Towards an Equivalence Theorem for Computer Simulation Experiments?

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Based on joint work with M. Stehlík and Luc Pronzato (started a week ago)
I take on challenge #1 from David’s list:

„create designs that are tied to our methods of analysis“

D. Steinberg (2009), ENBIS-EMSE workshop
The Setup

Random field: \[ y(z) = \eta\left(x(z), \beta\right) + \varepsilon(z) \]

with \[ E[\varepsilon(z)\varepsilon(z')] = c(z, z'; \theta) = c(d, \theta). \]

Two purposes: **prediction** or **estimation**

**Universal Kriging**: using the EBLUP and the corresponding GLS-estimator.

**Alternative**: Full ML or REML of \((\beta, \theta)\) and insert above.
Optimal Designs (for estimation)

Classical: select the inputs (and weights)

\[ \xi_N = \left\{ p_1, p_2, \cdots, p_n \right\} \]

such that a prespecified criterion

\[ \max_{z_i, p_i} \Phi \left[ M \left( \xi_N \right) \right] \]

is optimized.

Well developed theory for standard (uncorrelated) regression based on Kiefer’s (1959) concept of design measures.
Three Practical Cases:

**Case 1:** We are interested only in the trend parameters $\beta$ and consider $\theta$ as known or a nuisance.

**Case 2:** We are interested only in the covariance parameters $\theta$

(sometimes we set $\beta = 0$).

**Case 3:** We are interested in both sets of parameters equally.
D-optimal designs for estimating trend and covariance parameters

For the full parameter set the information matrix is

\[ E \left\{ \begin{array}{c}
-\frac{\partial \ln L(\beta, \theta)}{\partial \beta \partial \beta^T} \\
\frac{\partial \ln L(\beta, \theta)}{\partial \theta \partial \theta^T}
\end{array} \right\} = \begin{pmatrix}
M_\beta(\xi; \theta, \beta) & 0 \\
0 & M_\theta(\xi; \theta)
\end{pmatrix}. \]

Use the (weighted) product of the respective determinants as an optimum design criterion (Müller and Stehlík, 2009):

\[ \Phi'[M_\beta, M_\theta] = |M_\beta(\xi)|^\alpha \cdot |M_\theta(\xi)|^{1-\alpha} \]

Compound Designs

Single purpose criterion is inefficient, thus construct weighted averages

$$\Phi[\xi | \alpha] = \alpha \Phi[M(\xi)] + (1 - \alpha) \Phi'[M'(\xi)].$$

were introduced by Läuter (1976), related to constrained designs:

$$\xi^* = \arg \max_{\xi \in \Xi} \Phi[M(\xi)] \quad \text{s.t.} \quad \Phi'[M'(\xi)] > \kappa(\alpha),$$

(cf. Cook and Wong, 1994); sometimes standardized (Mcgree et al., 2008):

$$\Phi[\xi | \alpha] = \alpha \Phi[M(\xi)] / \Phi[M(\xi^*)] + (1 - \alpha) \Phi'[M'(\xi)] / \Phi'[M'(\xi^*)].$$
7 (9) Issues (surveyed in Müller & Stehlík, 2009)

1. Nonconvexity
2. Asymptotic unidentifiability ($M_\theta$)
3. Nonreplicability
4. Non-additivity
5. Smit’s paradox
6. Näther’s paradox
7. Impact of dependence on information (M&S paradox)
8. Choice of dependence structure
9. Singular designs (the role of the nugget effect)
The Impact of Dependence

Information from D-optimal design:

when \( \theta \) is estimated or not estimated respectively.
(Müller & Stehlík, 2004)
Design for prediction (EK-optimality)

Criterion often based on kriging variance, e.g.

\[
\min_{\xi} \max_{z} E[(\hat{y}(z) | \xi) - y(z))^2]
\]

Additional uncertainty from estimation of \( \theta \) is taken into account by Zhu (2002) and Zimmerman (2006):

\[
\min_{\xi} \max_{z} \left\{ \text{Var}[\hat{y}(z)] + \text{tr}\left\{ M_{\theta}^{-1} \text{Var}[\partial \hat{y}(z) / \partial \theta] \right\} \right\}
\]

