K-optimal designs for regression models driven by Ornstein-Uhlenbeck processes and fields

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Optimal Designs

$Z_\theta(x),\ x \in \mathcal{X}$: stochastic process (random field) with unknown parameter $\theta \in \Theta$.

$\boldsymbol{\xi} = \{x_1, x_2, \ldots, x_n\} \subset \mathcal{X}$: time points (locations) where $Z_\theta(x)$ is observed; design set.

Optimal design: design set optimizing some specified criterion[1].

Parameter estimation: most criteria are based on the Fisher information matrix (FIM).

- D-optimal design: maximizes the determinant[2] of the FIM of the observations;
- E-optimal design: maximizes the smallest eigenvalue[2] of the FIM;
- T-optimal design: maximizes the trace[2] of the FIM;
- A-optimal design: minimizes the trace of the inverse[2] of the FIM;
- K-optimal design: minimizes the condition number[3] of the FIM.

Recently most attention is focused on models with correlated errors[4,5].

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1 Müller, W. G. (2007) *Collecting Spatial Data. Third Edition.* Springer, Heidelberg.

2 Pukelsheim, F. (1993) *Optimal Design of Experiments.* Wiley, New York.

3 Ye, J. and Zhou, J. (2013) Minimizing the condition number to construct design points for polynomial regression models. *Siam. J. Optim.* **23**, 666–686.

4 Dette, H., Pepelyshev, A. and Zhigljavsky, A. (2015) Design for linear regression models with correlated errors. In: Dean, A., Morris, M., Stufken, J. and Bingham, D. (eds.), *Handbook of Design and Analysis of Experiments.* Chapman & Hall/CRC, Boca Raton, pp. 237–278.

5 Dette, H., Pepelyshev, A. and Zhigljavsky, A. (2016) Optimal designs in regression with correlated errors. *Ann. Statist.* **44**, 113–152.

General Properties of K-optimal Designs

K-optimal design

- Tries to minimize the error sensitivity of experimental measurements resulting in more reliable least squares estimates[1].
- Minimization of the condition number of the FIM avoids multicollinearity[2].
- The required optimization problem is not convex[3].
- Invariant to the multiplication of the FIM by a scalar; does not measure the amount of information on the unknown parameters.
- Does not have a meaning for one-parameter models.
- No results so far for correlated processes.

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[1] Maréchal, P., Ye, J. and Zhou, J. (2015) K-optimal design via semidefinite programming and entropy optimization. *Math. Oper. Res.* **40**, 495–512.

[2] Rempel, M. F. and Zhou, J. (2014) On exact K-optimal designs minimizing the condition number. *Comm. Statist. Theory Methods* **43**, 1114–1131.

[3] Yue, Z., Zhang, X., van den Driessche, P. and Zhou, J. (2022) Constructing K-optimal designs for regression models. *Stat. Papers*, doi:10.1007/s00362-022-01317-9.

Statistical Model

Ornstein-Uhlenbeck (OU) process with linear trend:

$$Y(s) = \alpha_0 + \alpha_1 s + U(s), \qquad s \in [a,b] \subset \mathbb{R}.$$

$U(s)$, $s \in \mathbb{R}$: stationary OU process. Zero mean Gaussian process with covariance structure

$$\mathsf{E}\, U(s)U(t) = \frac{\sigma^2}{2\beta} \exp\big(-\beta|s-t|\big), \qquad \beta > 0, \quad \sigma > 0.$$

Representation:

$$U(s) = \frac{\sigma}{\sqrt{2\beta}} \mathrm{e}^{-\beta s} \mathcal{W}\big(\mathrm{e}^{2\beta s}\big).$$

$\mathcal{W}(s)$, $s \in \mathbb{R}$: standard Brownian motion. β, σ: known parameters, variance is set to 1.

Aim: Compare D- and K-optimal designs for estimation of regression parameters α_0 and α_1.

Design: $\boldsymbol{\xi}_n = \{s_1, s_2, \ldots, s_n\}, \quad a \leq s_1 < s_2 < \cdots < s_n \leq b, \quad n \geq 2.$

Baran, S. (2017) K-optimal designs for parameters of shifted Ornstein-Uhlenbeck processes and sheets. *J. Stat. Plan. Inference* **186**, 28–41.

Fisher Information Matrix

Model: $Y(s) = \alpha_0 + \alpha_1 s + U(s),\ s \in [a, b] \subset \mathbb{R}$.

