Efficient Prediction Designs for Random Fields

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The Setup (continuously indexed)

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

$$y(z) = \eta\left(x\left(z\right), \beta\right) + \varepsilon\left(z\right)$$

Noise ε is usually assumed to have zero mean, finite variances and a parametrized covariance

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

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

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

Alternative: Full ML or REML of (β,θ) and insert above.

Find good input designs ξ:

Objective often based on kriging variance, e.g.

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

naturally leads to

S p a c e – f i l l i n g n e s s !

Design ξ for prediction (EK-optimality)

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

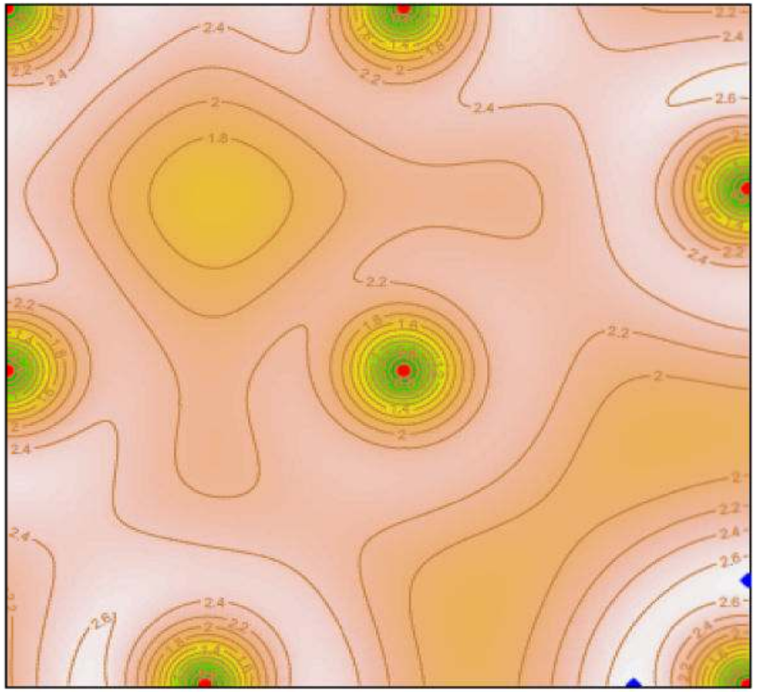
$$\min_{\xi} \max_{z} \left\{ \mathrm{var}[\hat{y}(z)] + \mathrm{tr}\left\{ M'^{-1}_{\theta} \, \mathrm{var}[\partial \hat{y}(z) / \partial \theta] \right\} \right\}$$

Computationally extremely demanding!

Simple example : bivariate O-U process ...

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

7-point Maximin design
and EK-Isolines:

