G-optimal retrospective grid designs

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Objective

Find the best possible retrospective designs for kriging models over two-dimensional grids under both frequentist and Bayesian paradigms.

Kriging model

$Z(x, y)$ sampled at $\mathcal{S} = \{x_1, \ldots, x_n\} \times \{y_1, \ldots, y_m\} \subseteq [0,1] \times [0,1] = \mathcal{D}$.

$x_i < x_{i'}$ and $y_j < y_{j'}$ whenever $i < i'$ and $j < j'$.

$$Z(x, y) = \boldsymbol{f}^T(x, y)\boldsymbol{\pi} + \epsilon(x, y) \text{ and}$$
$$Cov(\epsilon(x, y), \epsilon(x', y')) = \sigma^2 \, e^{-\alpha|x-x'|} \, e^{-\beta|y-y'|}.$$

$$\boldsymbol{\Theta} = (\sigma^2, \alpha, \beta)$$

Design Setup and criteria

Design

Set $\mathcal{S}$, equivalently $\boldsymbol{\xi} = (\boldsymbol{d}, \boldsymbol{\delta})$.
$\boldsymbol{d} = (d_1, \ldots, d_{n-1})$ and $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_{m-1})$ where, $d_i = x_{i+1} - x_i$ and $\delta_j = y_{j+1} - y_j$.

Design Criteria

Minimize the objective functions based on the mean squared prediction error($MSPE$):

$$SMSPE(\boldsymbol{\xi}, \boldsymbol{\Theta}) = \sup_{(x_0, y_0) \in \mathcal{D}} MSPE((x_0, y_0), \boldsymbol{\xi}, \boldsymbol{\Theta}).$$

$$\mathcal{R}(\boldsymbol{\xi}) = E_{\boldsymbol{\Theta}}[SMSPE(\boldsymbol{\xi}, \boldsymbol{\Theta})].$$

Evenness of Designs

$\boldsymbol{\xi}$ is more evenly spread than design $\boldsymbol{\xi}' \equiv (\boldsymbol{d}', \boldsymbol{\delta}')$ if $\boldsymbol{d} \prec \boldsymbol{d}'$ and $\boldsymbol{\delta} \prec \boldsymbol{\delta}'$, where '$\prec$' is majorization.

Retrospective designs - Simultaneous deletion of existing points

- Algorithm 3 reduces the size of the choice set for finding the best possible design from '9009' to '3'
- Best possible retrospective design $\boldsymbol{\xi}^-_{a3}$ is the most evenly spaced design among the choice set