$\mathcal{I}_{\alpha_0,\alpha_1}(n)$: FIM on parameters $\alpha_0,\ \alpha_1$ based on observations $\{Y(s),\ s \in \boldsymbol{\xi}_n\}$.

General form[1]:

$$\mathcal{I}_{\alpha_0,\alpha_1}(n) = H(n)C(n)^{-1}H(n)^\top, \qquad \text{where} \qquad H(n) := \begin{bmatrix} 1 & 1 & \cdots & 1 \\ s_1 & s_2 & \cdots & s_n \end{bmatrix}.$$

$C(n)$: covariance matrix of observations. $C(n)^{-1}$ is tridiagonal[2].

$$\mathcal{I}_{\alpha_0,\alpha_1}(n) = \begin{bmatrix} L_1(n) & L_2(n) \\ L_2(n) & L_3(n) \end{bmatrix},$$

$$L_1(n) := 1 + \sum_{i=1}^{n-1} \frac{1-p_i}{1+p_i}, \qquad L_2(n) := s_1 + \sum_{i=1}^{n-1} \frac{s_{i+1} - s_i p_i}{1+p_i}, \qquad L_3(n) := s_1^2 + \sum_{i=1}^{n-1} \frac{(s_{i+1} - s_i p_i)^2}{1-p_i^2},$$

where $p_i := \exp(-\beta d_i)$ and $d_i := s_{i+1} - s_i,\ i = 1, 2, \ldots, n-1$.

[1] Pázman, A. (2007) Criteria for optimal design of small-sample experiments with correlated observations. *Kybernetika* **43**, 453–462.

[2] Kiseľák, J. and Stehlík, M. (2008) Equidistant D-optimal designs for parameters of Ornstein-Uhlenbeck process. *Statist. Probab. Lett.* **78**, 1388–1396.

D- and K-optimal Designs

Observations: $\{Y(s),\ s \in \boldsymbol{\xi}_n\}$, where $\boldsymbol{\xi}_n = \{s_1, s_2, \ldots, s_n\}$.

FIM:

$$\mathcal{I}_{\alpha_0,\alpha_1}(n) = \begin{bmatrix} L_1(n) & L_2(n) \\ L_2(n) & L_3(n) \end{bmatrix}.$$

Function of the distances $d_i := s_{i+1} - s_i,\ i = 1, 2, \ldots, n-1$. Assumption: $s_1 = 0$.

D-optimal design: maximizes in $\boldsymbol{d} = (d_1, d_2, \ldots, d_{n-1})$ the determinant of the FIM.

$$\mathcal{D}(\boldsymbol{d}) := \det\left(\mathcal{I}_{\alpha_0,\alpha_1}(n)\right) = L_1(n)L_3(n) - L_2^2(n).$$

K-optimal design: minimizes in $\boldsymbol{d}$ the condition number $\mathcal{K}(\boldsymbol{d})$ of the FIM.

$$\mathcal{K}(\boldsymbol{d}) = g\big(\mathcal{R}(\boldsymbol{d})\big), \qquad \text{where} \qquad g(x) := \frac{1}{4}\left(\sqrt{x} + \sqrt{x-4}\right)^2, \quad x \geq 4,$$

$$\mathcal{R}(\boldsymbol{d}) := \big(L_1(n) + L_3(n)\big)^2 \big/ \big(L_1(n)L_3(n) - L_2^2(n)\big) \geq 4.$$

$g(x)$ is strictly monotone increasing. It suffices to minimize $\mathcal{R}(\boldsymbol{d})$.

Example. Three-point Restricted Design

Design space: $\mathcal{X} = [0, 1]$.

Three-point restricted design: $s_1 = 0,\ s_2 := d,\ s_3 = 1$ with $0 \le d \le 1$.

D-optimal design: maximizer in d of

$$\mathcal{D}(d) = 2\frac{(1 - \mathrm{e}^{-\beta d}) + d(\mathrm{e}^{-\beta d} - \mathrm{e}^{-\beta(1-d)}) - d(1-d)(1 - \mathrm{e}^{-\beta})}{(1 - \mathrm{e}^{-2\beta d})(1 - \mathrm{e}^{-2\beta(1-d)})}.$$