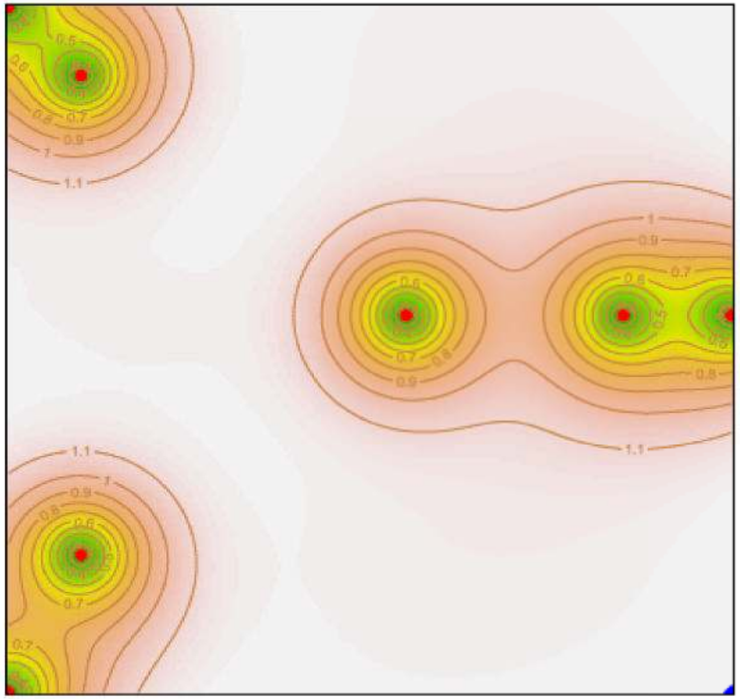


EK-value = 2.68

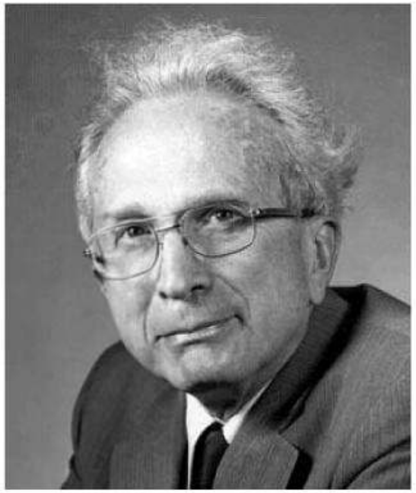
… example continued

7-point EK-optimal design:

EK-value = 1.18



Recall the Kiefer-Wolfowitz (1960) Equivalence Theorem



(uncorrelated errors)

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

and G-criterion: $\min_{\xi} \max_{z} \mathrm{Var}[\hat{y}(z) \mid \xi]$

yield same (approximate) optimal designs.

Designs for estimating trend and covariance parameters

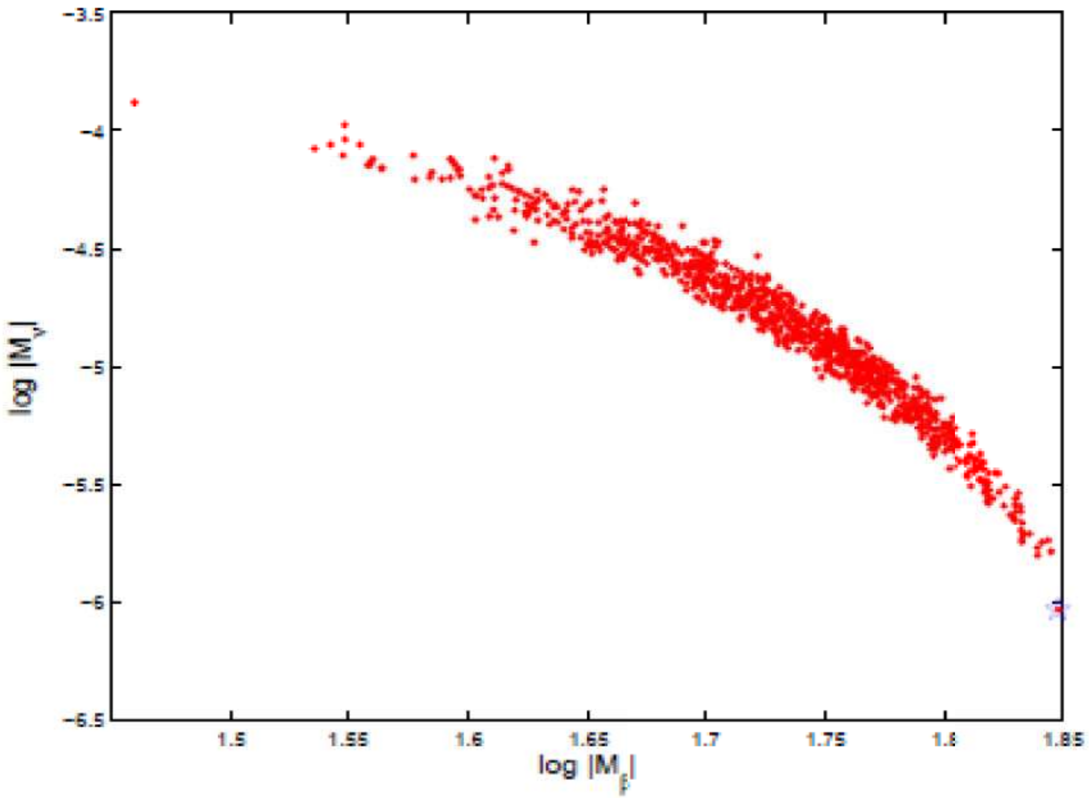
For the full parameter set the information matrix is

