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CatMADS: categorical variables with the MADS algorithm

Solving optimization problems where functions are blackboxes and variables involve different types poses significant theoretical and algorithmic challenges. Nevertheless, such settings frequently occur in simulation-based engineering design and machine learning. This paper extends the Mesh Adaptive Direct Search (MADS) algorithm to address mixed-variable problems with categorical, integer and continuous variables. MADS is a robust derivative-free optimization framework with a well-established convergence analysis for constrained quantitative problems. CatMADS generalizes MADS by incorporating categorical variables, handled via distance-induced neighborhoods. An exhaustive convergence analysis of CatMADS is provided, with flexible choices balancing computational cost and local optimality strength. Four types of mixed-variable local minima are introduced, corresponding to progressively stronger notions of local optimality. CatMADS integrates the progressive barrier strategy for handling constraints with guarantees. An instance of CatMADS employs cross-validation to construct problem-specific categorical distances. This instance is benchmarked against state-of-the-art solvers on 32 mixed-variable problems, half of which are constrained. Data profiles show that CatMADS achieves the best results, demonstrating that the framework is empirically efficient in addition to having strong theoretical foundations.