K-optimal design: minimizer in d of

$$\mathcal{R}(d) = \mathcal{R}_1^2(d)/\mathcal{R}_2(d), \qquad \text{where}$$

$$\begin{aligned}\mathcal{R}_1(d) :=& (1-\mathrm{e}^{-\beta(1-d)})^2(1-\mathrm{e}^{-2\beta d}) + (1-\mathrm{e}^{-\beta d})^2(1-\mathrm{e}^{-2\beta(1-d)}) + (1-\mathrm{e}^{-2\beta d})(1-\mathrm{e}^{-2\beta(1-d)}) \\ &+ d^2(1-\mathrm{e}^{-2\beta(1-d)}) + (1-d\mathrm{e}^{-\beta(1-d)})^2(1-\mathrm{e}^{-2\beta d}),\end{aligned}$$

$$\mathcal{R}_2(d) := 2(1 - \mathrm{e}^{-2\beta d})(1-\mathrm{e}^{-2\beta(1-d)})\big(1-\mathrm{e}^{-\beta d} + d^2(1-\mathrm{e}^{-\beta}) - d(1+\mathrm{e}^{-\beta(1-d)})(1-\mathrm{e}^{-\beta d})\big).$$

Example. Optimal Three-point Restricted Designs

Three-point restricted design: $s_1 = 0,\ s_2 = d,\ s_3 = 1$ with $0 \le d \le 1$.

D-optimal design

For all $\beta > 0$ the maximizer of $\mathcal{D}(d)$ is $d = 1/2$. Equidistant design.

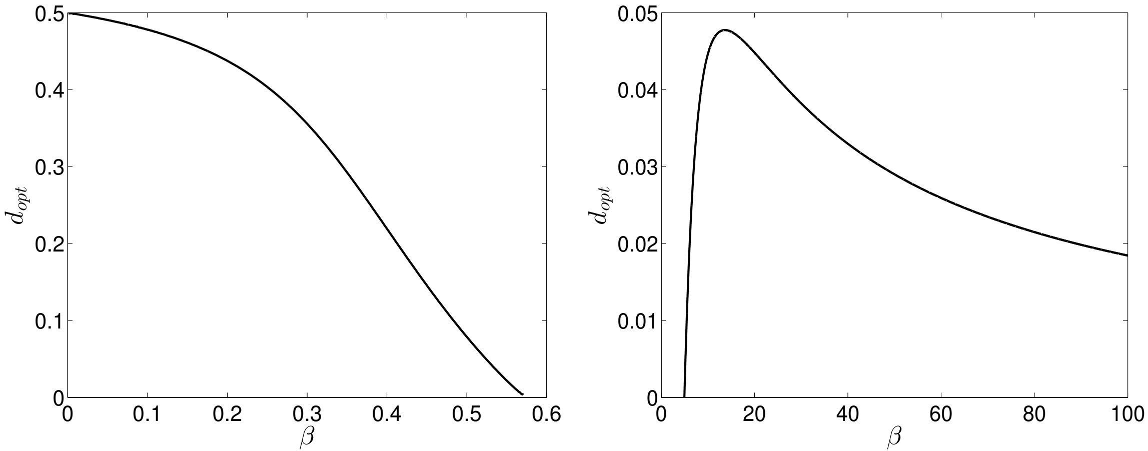
K-optimal design

$\beta^* \approx 0.5718,\ \beta^{**} \approx 4.9586$: only positive roots of

$$(\beta^2 - 6\beta + 4)\mathrm{e}^{4\beta} + (6\beta^2 + 6\beta - 10)\mathrm{e}^{3\beta} - (11\beta^2 - 10\beta - 2)\mathrm{e}^{2\beta} + (2\beta^2 - 6\beta + 10)\mathrm{e}^{\beta} - 2\beta^2 - 4\beta - 6 = 0.$$

- $\beta \in [\beta^*, \beta^{**}]$: $\mathcal{R}(d)$ has minima at $d = 0$ and $d = 1$. K-optimal design collapses.
- $\beta \notin [\beta^*, \beta^{**}]$: a K-optimal three-point design $\{0, d_{opt}, 1\}$ exists. $d_{opt} \to 0$ as $\beta \to \infty$.

Example. K-optimal Three-point Restricted Designs



K-optimal value d_{opt} for the three point design $\boldsymbol{\xi}_3 = \{0, d, 1\}$ for the intervals $]0, \beta^*[$, $\beta^* \approx 0.5718$, and $]\beta^{**}, 100]$, $\beta^{**} \approx 4.9586$.

Equidistant Designs

$\xi_n = \{0, d, 2d, \ldots, (n-1)d\}$: equidistant increasing domain design with step size $d > 0$.