$$E\begin{Bmatrix} -\frac{\partial lnL(\beta,\theta)}{\partial\beta\partial\beta^T} & -\frac{\partial lnL(\beta,\theta)}{\partial\beta\partial\theta^T} \\ -\frac{\partial lnL(\beta,\theta)}{\partial\theta\partial\beta^T} & -\frac{\partial lnL(\beta,\theta)}{\partial\theta\partial\theta^T} \end{Bmatrix} = \begin{pmatrix} M_\beta(\xi;\theta,\beta) & 0 \\ 0 & M_\theta(\xi;\theta) \end{pmatrix}.$$

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

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

Contradicting criteria



Compound Designs

Single purpose criterion is inefficient, thus construct weighted averages

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

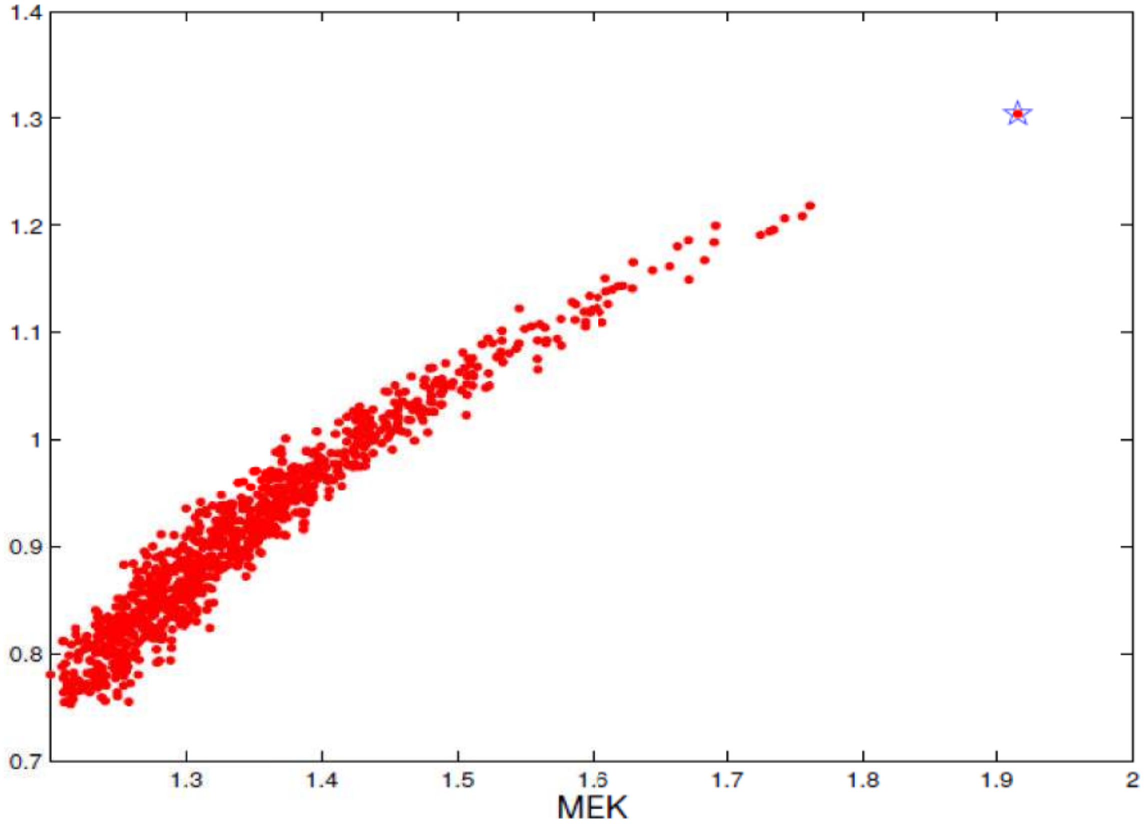
were introduced by Läuter (1976), related to constrained designs:

