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On-line surrogate-based optimization with multiple kernel regression for continuous and categorical variables

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Design optimization of mechanical components or systems is often confronted to mixed-variate problems characterized by continuous and categorical variables. The former can be modeled seamlessly by real parameters, the latter–representing any non-numerical data, like the selection of a geometrical shape ('circle', 'square', 'triangle'), or the choice of a material ('steel', 'titanium', 'aluminum')–must undergo a conversion process from categories to numbers. This specificity has a double impact: first, the optimization algorithm should be able to deal with mixed variables. Then, when expensive (high fidelity) simulations are required to assess the responses $\mathbf{y}(\mathbf{x})$ for a given variable vector $\mathbf{x} = \{\mathbf{x}^{cont}\ \mathbf{x}^{categ}\}$, surrogate models or metamodels tailored for mixed variables must be used to reduce drastically the number of calls to the simulation.

In a preliminary study [1], the authors have proposed a general framework for multi-objective surrogate-based optimization, combining an evolutionary algorithm with a multiple kernel regression metamodel: after a preliminary step devoted to the construction of the approximation (based on a design of experiments performed with the expensive simulation), an evolutionary algorithm adapted to mixed variables is directly coupled to the metamodel, without any call to the high fidelity model. However, for structural design examples, a lower accuracy of the metamodel was observed when the optimizer converged to the multi-objective Pareto front; in other words, the metamodel built on an initial training database was not reliable enough when the evolutionary algorithm further explored the design space towards optimal solutions.

Therefore, the aim of this contribution is to propose a novel surrogate-based optimization algorithm leaning on an online procedure filling in the training database during the generations of the evolutionary optimization [2]. The main feature of the method lies in algorithmic developments allowing to update the multiple kernel regression metamodel at a very economical computational cost.

The full paper will include a complete validation process on analytical benchmark test cases in single-objective optimization, as well as on multi-objective applications, i.e. in truss sizing. Both are characterized by continuous and categorical parameters.

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