FIM:

$$\mathcal{I}_{\alpha_0,\alpha_1}(n) = \begin{bmatrix} L_1(n) & L_2(n) \\ L_2(n) & L_3(n) \end{bmatrix}, \qquad \text{where}$$

$$L_1(n) = \frac{2 - n + n\mathrm{e}^{\beta d}}{\mathrm{e}^{\beta d} + 1}, \qquad L_2(n) = \frac{d(n-1)}{2} L_1(n),$$

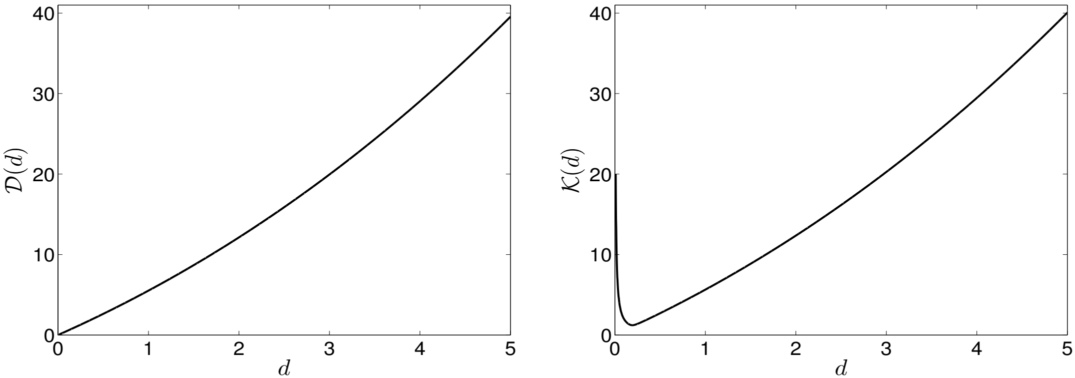
$$L_3(n) = \frac{d^2(n-1)}{\mathrm{e}^{2\beta d} - 1} \left(\frac{n(2n-1)(\mathrm{e}^{\beta d} - 1)^2}{6} + n\big(\mathrm{e}^{\beta d} - 1\big) + 1 \right).$$

D-optimal design: maximizes $\mathcal{D}(d) = L_1(n)L_3(n) - L_2^2(n)$.

K-optimal design: minimizes $\mathcal{R}(d) = \big(L_1(n) + L_3(n)\big)^2 / \big(L_1(n)L_3(n) - L_2^2(n)\big)$.

Theorem. *For an OU process with linear trend $Y(s) = \alpha_0 + \alpha_1 s + U(s)$ and equidistant increasing domain design with step size $d > 0$, function $\mathcal{D}$ is monotone increasing in d, whereas $\mathcal{R}$ has at least one global minimum point, that is, there exists a K-optimal design.*

Two-point designs



Objective functions for two-point D-optimal and K-optimal designs with $\beta = 0.1$.

Theorem. *For an OU process with linear trend* $Y(s) = \alpha_0 + \alpha_1 s + U(s)$ *there exists a unique K-optimal two-point design* $\{0, d_{opt}\}$, *where* d_{opt} *is the unique solution of*

$$\left(d^2 - 2\right)\mathrm{e}^{3\beta d} + 2(\beta d + 1)\mathrm{e}^{2\beta d} - \left(\beta d^3 + d^2 + 2\beta d - 2\right)\mathrm{e}^{\beta d} - 2 = 0.$$

Simulation Study

Model: $Y(s) = \alpha_0 + \alpha_1 s + U(s),\ s \in [0,1]$. $U(s)$: stationary OU process with $\sigma = 1/4$.

True parameters: $\alpha_0 = \alpha_1 = 1$.

Design: three-point restricted design $\{0, d, 1\}$.

D-optimal design: $\{0, 1/2, 1\}$.

K-optimal design: exists for $0 < \beta < \beta^* \approx 0.5718$ and $\beta > \beta^{**} \approx 4.9586$.

