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Bayesian Geostatistical Design: Optimal Site Investigation When the Geostatistical Model is Uncertain

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Geostatistical optimal design optimizes subsurface exploration for maximum information towards task-specific prediction goals. Until recently, geostatistical design studies have assumed that the geostatistical description (i.e., the mean, trends, covariance models and their parameters) is given a priori, even if only few or no data offer support for such assumptions. This is in contradiction with the fact that the bulk of data acquisition is merely being planned at this stage.

We believe that geostatistical design should comply with the following four guidelines:

1. Avoid unjustified a priori assumptions on the geostatistical description such as claiming certainty in the geostatistical model, but to acknowledge the inevitable uncertainty of geostatistical descriptions,
2. Reduce geostatistical model uncertainty as secondary design objective,
3. Rate this secondary objective optimal for the overall prediction goal and
4. Be robust even under inaccurate geostatistical assumptions.

Bayesian Geostatistical Design (Diggle und Lophaven, 2006) follows the above four guidelines by considering uncertain covariance model parameters. These authors considered a kriging-like prediction task, using the spatial average of the estimation variance as objective function for the design. We transfer their concept from kriging-like applications to geostatistical inverse problems, thus generalizing towards arbitrary hydrogeological or geophysical data and prediction goals.

A remaining concern is that we deem it inappropriate to consider parametric uncertainty only within a single covariance model. The Matérn family of covariance functions has an additional shape parameter, and so allows for uncertain smoothness and shape of the covariance function (Zhang and Rubin, submitted to WRR). Controlling model shape by a parameter converts covariance model selection to parameter identification and resembles Bayesian model averaging over a continuous spectrum of covariance models.

We illustrate how our approach fulfills the above four guidelines in a series of synthetic test cases. The underlying scenario is a hypothetical or recent ground water contamination that may contaminate a sensitive location (e.g., a drinking water well). We minimize the prediction variance of contaminant concentration at the sensitive location by optimal placement of 24 hydraulic head and log-conductivity measurements. For the synthetic test cases, we developed and implemented a lightweight first-order approximation of Bayesian Geostatistical Design based on Ensemble Kalman Filters.

By varying the level of uncertainty in the geostatistical description in several variations of the scenario, we demonstrate and discuss the impact of structural uncertainty on geostatistical design. The sampled lag-distances change with increasing uncertain covariance function. The resulting designs efficiently reduce geostatistical uncertainty to a degree acceptable for the prediction task, and behave robust under a wide range of different geostatistical models.