min \mathrm{PR} = \min \Phi_{Mm}$ on projections

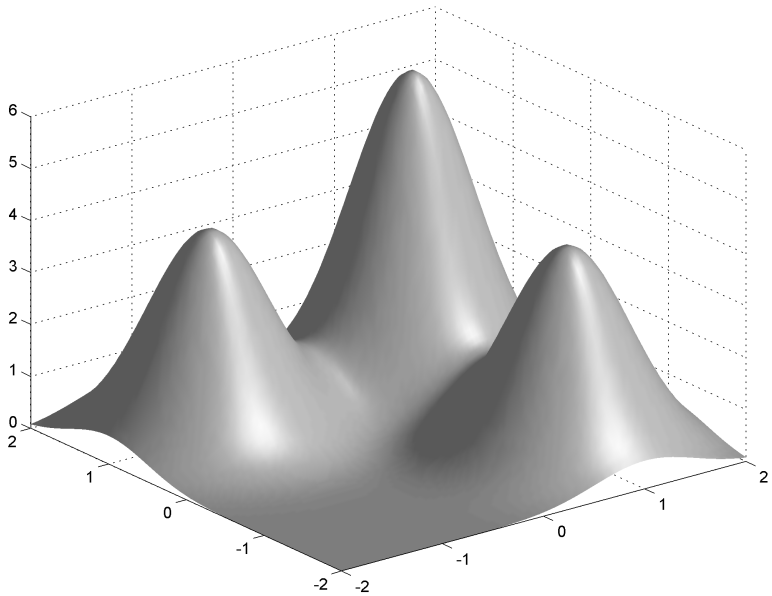
$\diamondsuit$ $\mathbf{X}_{100}^{S}$, $\triangledown$: $\mathbf{X}_{100}^{VD}$, $\bigstar$: $\mathbf{X}_{100}^{VDopt}$

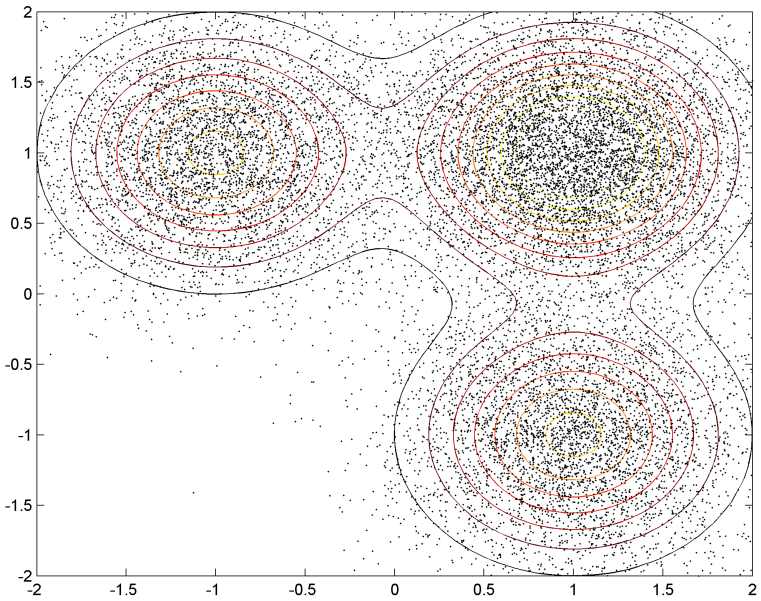


Kernel herding is not restricted to μ being uniform:

Example: Gaussian mixture $\mu = \sum_{j=1}^{3} \beta_j \, \mu_{\mathcal{N}}(\mathbf{a}_j, \sigma_j)$, $Q = 2^{14} = 16\,384$

(for $K_\theta(\mathbf{x}, \mathbf{x}') = \exp -(\theta \, \|\mathbf{x} - \mathbf{x}'\|^2)$, we know $P_\mu(\cdot)$ and $\mathscr{E}_K(\mu)$)