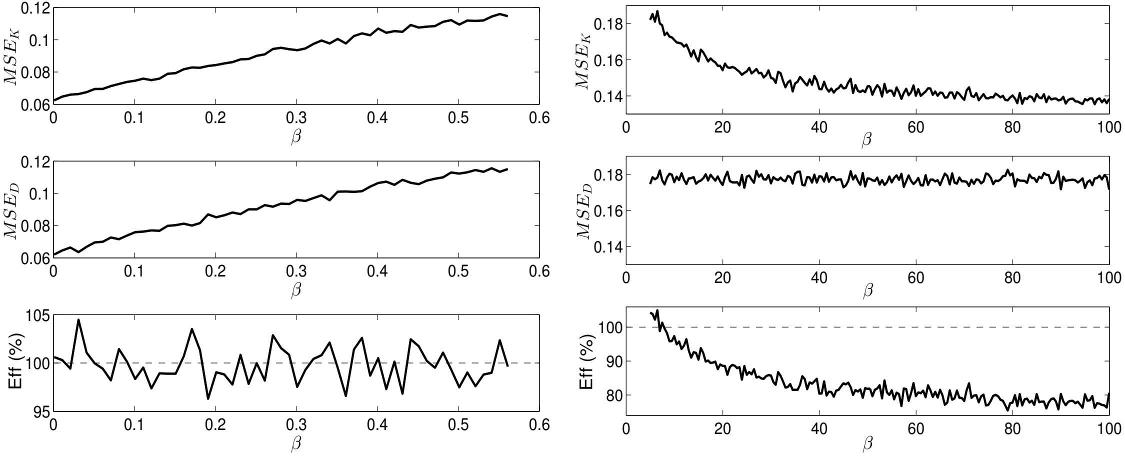
Simulation settings: 10000 independent samples of the driving Gaussian process.

$\mathrm{MSE}_K,\ \mathrm{MSE}_D$: average mean squared errors of GLS estimates of (α_0, α_1).

Relative efficiency:

$$\mathrm{Eff} := \frac{\mathrm{MSE}_K}{\mathrm{MSE}_D} \times 100\,\%.$$

Simulation Results



Average mean squared errors MSE_K and MSE_D of GLS estimates of parameters based on three-point restricted K- and D-optimal designs and relative efficiency $(\mathrm{Eff} := \mathrm{MSE}_K/\mathrm{MSE}_D \times 100\,\%)$.

Statistical Model

Ornstein-Uhlenbeck (OU) field with linear trend:

$$Y(s,t) = \alpha_0 + \alpha_1 s + \alpha_2 t + U(s,t), \qquad (s,t) \in [a_1, b_1] \times [a_2, b_2] \subset \mathbb{R}^2.$$

$U(s,t),\ s,t \in \mathbb{R}$: stationary OU field. Centered Gaussian sheet with covariance structure

$$\mathrm{E}\, U(s_1,t_1)U(s_2,t_2) = \frac{\sigma^2}{4\beta\gamma} \exp\big(-\beta|s_1 - s_2| - \gamma|t_1 - t_2|\big), \qquad \beta > 0, \quad \gamma > 0, \quad \sigma > 0.$$

Representation[1]:

$$U(s,t) = \frac{\sigma}{2\sqrt{\beta\gamma}} \mathrm{e}^{-\beta s - \gamma t} \mathcal{W}\big(\mathrm{e}^{2\beta s}, \mathrm{e}^{2\gamma t}\big).$$

$\mathcal{W}(s,t),\ s,t \in \mathbb{R}$: standard Brownian sheet. $\beta,\ \gamma,\ \sigma$: known parameters.

Regular grid design[2]:

$$\xi_{n,m} = \big\{(s_i, t_j):\ i = 1,2,\ldots,n,\ j = 1,2,\ldots,m\big\} \subset [a_1, b_1] \times [a_2, b_2],$$

$a_1 \le s_1 < s_2 < \ldots < s_n \le b_1$ and $a_2 \le t_1 < t_2 < \ldots < t_m \le b_2$, $n,m \ge 2$.

[1] Baran, S., Pap, G. and Zuijlen, M.v. (2003) Estimation of the mean of stationary and nonstationary Ornstein-Uhlenbeck processes and sheets. *Comput. Math. Appl.* **45**, 563–579.

[2] Baran, S., Sikolya, K. and Stehlík, M. (2015) Optimal designs for the methane flux in troposphere. *Chemometr. Intell. Lab.* **146**, 407–417.

Fisher Information Matrix

Model: $Y(s,t) = \alpha_0 + \alpha_1 s + \alpha_2 t + U(s,t), \quad (s,t) \in \mathcal{X} = [a_1, b_1] \times [a_2, b_2].$

$I_{\alpha_0,\alpha_1,\alpha_2}(n,m)$: FIM on parameters $\alpha_0, \alpha_1, \alpha_2$ based on observations $\{Y(s,t),\ (s,t) \in \xi_{n,m}\}$.

