

Surrogate GSA with categorical and continuous inputs.

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Many real-world problems combine qualitative and quantitative input features. To address these, we perform Global Sensitivity Analysis in the presence of categorical (i.e. discrete valued) inputs alongside continuous ones. The strategy employed is to treat each categorical combination or state as a separate output in a multi-output Gaussian process (MOGP), using an RBF kernel for continuous inputs. Sobol' indices are extended to assess the influence of continuous inputs on the correlation between categorical states. This in turn is related to the influence of the categorical state on the Sobol' indices of the output. In this way one may effectively consider cooperation between categorical and continuous inputs to influence the output. The possibility of multi-task learning, where different categorical states inform each other via the MOGP is investigated, and its effect on GSA is outlined.

Applications are presented to engineering problems, such as a synthesis where certain chemical analyses may fail under some conditions, or certain categorical combinations have only been sparsely investigated as they are considered unpromising. An important application is to syntheses where the categorical inputs are the choice of ingredients or conditions, recently explored using a related approach [1].

The ultimate benefit of GSA is often to reduce the number of inputs in order to aid experimental design and optimisation of the synthesised material. The approach outlined here is particularly suited to situations where training data is sparse, and must be utilised to maximum effect, for example in pharmaceutical production where syntheses may be extremely expensive. This should also prove useful in wider applications, not related to synthesis.

[1] Y. Comlek, L. Wang, and W. Chen, "Mixed-Variable Global Sensitivity Analysis for Knowledge Discovery and Efficient Combinatorial Materials Design.", *ASME. J. Mech. Des.*, **146**(5):1–10, 2024.

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