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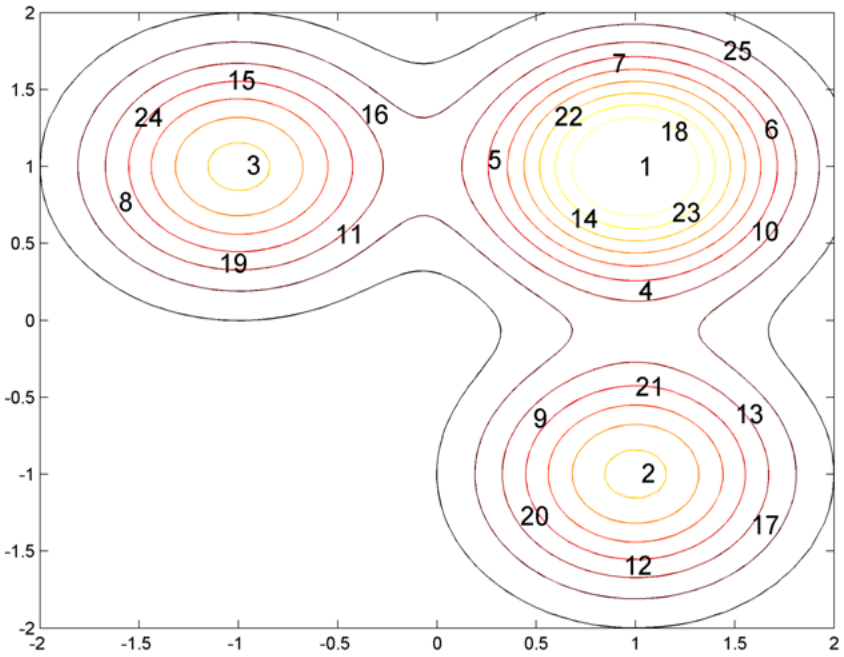
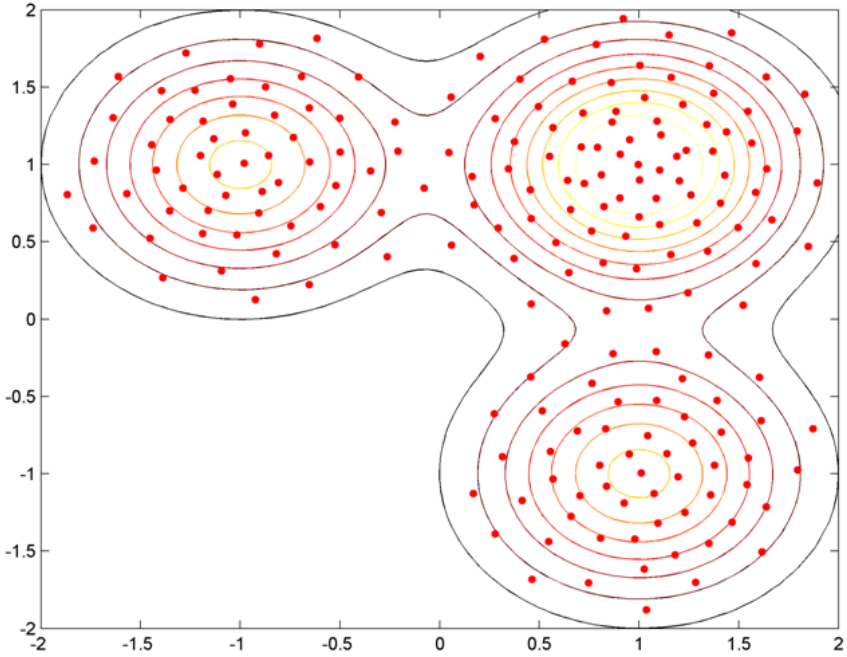


