Nature-Inspired Meta-heuristic Algorithms for Generating Optimal Experimental Designs

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Abstract

Nature-inspired meta-heuristic algorithms are general-purpose optimization algorithms that require little assumptions for them to work quite well. They are increasingly used across disciplines to solve complex optimization problems. Interestingly, these algorithms are rarely used in mainstream statistical research even though they are simple to implement, very flexible, computationally efficient and able to find an optimum or a nearly optimal solution quickly. The algorithms have tuning parameters, stochastic components and invariably, do not come with rigorous proofs of convergence to the global optimum.

I provide an overview of such algorithms and demonstrate their effectiveness using an exemplary algorithm called Particle Swarm Optimization (PSO). Applications will include finding different types of optimal designs for nonlinear models in toxicology and dose response studies. I will also present web-based tools based on PSO to facilitate toxicologists' search for an optimal design to estimate various benchmark doses or help clinical researchers implement an early phase trial for estimating the biologically optimal dose under a continuation ratio model.

Key words: approximate design, biologically optimal dose, equivalence theorem, hormesis, information matrix, multiple-objective optimal design.