Efficient Prediction Designs for Random Fields

Werner G. Müller
Department of Applied Statistics

Joint work with L. Pronzato, J. Rendas, and H. Waldl

SAMO, Nice, 21 March 2013
The Setup (continuously indexed)

Data $y$ is observed at coordinates $z \in Z \subset \mathbb{R}^2$ as being generated by a random field:

$$y(z) = \eta(x(z), \beta) + \epsilon(z)$$

Noise $\epsilon$ is usually assumed to have zero mean, finite variances and a parametrized covariance

$$E[\epsilon(z)\epsilon(z')] = c(z, z'; \theta) = c(d, \theta).$$
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.
Find good input designs $\xi$:

Objective often based on kriging variance, e.g.

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

naturally leads to

**Space-fillingness!**
Design $\xi$ for prediction (EK-optimality)

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

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

**Computationally extremely demanding!**
Simple example: bivariate O-U process...

Constant trend $\eta(.) = \beta$

$\text{cov}(z, z') = \sigma^2 e^{-\frac{|z-z'|}{\theta}}$

7-point Maximin design and EK-Isolines:

EK-value = 2.68

SAMO, Nice, 21 March 2013
... example continued

7-point EK-optimal design:

EK-value = 1.18

SAMO, Nice, 21 March 2013
Recall the Kiefer-Wolfowitz (1960) Equivalence Theorem

(uncorrelated errors)

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

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

yield same (approximate) optimal designs.
Designs for estimating trend and covariance parameters

For the full parameter set the information matrix is

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

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

\[
\{M_\theta(\xi_N)\}_{ij} = \frac{1}{2} \text{tr} \left\{ C^{-1}(\xi_N, \theta) \frac{\partial C(\xi_N, \theta)}{\partial \theta_i} C^{-1}(\xi_N, \theta) \frac{\partial C(\xi_N, \theta)}{\partial \theta_j} \right\}
\]

SAMO, Nice, 21 March 2013
Contradicting criteria
Compound Designs

Single purpose criterion is inefficient, thus construct weighted averages

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

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

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

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

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

SAMO, Nice, 21 March 2013
Relation prediction vs. estimation criterion
A simplified exchange algorithm
CD-optimal design and EK-Isolines

7-point CD-optimal design:

EK-value = 1.211
Designs generated with comparative effort
Extensions and Conclusions

- 11 < 2000 evaluations of expensive criterion;
- quick and reliable procedure whenever non-space-filling designs are required;
- particularly when observations are costly.

- More elaborate iterative procedure is available.
- Example from a real computer experiment: water quality in the North Sea is in the paper.
Submit good papers to:

Impact factor 0.683 (2012)
Find further stuff in my book:

1\textsuperscript{st} edition 1998

2\textsuperscript{nd} edition 2001

3\textsuperscript{rd} edition 2007

SAMO, Nice, 21 March 2013
New book:

Out now!

SAMO, Nice, 21 March 2013