A new mixed-categorical correlation kernel for Gaussian process

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PhD expected duration: Oct. 2020 – Sep. 2023

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Abstract

Expensive-to-evaluate blackbox simulations play a key role for many engineering and industrial applications. In this context, surrogate models have been widely used to adress a large range of applications, e.g., aircraft design [9], deep neural networks [10], coastal flooding prediction [6], agriculture forecasting [4] or seismic imaging [2]. In general, these blackbox simulations are complex and may involve mixed-categorical input variables. Typically, an aircraft design tool may need to consider variables such as the number of panels, the list of cross sectional areas or the material choices. As a result, there has been a growing interest for mixed-categorical models based on Gaussian process (GP) surrogates, particularly in the context of Bayesian optimization.

In this setting, several existing approaches use different strategies to handle mixed-categorical variables. These approaches either use continuous kernels (e.g., continuous relaxation [3] and Gower distance based [5] GP) or use a direct estimation of the correlation matrix such as the Homoscedastic Hypersphere (HH) kernel [7]. To combine both approaches, we developed a kernel-based approach that extends continuous exponential kernels to handle mixed-categorical variables denoted Exponential Homoscedastic Hypersphere (EHH) kernel [8]. The proposed kernel leads to a new GP surrogate that generalizes both the continuous relaxation and the Gower distance based GP models.

However, the EHH and HH kernels significantly increase the number of hyperparameters related to the surrogate GP model. Therefore, a second contribution addresses this issue by constructing the surrogate model with fewer hyperparameters. The reduction process is based on the Partial Least Squares (PLS) regression [1] which has previously been developed for the continuous relaxation based GP [9]. We show how to generalize Kriging with PLS for the more general HH kernel using an extension of the PLS regression to matrices.

We demonstrate, on both analytical and engineering problems, that our proposed GP models give a higher likelihood and a smaller residual error than the other kernel-based state-of-the-art models.

Our methods are available in the open-source software SMT.

Short biography

This work is part of the activities of ONERA - ISAE - ENAC joint research group. This research is performed in the framework of the AGILE 4.0 project and has received funding from the European Union Horizon 2020 Programme under grant agreement n° 815122.

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