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Gradient-Based Line Search for Continuous Optimal Designs in Spatial Statistics

In spatial statistics, optimal designs select sampling locations such that a specific optimality criterion - for instance, maximizing the precision of parameter estimation or prediction accuracy - is satisfied. This task is particularly challenging in high-dimensional design spaces. Frequently, space-filling designs are used as an alternative; however, these perform well only under certain idealized conditions and fail to cover the area effectively as the dimensionality of the input space increases.

Search methods, such as the well-known sequential Wynn algorithm or the Fedorov exchange algorithm, usually add or exchange sampling locations from a finite set of candidate points, often relying on a trial-and-error approach. In the context of these algorithms, the term "gradient" is sometimes used misleadingly to denote the marginal gain in the optimality criterion resulting from a point exchange.

In this talk, the gradient is used in its genuine mathematical sense within an exchange algorithm. The presented method is compatible with continuous and differentiable optimality criteria, such as GV-optimality (Waldl & Müller, 2023). It computes the gradient of the criterion function with respect to the coordinates of the sampling locations. This gradient is then utilized within a line-search method as a descent direction to minimize the objective function. From a theoretical perspective, line-search methods are less susceptible to the curse of dimensionality than exchange algorithms that rely on a finite set of candidate points.

This strategy considerably reduces the number of criterion function evaluations, thereby identifying locally optimal designs faster than conventional exchange algorithms. Computer simulations in low-dimensional settings demonstrate interesting and promising preliminary results.

Special/ Invited session

Classification

Mainly methodology

Keywords

optimal design, exchange algorithms, gradient

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Track Classification: Design of Experiments