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

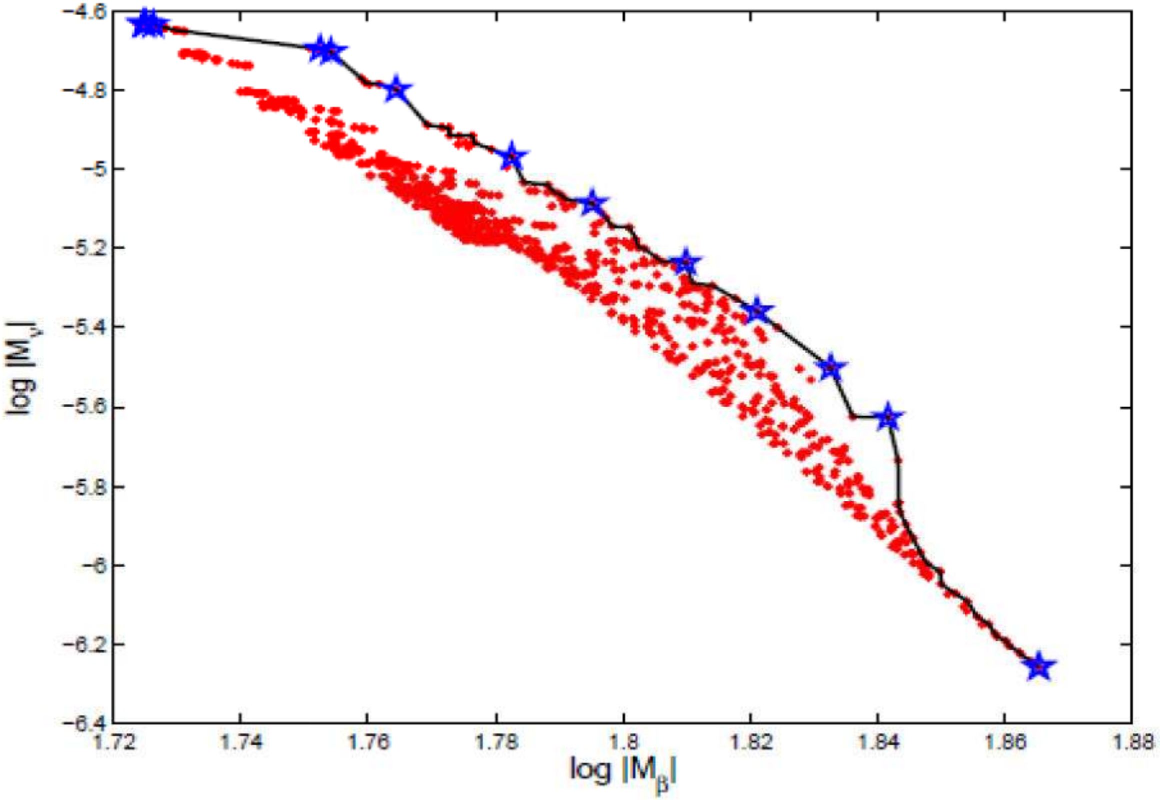
Use the (weighted) product of the respective determinants as an optimum design criterion (Müller and Stehlík, 2009, Environm.):

