Bayesian optimization for mixed continuous and categorical variables: A latent variable approach

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Abstract:

Physical experiments are necessary during the design stage of new industrial components. However, these experiments are expensive and time consuming. Thus, most of the time, designers rely on numerical optimization involving a physical simulator, based for instance on finite element method, Monte Carlo, etc., that provides an approximation of the physical behavior of the system. This simulation process takes into account the actual physical parameters, which can be separated into two kinds: continuous variables (e.g. width, length, temperature) and categorical, or discrete variables (e.g. material, shape, number of components).

Resorting to simulators allow the analysis of a large set of possible solutions, from which one can extract a reduced set of promising configurations to be tested in expensive physical experiments. This search for configurations can be seen as the resolution of an optimization problem, which can be very demanding in terms of computing time, especially in the case of mixed problems, involving both continuous and categorical variables.

Optimization involving expensive simulators is a topic widely studied in the literature [6], [1]. In this work, we focus on Bayesian optimization (BO), which is particularly suitable for solving such problems [2]. More precisely, Bayesian optimization is a sequential design strategy that requires a data-driven mathematical model or metamodel and a selection criterion. Where, the metamodel is trained from a reduced set of simulation data and the selection criteria is used to propose new configurations to be simulated in the next iteration. This continues until convergence or the maximal computational budget is reached.

Efficient global optimization (EGO) [4] is an adaptive sampling approach to global optimization that combines kriging as the metamodeling strategy and expected improvement (EI) as the selection criterion. EGO often outperforms other state-of-the-art approaches due to its properties of simultaneously improving the metamodel approximation at each iteration (exploration) and finding the optimal value of the function (exploitation) [7].

When it comes to mixed inputs, the most common approach is to adapt metamodels and selection criteria to exploit information from both continuous and non-continuous variables and preserve desirable mathematical properties in the search for the global optimum [5].

However, recent developments in metamodels involving mixed variables show that it is possible to transform categorical variables into a set of continuous ones by estimating a set of latent variables

[8], [3]. Latent variables emulate the properties of the original variables and their contribution to the metamodel prediction. Motivated by this, and by the fact that categorical variables in physical problems can often be explained by a smaller set of unknown continuous variables, we developed the LV-EGO algorithm, as a modified version of the EGO algorithm that proposes a relaxation from categorical to continuous variables, through a latent variable mapping.

In LV-EGO, we start with the original mixed variables, then estimate the latent variables that will be used to train the kriging surrogate in a full continuous framework. Then we use a modified EI criterion to select a new candidate as a feasible point in the original mixed space. With this, we can continue the regular BO and use the already known advantages of the EGO in continuous variables for a scenario with mixed variables.

We compare our approach to approaches working directly on the mixed input space and adapting the EGO with state of the art mixed variables surrogates in a deterministic example. Finally, we discuss applications to real design problems and the future of our approach in terms of generalizing optimization in the presence of mixed variables.

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Short biography – Jhouben Cuesta Ramirez, is a PhD. student at CEA-LETI and Mines Saint Etienne. He received his BSc. in Electrical Engineering in the Universidad Tecnológica de Pereira, Pereira Colombia, in 2013 and his MSc. degree in Electrical Engineering in the Universidad Tecnológica de Pereira, in 2015. He is a former associate professor in Corporación Universitaria Minuto de Dios in 2018, and lecturer in Universidad Tecnológica de Pereira in 2016.