

DIMENSIONALITY REDUCTION-BASED AFFINITY LEARNING FOR CATEGORICAL VARIABLES IN SURROGATE-BASED OPTIMIZATION - APPLICATION TO STRUCTURAL AND MECHANICAL DESIGN

Charlotte Beauthier⁽¹⁾, Christophe Dumeunier⁽¹⁾, Rajan Filomeno Coelho⁽¹⁾, Rémy Nigro⁽¹⁾,
Caroline Sainvitu⁽¹⁾, Annick Sartenaer⁽²⁾

⁽¹⁾Cenaero

⁽²⁾University of Namur, Namur Institute for Complex Systems (naXys)

Keywords: Surrogate-based optimization, Mixed-variable optimization, Evolutionary algorithms, Derivative-free optimization, Categorical variables, Mixed distance, Affinity, Dimensionality Reduction

Abstract

Because many industrial applications involve both continuous and categorical variables, this work focuses on the efficient handling of mixed variables within a surrogate-based optimization framework. Since both surrogate model construction and the optimization process require meaningful comparisons between individuals characterized by mixed variable types, we propose a variant of a heterogeneous distance function that inherently relies on metrics tailored to each variable type. In particular, the overlap metric traditionally used for categorical variables is enhanced by introducing the concept of affinities between the possible categorical values, referred to as attributes. These affinities represent weighted relationships between attributes and reflect their relative influence on the output responses. They are typically defined based on the designer's physical insight, allowing the distances between attributes to be adjusted so as to modify the topological representation of the design space.

To alleviate this reliance on expert knowledge, an automatic procedure for defining attribute affinities is proposed, based on a dimensionality reduction technique known as Uniform Manifold Approximation and Projection (UMAP). UMAP aims to uncover intrinsic topological structures by preserving neighborhood relationships. In the proposed setting, samples yielding similar responses are mapped close to one another, while samples exhibiting significantly different behaviors are placed farther apart, resulting in a clustering-based approach for identifying attribute affinities.

Numerical results on benchmark problems inspired by structural, thermal and mechanical design applications are presented to assess the impact of the proposed strategy. Moreover, results are also shown on a demonstrator (namely, a multi-stage compressor) where the goal consists in finding the optimal design of the compressor. In this case, a pre-design tool is used to quickly assess the aerodynamical performances. The challenge of this optimization problem, which is

high-dimensional, with mixed variables, and highly constrained, helps us to prove the importance of efficiently handle natively mixed variables in a surrogate-based optimization framework.