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

Relation prediction vs. estimation criterion



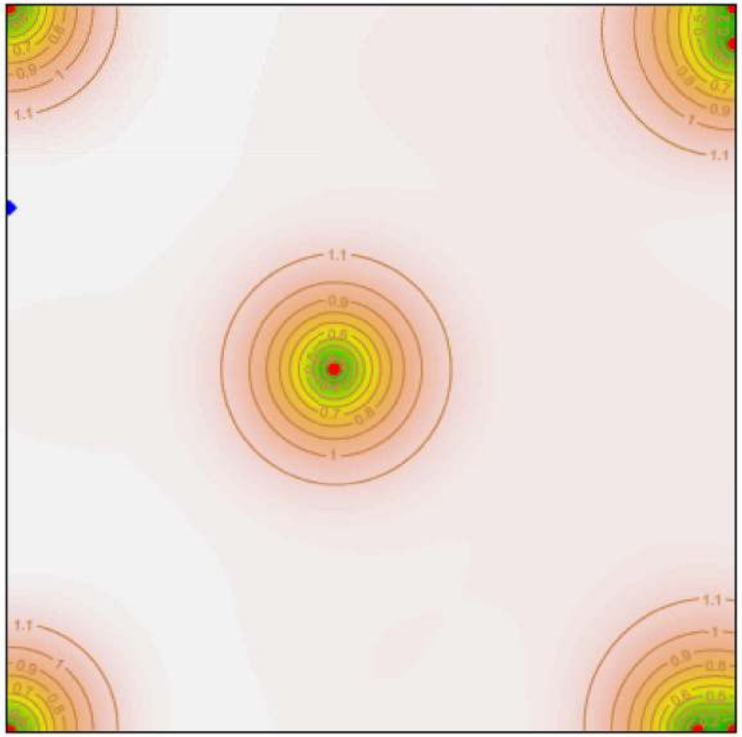
A simplified exchange algorithm



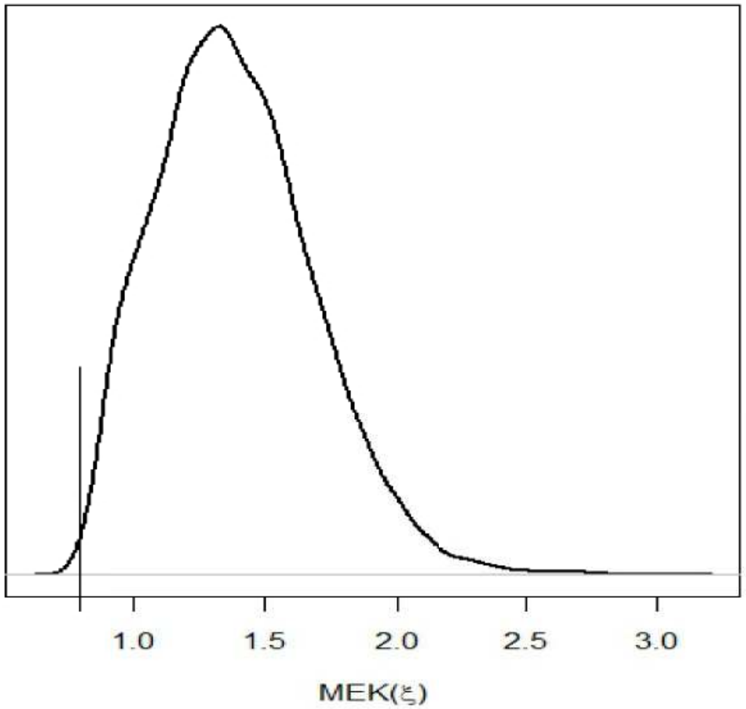
CD-optimal design and EK-Isolines

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.

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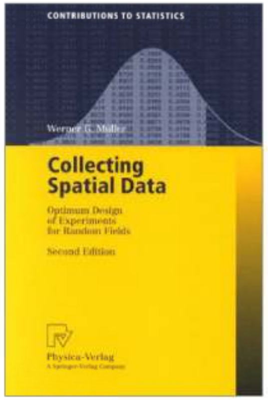

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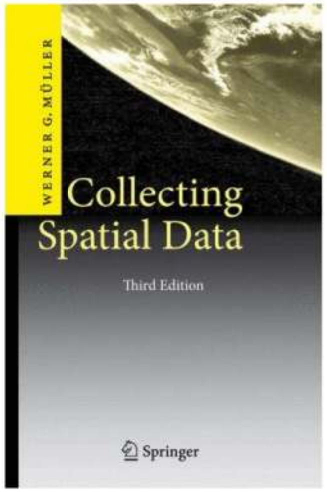