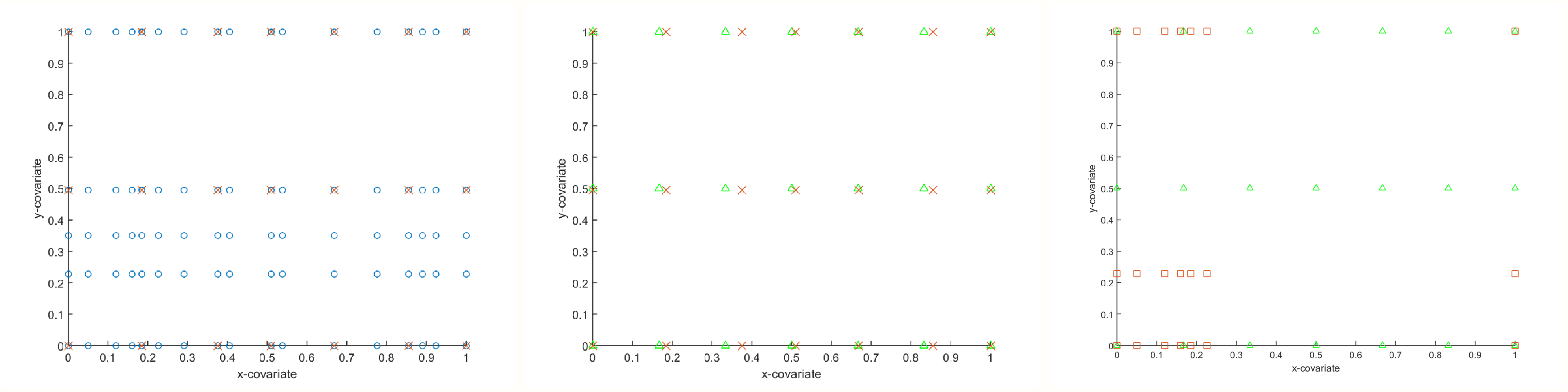

Figure 1: Comparison of design $\boldsymbol{\xi}$ Vs $\boldsymbol{\xi}^-_{a3}$ (left); $\boldsymbol{\xi}^-_{eq7\times3}$ Vs $\boldsymbol{\xi}^-_{a3}$ (middle); $\boldsymbol{\xi}^-_{eq7\times3}$ Vs $\boldsymbol{\xi}^-_{a3-worst}$ (right).
'○' - $\boldsymbol{\xi}$: Original design grid of size 17×5. '×' - $\boldsymbol{\xi}^-_{a3}$: Best possible retrospective design of size 7×3.
'△' - $\boldsymbol{\xi}^-_{eq7\times3}$: An equispaced grid of size 7×3. '□' - $\boldsymbol{\xi}^-_{a3-worst}$: Worst possible retrospective design of size 7×3.

Table 1: Efficiencies of $\boldsymbol{\xi}^-_{a3}$ and $\boldsymbol{\xi}^-_{a3-worst}$ with respect to $\boldsymbol{\xi}$ and $\boldsymbol{\xi}^-_{eq7\times3}$.

(α, β)	$eff(\boldsymbol{\xi}^-_{a3-worst} : \boldsymbol{\xi})^{**}$	$eff(\boldsymbol{\xi}^-_{a3} : \boldsymbol{\xi})^{\dagger}$	$eff(\boldsymbol{\xi}^-_{a3-worst} : \boldsymbol{\xi}^-_{eq7\times3})^{**}$	$eff(\boldsymbol{\xi}^-_{a3} : \boldsymbol{\xi}^-_{eq7\times3})^{\dagger\dagger}$
(.5, .7)	0.4973	0.9415	0.5116	0.9687
(1, 5)	0.8133	0.9884	0.8168	0.9927
(10, 15)	0.9335	0.9757	0.9559	0.9991

† Efficiency of the new design is quite closer to the initial design.
†† Best possible retrospective design is close to the G-optimal prospective design.
** Removing points without analyzing could lead to a considerable loss of efficiency. For the worst possible choice of removal of points, the efficiencies are reduced considerably.

Important definitions

- **Prospective design**- The new design is developed before the experiment is conducted
- **Retrospective design**- The new design is constructed by adding points to or deleting points from an already existing design
- **Efficiency of design** $\boldsymbol{\xi}_1$ with respect to $\boldsymbol{\xi}_2$ - $eff(\boldsymbol{\xi}_1 : \boldsymbol{\xi}_2) = SMSPE(\boldsymbol{\xi}_2)/SMSPE(\boldsymbol{\xi}_1)$. Higher the efficiency, better the design $\boldsymbol{\xi}_1$.

Our contribution

- A criterion to compare the evenness of two-dimensional grid designs
- **Algorithm 1** - Deterministic algorithm to find the best possible retrospective design (with respect to SMSPE criterion) by sequentially adding points to an existing design
- **Algorithm 2** - Deterministic algorithm to find the best possible retrospective design by simultaneously adding all points to an existing design
- **Algorithm 3** - Deterministic algorithm to find the best possible retrospective design by simultaneously deleting the required number of points from an existing design

Prospective design result

Theorem 1. *For ordinary kriging models with separable exponential structures, an* ***equispaced*** *grid in both coordinates is the* ***prospective design*** *G-optimal design under both frequentist and Bayesian paradigm.*