Abt (1999) and Zhu and Stein (2007) supplement this by

\[
\left( \frac{\partial \text{Var}[\hat{y}(z)]}{\partial \theta} \right)^T M_{\theta}^{-1} \left( \frac{\partial \text{Var}[\hat{y}(z)]}{\partial \theta} \right).
\]
Recall the Kiefer-Wolfowitz Equivalence Theorem (1960)

(Case 1 with uncorrelated errors)

D-criterion: \[ \max_{\xi} \left| M_\beta (\xi) \right| \]

and G-criterion: \[ \min \max_{\xi} \text{Var}[\hat{y}(z) | \xi] \]

yield same (approximate) optimal designs.
Conjecture:

One can always find an $\alpha$ such that the compound design based upon

$\Phi'[M_\beta, M_\theta]$ is (in some to be defined sense) close to designs

following from Zhu’s EK-(empirical kriging)-optimality.
Example: Ornstein-Uhlenbeck process

- Constant trend $\eta(.) = \beta$
- $\text{cov}(z, z') = \sigma^2 e^{-\frac{d}{\theta}}$

**Case 1** (Kiselak and Stehlík, 2007, Dette et al., 2007): uniform (space-filling) design is D-optimal!

**Case 2** (Müller and Stehlik, 2009, Zagoraiou and Baldi-Antognini, 2009): D-optimal design collapses!

**Case 3**: regulatory version.
Exchange algorithms (Fedorov/Wynn, 1972)

consist in a simple exchange of points from the two sets $S_{ξ}$ and $X_s \setminus S_{ξ}$ at every iteration, namely

$$ξ_{s+1} = \left\{ ξ_s \setminus \left\{ x_s^-, \frac{1}{n_s} \right\} \right\} \cup \left\{ x_s^+, \frac{1}{n_s} \right\},$$

where

$$x_s^+ = \arg \max_{x \in X_s \setminus S_{ξ}} \phi(x, ξ_s) \quad \text{and} \quad x_s^- = \arg \min_{x \in S_{ξ}} \phi(x, ξ_s).$$

Version: Cook and Nachtsheim, 1980
Survey: Royle, 2002
Suggested Variant: Hybrid with Simulated Annealing

- Make the best exchange between a point from sets $S_{\xi_s}$ and a randomly chosen point from $\bar{X}_s \setminus S_{\xi_s}$ at every iteration.
- If there is no improvement, give more weight to points farther from the selected and draw anew.
- Perhaps use a stochastic acceptance operator (decreasing temperature) to improve performance.
Case 3 for $\theta = 1$ and varying $\alpha = 0, 0.7, 1$
Case 3 for $\alpha=0.9$ and varying $\theta=0.1,1,10$
Efficiency Comparison

![Graph showing efficiency comparison]

Key:
- Brimkulov et al. (1986)
- M. & Pazman (1999)
References (www.ifas.jku.at)


Müller, W.G. and Stehlík, M., “Compound Optimal Spatial Design”, accepted for *Environmetrics*.

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Problem #1: Non-additivity of the Information Matrix

Leads to unseparability of information contributions through design measures!

\[
M (\xi_N) = \frac{1}{N} \sum_{z} \sum_{z'} X(z) \left[ C^{-1} (\xi_N) \right]_{z,z'} X^T (z')
\]

Remedy: e.g. interpretation of design measures as amount of noise suppression (Pázman & M., 1998, M.+P., 2003)
Problem #2: Use of Fisher Information Matrix

If covariance parameters $\theta$ are included in the estimation (cases 2 & 3), the FI matrix contains a block

$$M'(\xi, \theta)_{ij} = \frac{1}{2} tr \left\{ C^{-1}(\xi, \theta) \frac{\partial C(\xi, \theta)}{\partial \theta_i} C^{-1}(\xi, \theta) \frac{\partial C(\xi, \theta)}{\partial \theta_j} \right\}$$

Then its interpretation as being inversely proportional to asymptotic covariance matrix of parameters fails (Abt & Welch, 1998).