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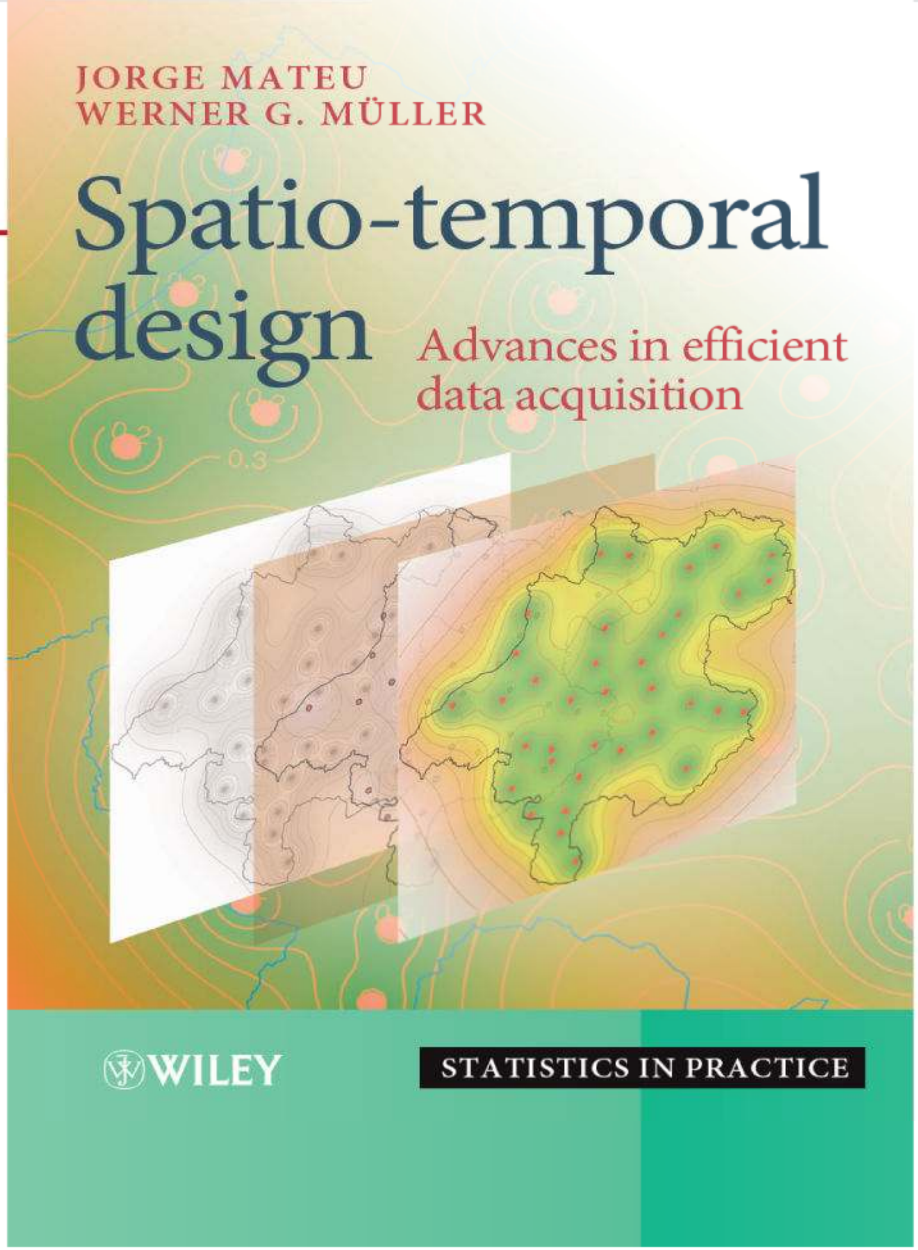

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