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Ascent with Quadratic Assistance for the Construction of Exact Experimental Designs

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In the area of experimental design, there is a large body of theoretical knowledge and computational experience concerning so-called optimal approximate designs. However, for an approximate design to be executed in a practical setting, it must be converted into an exact design, which is usually done via rounding procedures.

The first notable rounding method was suggested by Kiefer [3], who formulated the rounding problem as the minimization of the maximum of the difference between the exact and approximate design weights. By using techniques similar to those applied in voting apportionment, the authors of [4] arrived at a criterion-independent rounding algorithm known as efficient rounding (ER). More recent proposals include randomized rounding heuristics (see [1] and [5]); however, these methods are only applicable if the criterion function is submodular (e.g., D-optimality). Although generally rapid, rounding procedures have several drawbacks; in particular, they often yield worse exact designs than heuristics that do not require approximate designs at all.

In the talk, we will present a model- and criterion-based hill-climbing method, which we call ascent with quadratic assistance (AQuA), based on a quadratic simplification of the optimality criterion in the neighborhood of the optimal approximate information matrix, extending the approach of [2]. AQuA overcomes almost all of the disadvantages of ER and similar methods. In particular, the proposed method does not depend on the choice of the optimal approximate design (if the approximate design is not unique), it is not restricted to the support of the optimal approximate design, and the resulting designs are usually significantly more efficient than the designs computed via ER and somewhat more efficient than the results produced via heuristic methods that do not use approximate designs. Unlike the method proposed in [2], AQuA does not require advanced integer quadratic solvers; moreover, it is generally more efficient, and its applicability is not restricted to problems of D-optimality but rather extends to a much broader spectrum of criteria.

We numerically demonstrate the generally superior performance of AQuA relative to both rounding procedures and standard heuristics for a problem of optimal mixture experimental design.

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