Summary: Optimizing expensive black-box systems with limited data is an extremely challenging problem. As a resolution, we present a new surrogate optimization approach by addressing two gaps in prior research – unimportant input variables and inefficient treatment of uncertainty associated with the black-box output. We first design a new flexible non-interpolating parsimonious surrogate model using a partitioning-based multivariate adaptive regression splines approach, Tree Knot MARS (TK-MARS). The proposed model is specifically designed for optimization by capturing the structure of the function, bending at near-optimal locations, and is capable of screening unimportant input variables. Furthermore, we develop a novel replication approach called Smart-Replication, to overcome the uncertainty associated with the black-box output. The Smart-Replication approach identifies promising input points to replicate and avoids unnecessary evaluations of other data points. Smart-Replication is agnostic to the choice of a surrogate and can adapt itself to an unknown noise level. Finally to demonstrate the effectiveness of our proposed approaches we consider different complex global optimization test functions from the surrogate optimization literature. The results indicate that TK-MARS outperforms original MARS within a surrogate optimization algorithm and successfully detects important variables. The results also show that although non-interpolating surrogates can mitigate uncertainty, replication is still beneficial for optimizing highly complex black-box functions. The robustness and the quality of the final optimum solution found through Smart-Replication are competitive with that using no replications in environments with low levels of noise and using a fixed number of replications in highly noisy environments.

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