Retrospective designs - Simultaneous addition of new points

- Algorithm 2 reduces the size of choice set for selecting best possible design from 'infinity' to '100'
- The best possible retrospective design $\boldsymbol{\xi}^+_{a2}$ is the most evenly spaced

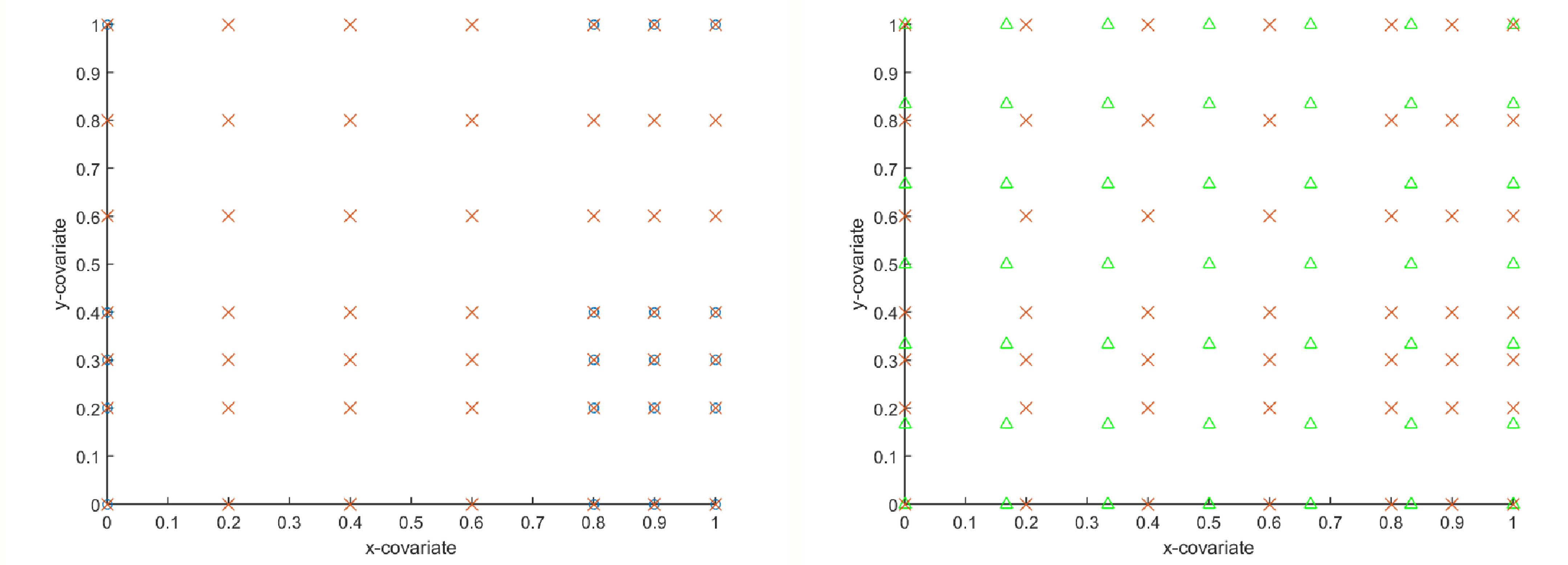

Figure 2: Comparison of design $\boldsymbol{\xi}$ Vs $\boldsymbol{\xi}^+_{a2}$ (left); $\boldsymbol{\xi}^+_{eq7\times7}$ Vs $\boldsymbol{\xi}^+_{a2}$ (right).
'○' - $\boldsymbol{\xi}$: Original design grid ofsize 4×5. '×' - $\boldsymbol{\xi}^+_{a2}$: Best possible retrospective design of size 7×7.
'△' - $\boldsymbol{\xi}^+_{eq7\times7}$: An equispaced grid of size 7×7.

References

[1] Peter Diggle and Søren Lophaven. Bayesian geostatistical design. *Scandinavian Journal of Statistics*, 33:53–64, 2006.

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