Likelihood-free Simulation-based Optimal Design with an Application to Spatial Extremes

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Abstract

Simulation-based optimal design techniques are a convenient tool for solving optimal design problems with potentially complex model structures. The goal is to find the optimal configuration of factor settings with respect to an expected utility criterion. In addition, we assume that the model likelihood function is intractable but that sampling from the probability model is possible. Therefore, we utilize likelihood-free inference methods to estimate the expected utility criterion.

The methodology is applied to find the optimal design for a network of temperature measuring stations when the main interest is in inference for extreme events. The likelihood function of the multivariate extreme value distribution (Schlather model) is not available in closed form for dimensions greater than two.

Keywords: approximate Bayesian computation; expected utility; max-stable process; Schlather model.

1 Simulation-based Optimal Design

The general aim of simulation-based optimal design is to find the optimal configuration $\xi^* = \arg\sup_{\xi} U(\xi)$ for the expected utility integral (see [5])

$$U(\xi) = \int_{z \in \mathcal{Z}} \int_{\vartheta \in \Theta} u(z, \xi, \vartheta) p(z|\vartheta, \xi) p(\vartheta) d\vartheta dz.$$

If it is possible to obtain a sample $\{z^{(t)}, \vartheta^{(t)}\}_{t=1}^{T}$ from the joint distribution of the data z and the parameters ϑ conditional on the design ξ, $p(z, \vartheta|\xi)$, a straightforward way to approximate $U(\xi)$ is to use Monte Carlo integration:

$$U(\xi) \approx \hat{U}(\xi) = \frac{1}{T} \sum_{t=1}^{T} u(z^{(t)}, \xi, \vartheta^{(t)}). \tag{1}$$

This function can then be maximized using a suitable optimization algorithm. Approaches based on MCMC or particle methods are also possible (see [1], [5]).

When the goal is to optimize the experiment's expected gain in information, the most natural choice for $u(.)$ is the Kullback-Leibler divergence between the posterior and the prior distribution. If the posterior distribution has a regular shape, a useful and easy to estimate alternative for measuring the posterior precision is the inverse of the determinant of the posterior's variance-covariance matrix.

2 Likelihood-free inference

If the likelihood function is intractable, but it is possible to simulate from it, then an approximate sample from the posterior distribution can be obtained by employing *likelihood-free* methods, also called *approximate Bayesian computation (ABC)* (see e.g. [4]). The idea is to generate a joint sample of the parameters ϑ^* and the data z^* and to keep those ϑ^* for which the simulated data z^* are close to the actual data z. If the data are high-dimensional, summary statistics have to be used to mitigate the curse of dimensionality.

However, in (1) the posterior has to be computed for each simulated conditional value $z^{(t)}$, $t = 1, \ldots, T$. Performing ABC sampling separately for each $z^{(t)}$ would be computationally prohibitive. If memory capacity permits, one solution to this problem is to generate a large joint sample of ϑ^* and z^* at all possible design points before running the actual design algorithm. The sample is then re-used in every step as input to a fast ABC rejection sampler. This approach was also pursued by [2].

A second method for estimating the posterior builds on importance sampling ideas. The importance weights of the prior sample ϑ^* are updated to obtain an approximate sample from the posterior distribution. Due to the intractable likelihood, ABC is used to compute the weight updates. This approach is useful in a sequential setting, when the sample ϑ^* is a sample from an ABC posterior based on previously available observations. As before, if possible it is beneficial to create a large sample in advance and to re-use it in every step.

3 LF Simulation-based Design for Spatial Extremes

As an example, we consider optimal design for spatial data which follow an extreme value distribution (e.g. maximum monthly temperature, maximum daily rainfall). We take the data-generating process to be a max-stable process. In particular, we assume that the data are distributed according to the Schlather model ([6]). Optimal design is performed with respect to the correlation parameters, especially the range parameter of a Whittle-Matérn correlation function. Unfortunately, no likelihood function is available for the Schlather model if the dimension is greater than two, so the application of likelihood-free methods is a sensible option.

We perform likelihood-free simulation-based optimal design for a network of temperature measuring stations (c.f. [3]), for which we try out different summary statistics. The optimal design is found among a given set of candidate designs.

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