General form:

$$\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m) = G(n,m) C(n,m)^{-1} G(n,m)^\top.$$

$$G(n,m) := \begin{bmatrix} 1 & 1 & \cdots & 1 & 1 & 1 & \cdots & 1 & \cdots & 1 & 1 & \cdots & 1 \\ s_1 & s_1 & \cdots & s_1 & s_2 & s_2 & \cdots & s_2 & \cdots & s_n & s_n & \cdots & s_n \\ t_1 & t_2 & \cdots & t_m & t_1 & t_2 & \cdots & t_m & \cdots & t_1 & t_2 & \cdots & t_m \end{bmatrix}.$$

$C(n,m)$: covariance matrix of observations.

$$C(n,m) = P(n) \otimes Q(m), \quad \text{so} \quad C^{-1}(n,m) = P^{-1}(n) \otimes Q^{-1}(m).$$

$P(n),\ Q(m)$: covariance matrices of observations of OU processes with covariance parameters $\beta > 0$ and $\gamma > 0$ in time points $s_1 < s_2 < \ldots < s_n$ and $t_1 < t_2 < \ldots < t_m$.

Exact Form of the Fisher Information Matrix

Theorem. *For an OU field with linear trend* $Y(s,t) = \alpha_0 + \alpha_1 s + \alpha_2 t + U(s,t)$ *observed on regular grid* $\boldsymbol{\xi}_{n,m}$

$$\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m) = \begin{bmatrix} L_1(n)M_1(m) & L_2(n)M_1(m) & L_1(n)M_2(m) \\ L_2(n)M_1(m) & L_3(n)M_1(m) & L_2(n)M_2(m) \\ L_1(n)M_2(m) & L_2(n)M_2(m) & L_1(n)M_3(m) \end{bmatrix}$$

with

$$L_1(n) := 1 + \sum_{i=1}^{n-1} \frac{1-p_i}{1+p_i}, \qquad L_2(n) := s_1 + \sum_{i=1}^{n-1} \frac{s_{i+1} - s_i p_i}{1+p_i}, \qquad L_3(n) := s_1^2 + \sum_{i=1}^{n-1} \frac{(s_{i+1} - s_i p_i)^2}{1-p_i^2},$$

$$M_1(m) := 1 + \sum_{i=1}^{m-1} \frac{1-q_i}{1+q_i}, \qquad M_2(m) := t_1 + \sum_{i=1}^{m-1} \frac{t_{i+1} - t_i q_i}{1+q_i}, \qquad M_3(m) := t_1^2 + \sum_{i=1}^{m-1} \frac{(t_{i+1} - t_i q_i)^2}{1-q_i^2},$$

where $p_i := \exp(-\beta d_i)$ *with* $d_i := s_{i+1} - s_i$, $i = 1, 2, \ldots, n-1$, *and* $q_j := \exp(-\gamma \delta_j)$ *with* $\delta_j := t_{j+1} - t_j$, $j = 1, 2, \ldots, m-1$.

Spatial D- and K-optimal Designs

FIM: $\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)$ depends on distances $d_i := s_{i+1} - s_i$, $\delta_j := t_{j+1} - t_j$, $s_1 = t_1 = 0$.

D-optimal design: maximizes in $\boldsymbol{d} = (d_1, d_2, \ldots, d_{n-1})$ and $\boldsymbol{\delta} = (\delta_1, \delta_2, \ldots, \delta_{m-1})$

$$\mathcal{D}(\boldsymbol{d},\boldsymbol{\delta}) := \det\left(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\right) = L_1(n)M_1(m)\big(L_1(n)L_3(n) - L_2^2(n)\big)\big(M_1(m)M_3(m) - M_2^2(m)\big)$$

K-optimal design: minimizes in $\boldsymbol{d}$ and $\boldsymbol{\delta}$

$$\mathcal{K}(\boldsymbol{d},\boldsymbol{\delta}) = \frac{\mathrm{tr}\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) + \sqrt{6\mathrm{tr}\big(\mathcal{I}^2_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) - 2\mathrm{tr}^2\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big)}\cos(\varphi)}{\mathrm{tr}\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) + \sqrt{6\mathrm{tr}\big(\mathcal{I}^2_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) - 2\mathrm{tr}^2\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big)}\cos\left(\varphi + 2\pi/3\right)},$$

where $\varphi := \frac{1}{3}\arccos(\varrho) \in [0, \pi/3]$, with

$$\varrho := \frac{54\det\left(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\right) + \mathrm{tr}\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big)\Big(9\mathrm{tr}\big(\mathcal{I}^2_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) - 5\mathrm{tr}^2\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big)\Big)}{\sqrt{2}\Big(3\mathrm{tr}\big(\mathcal{I}^2_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big) - \mathrm{tr}^2\big(\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(n,m)\big)\Big)^{3/2}}.$$

Smith, O, K. (1961) Eigenvalues of a symmetric 3×3 matrix. *Commun. ACM* **4**, 168.