$n = 25$



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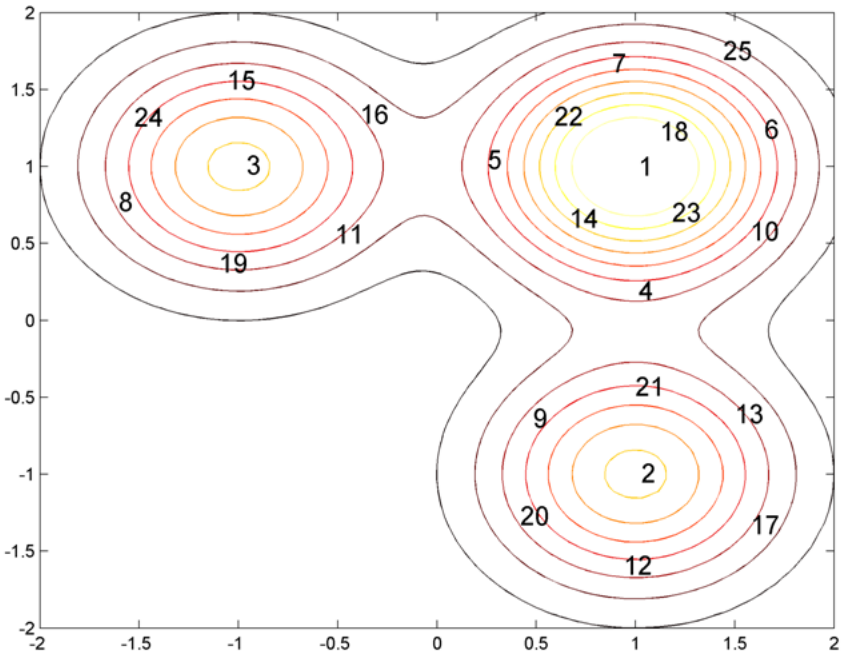

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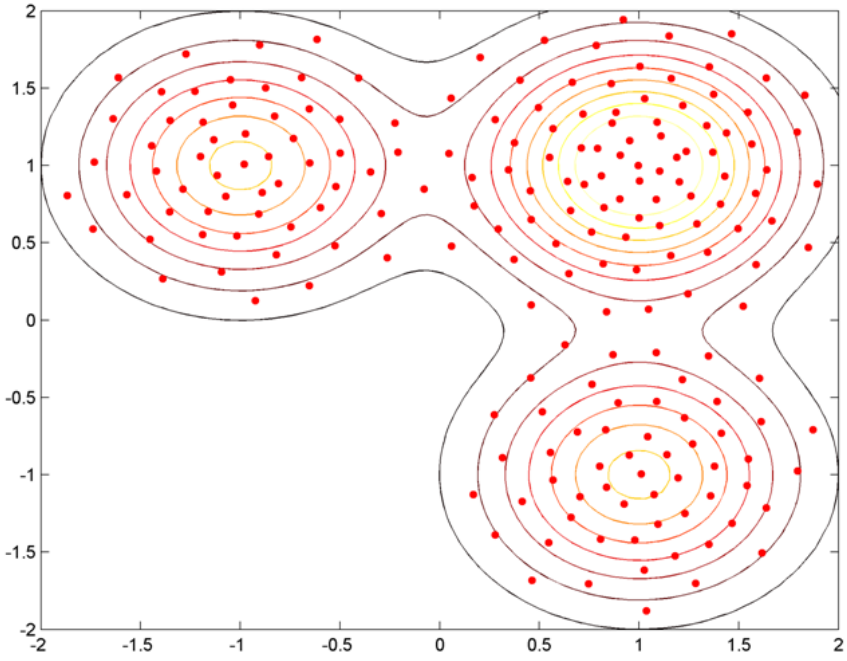

$n = 200$

- Comparison between kernel herding, greedy MMD minimisation and Sequential Bayesian Quadrature (P., 2021)
- Extension to Stein discrepancy (Teymur et al., 2020) (K'_μ such that $P_\mu(\cdot) \equiv 0$ and $\mathscr{E}_{K'_\mu}(\mu) = 0$ without knowing the normalising constant in μ)
- Singular kernels (via completely monotone functions) (P. & Zhigljavsky, 2021)

4 Conclusions

- Maximum Mean Discrepancy connects Bayesian quadrature, potential theory, design for parameter estimation, space filling design
  - For many kernels K: metric for the weak cv. of prob. measures, easier to compute than optimal transport (= Wasserstein)
  - (design for) Bayesian integration $\Leftrightarrow$ (design for) parameter estimation in a model with modified covariance

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- Optimisation algorithm for n fixed:
  Any nonlinear programming method (unconstrained) can be used
  (a Maj.-Min. approach is used in (Mak and Joseph, 2017, 2018))

A few more general questions and open issues:

- Space-filling performance? (discrepancy $\not\Leftrightarrow$ dispersion)
  Efficiency bounds for CR and PR?
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Thank you for your attention !

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