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Efficient Prediction Designs for Random Fields

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For estimation and prediction of random fields it is increasingly acknowledged that the kriging variance may be a poor representative of the true uncertainty. Experimental designs based on the more elaborate criteria that are appropriate for empirical kriging are very costly to determine. We investigate the possibility of using a compound criteria inspired by an equivalence theorem type relation cf.[1], to build designs sub-optimal for the empirical kriging variance.

The model underlying our investigations is the correlated scalar random field given by

$$Y(x) = \eta(x, \beta) + \varepsilon(x)\,.$$

Here, β is an unknown vector of parameters in R^p, $\eta(\cdot,\cdot)$ a known function and the random term $\varepsilon(x)$ has zero mean, (unknown) variance σ^2 and a parameterized spatial error correlation structure such that $E[\varepsilon(x)\,\varepsilon(x')] = \sigma^2 c(x, x'; \nu)$ with ν some unknown parameters.

We are interested in making predictions $\hat{Y}(\cdot)$ of $Y(\cdot)$ at unsampled locations x in a compact subset X of R^d using observations $Y(x_1), \ldots, Y(x_n)$ collected at a set of design points $\xi = (x_1, \ldots, x_n) \subset X^n$. Our objective is to select ξ (of given size n) in order to maximize the precision of the predictions $\hat{Y}(x)$ over X. One penalized design criterion for such designs is the corrected kriging variance:

$$MEK(\xi) = \max_{x \in X} \left\{ \mathrm{Var}[\hat{Y}(x)] + \mathrm{tr}\left\{ V_\nu \, \mathrm{Var}[\partial \hat{Y}(x)/\partial \nu] \right\} \right\}, \tag{1}$$

with V_ν the covariance of the ML estimator of the covariance parameters ν. Designs ξ that minimize this criterion are called EK(empirical kriging)-optimal. EK-optimal designs are typically not space-filling. This is particularly true for small numbers of observations, when prediction precision is the most sensitive to the detailed geometry of the design. Unfortunately, straightforward maximization of the EK-criterion is computationally demanding. In [4] the use of a convex composition of the two D-optimality criteria for the parameters β and ν is suggested as a surrogate for EK:

$$J_\alpha(\xi) = \alpha \log |M_\beta(\xi, \theta)| + (1 - \alpha) \log |V_\nu^{-1}(\xi, \nu)|, \qquad \alpha \in [0.1]\,, \tag{2}$$

where

$$\begin{pmatrix} M_\beta(\xi,\theta) & 0 \\ 0 & M_\theta(\xi,\theta) \end{pmatrix} = E \left\{ \begin{array}{cc} -\frac{\partial^2 \log L(\beta,\theta)}{\partial\beta\partial\beta'} & -\frac{\partial^2 \log L(\beta,\theta)}{\partial\beta\partial\theta'} \\ -\frac{\partial^2 \log L(\beta,\theta)}{\partial\theta\partial\beta'} & -\frac{\partial^2 \log L(\beta,\theta)}{\partial\theta\partial\theta'} \end{array} \right\},$$

with $L(\beta, \theta)$ the likelihood of β and $\theta = (\sigma^2, \nu)$, and $V_\nu(\xi, \nu)$ in the second term of (2) is the lower diagonal block of $M_\theta^{-1}(\xi, \theta)$.

Although, as it has been shown in [3], a strict equivalence between (1) and (2) does not hold, there is experimental evidence that that optimal designs for one of the criteria tend to perform well under the other, confirming the intuition that finding designs ξ that minimize the EK criterion (1) should be intimately related to finding designs that optimize a suitable combination of the D-optimality criteria for β and ν.

However, the ability to define a constructive experimental design method based on $J_\alpha(\cdot)$ is hampered by the lack of an efficient methodology to select α. In this paper we overcome this difficulty by considering simultaneous optimization of the two criteria $\log |M_\beta(\xi, \theta)|$ and $\log |V_\nu^{-1}(\xi, \nu)|$, and

constraining the candidate set Ξ for the minimization of (1) to the set of non-dominated designs for the corresponding multi-criteria optimization problem. The EK criterion (1) will thus play the role of a preference function for choosing designs in the reduced candidate set Ξ.

Other authors have addressed the determination of experimental designs that simultaneously optimize multiple criteria, constraining the set of possible solutions to the corresponding Pareto surface, *e.g.* [2] where the author discusses the advantages of explicit consideration of the individual criteria over the use of scalar "desirability functions" and proposes several methods to chose amongst the efficient solutions of the Pareto surface. The precise contribution of our work is to use the set of non-dominated solutions of the two identified D-optimality criteria, $\log|M_\beta(\xi,\theta)|$ and $\log|V_\nu^{-1}(\xi,\nu)|$, as a relevant (small) candidate set for EK-optimal designs. We call the designs of this constrained candidate set Pareto-optimal.

For simultaneous optimization of two criteria the Pareto surface reduces to a bounded curve (or to a finite subset of a curve when X is finite). Since the Pareto surface is also the set of maxima of all scalar functions monotone in each criterion, we can construct a finite set of candidate designs by optimizing the compound criterion $J_\alpha(\cdot)$ for a finite set of values of α. Evaluation of the corrected kriging variance over this finite subset allows the determination of a good approximation to the EK-optimal design. As the examples presented will demonstrate, our Pareto-optimal designs have high EK-efficiency, especially for designs with small size n.

References:

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