Example. Nine-point Restricted Regular Grid Design

Design space: $\mathcal{X} = [0,1]^2$.

Nine-point restricted design: $s_1 = t_1 = 0,\ s_2 = d,\ t_2 = \delta,\ s_3 = t_3 = 1$ with $0 \le d, \delta \le 1$.

$$\mathcal{I}_{\alpha_0,\alpha_1,\alpha_2}(d,\delta) = \begin{bmatrix} L_1(d)M_1(\delta) & L_2(d)M_1(\delta) & L_1(d)M_2(\delta) \\ L_2(d)M_1(\delta) & L_3(d)M_1(\delta) & L_2(d)M_2(\delta) \\ L_1(d)M_2(\delta) & L_2(d)M_2(\delta) & L_1(d)M_3(\delta) \end{bmatrix}$$

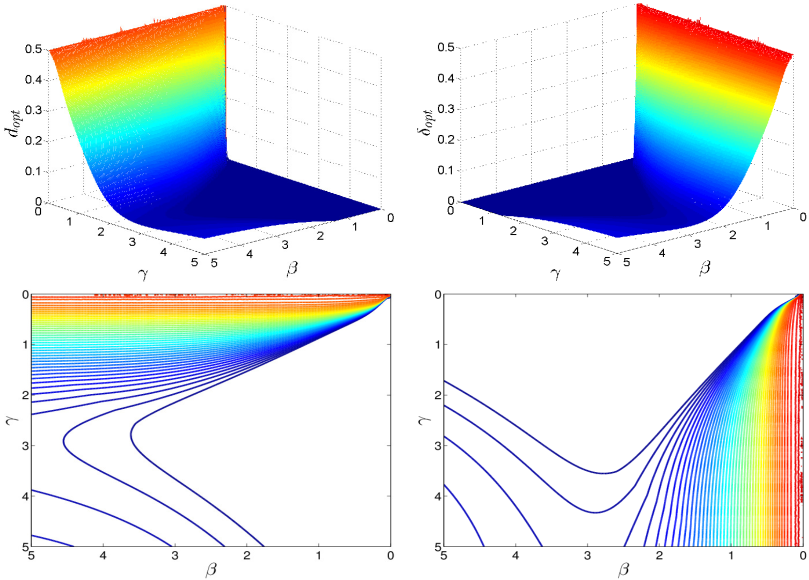
$$L_1(d) := \frac{2}{1+\mathrm{e}^{-\beta d}} + \frac{1-\mathrm{e}^{-\beta(1-d)}}{1+\mathrm{e}^{-\beta(1-d)}}, \qquad M_1(\delta) := \frac{2}{1+\mathrm{e}^{-\gamma\delta}} + \frac{1-\mathrm{e}^{-\gamma(1-\delta)}}{1+\mathrm{e}^{-\gamma(1-\delta)}},$$

$$L_2(d) := \frac{d}{1+\mathrm{e}^{-\beta d}} + \frac{1-d\mathrm{e}^{-\beta(1-d)}}{1+\mathrm{e}^{-\beta(1-d)}}, \qquad M_2(\delta) := \frac{\delta}{1+\mathrm{e}^{-\gamma\delta}} + \frac{1-\delta\mathrm{e}^{-\gamma(1-\delta)}}{1+\mathrm{e}^{-\gamma(1-\delta)}},$$

$$L_3(d) := \frac{d^2}{1-\mathrm{e}^{-2\beta d}} + \frac{(1-d\mathrm{e}^{-\beta(1-d)})^2}{1-\mathrm{e}^{-2\beta(1-d)}}, \qquad M_3(\delta) := \frac{\delta^2}{1-\mathrm{e}^{-2\gamma\delta}} + \frac{(1-\delta\mathrm{e}^{-\gamma(1-\delta)})^2}{1-\mathrm{e}^{-2\gamma(1-\delta)}}.$$

The maximizer of $\mathcal{D}(d,\delta)$ is $d = \delta = 1/2$ for all $\beta, \gamma > 0$. Equidistant design is D-optimal.

Example. K-optimal Nine-point Restricted Regular Grid Design



Minimizer of $\mathcal{K}(d, \delta)$:

$$(d_{opt}, \delta_{opt}).$$

Collapsing design:

$$d_{opt} = 0 \quad \text{or} \quad \delta_{opt} = 0.$$

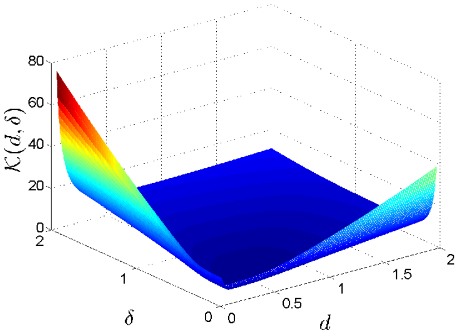
Non-collapsing K-optimal design exists outside a certain region of the (β, γ) parameter space.

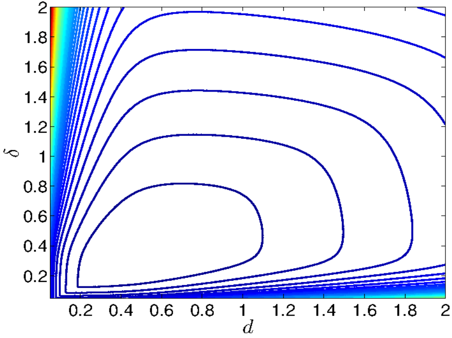
Directionally Equidistant Designs

Directionally equidistant regular grid design with step sizes $d > 0$, $\delta > 0$:

$$\xi_{n,m} = \{((i-1)d, (j-1)\delta) : \ i = 1, 2, \ldots, n, \ j = 1, 2, \ldots, m\}.$$

Theorem. *For an OU field with linear trend* $Y(s,t) = \alpha_0 + \alpha_1 s + \alpha_2 t + U(s,t)$ *observed on* $\xi_{n,m}$ *function* $\mathcal{D}(d, \delta)$ *is monotone increasing both in* d *and* δ.





Objective function $\mathcal{K}(d, \delta)$ of a four-point regular grid design $\{(0,0), (d,0), (0,\delta), (d,\delta)\}$ with $\beta = 0.2$, $\gamma = 0.3$.

Simulation Study

Model: $Y(s,t) = \alpha_0 + \alpha_1 s + \alpha_2 t + U(s,t)$.

$U(s,t)$: stationary OU field, $\sigma = 1/4$.

True parameters: $\alpha_0 = \alpha_1 = \alpha_2 = 1$.

Design: $\{0, d, 1\} \times \{0, \delta, 1\}$.

D-optimal design: $d = \delta = 1/2$.

Simulation settings: 10000 independent samples of the driving field.

MSE_K, MSE_D: average mean squared errors of GLS estimates of $(\alpha_0, \alpha_1, \alpha_2)$.

$$\mathrm{Eff} := \frac{\mathrm{MSE}_K}{\mathrm{MSE}_D} \times 100\,\%.$$

$\beta \setminus \gamma$	0.01	0.03	0.05	0.10	0.15
0.01	100.88	99.45	97.53	101.60	96.92
0.03	99.43	101.54	100.12	99.22	104.38
0.05	100.79	100.33	102.00	97.51	97.46
0.10	101.37	99.91	99.61	99.86	99.66
0.15	100.94	99.51	102.65	98.48	102.48

$\beta \setminus \gamma$	10	15	20	25	30
10	115.33	109.19	105.53	102.89	99.14
15	108.18	104.65	96.49	95.25	93.80
20	103.93	100.66	95.09	93.61	93.70
25	100.50	95.92	94.18	93.20	89.28
30	102.91	96.98	94.14	90.04	88.90

Relative efficiency Eff (100 %) of MSEs of GLS estimates of regression parameters.

Conclusions

- First study on K-optimal designs for correlated processes[1].
- Key differences between D-optimal and K-optimal designs are revealed.
- Dependence of the two designs on the covariance parameters of the driving process are investigated.
- Simulation studies: restricted K-optimal designs outperform D-optimal designs for large values of covariance parameters.

Possible further directions

- Extension of the results to complex OU processes[2,3].
- Investigation of more general regression models[4] (polynomial or trigonometric) in correlated setup.

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