

## PROPOSITION DE STAGE EN COURS D'ETUDES

Référence : **DTIS-2024-13**  
(à rappeler dans toute correspondance)

Lieu : Palaiseau

Département/Dir./Serv. : DTIS/M2CI

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### DESCRIPTION DU STAGE

Thématique(s) : Conception et Optimisation des Systèmes

Type de stage :  Fin d'études bac+5     Master 2     Bac+2 à bac+4     Autres

**Intitulé : Machine learning-based approach for quality-diversity conditional search space problems**

Sujet :

Complex engineering design problems, such as those involved in aerospace fields (e.g., reusable launcher, new aircraft configurations to reduce the environmental footprint), require the use of numerically costly simulation codes in order to predict the behavior and performance of the system to be designed. To perform the design of the systems, these codes are often embedded into an optimization process to provide the best design while satisfying the design constraints. For instance, for the design of a launch vehicle [1], classical objective function to be minimized can be: the launcher cost, the environmental impact, the propellant consumption, the Gross-Lift-Off-Weight and considered constraints might be the maximal allowed loads undertaken during the trajectory to ensure the structural integrity of the launcher and the satellites.

These optimization problems often involve mixed continuous, discrete and categorical design variables allowing to take into account technological choices into the design process [4,5]. Classical continuous variables might be the stage diameter, the masses of propellants, and the parameters of the guidance law for the trajectory. Discrete variables can be the number of rocket engines and categorical variables can be the type of material (e.g., composite, aluminum alloy) or the propellant type (e.g., LOx/LH2, LOX/CH4, LOx/RP1). In addition, in these design problems, another specific type of design variables called 'conditional variables' may be encountered which modify the structure of the optimization problem (e.g., the number of design variables, the number of constraints) depending on the value taken by these conditional variables [6]. For instance, the conditional variable 'propulsion type' for a rocket engine with two choices: 'propulsion type' = {'solid', 'liquid'} activates different continuous variables (e.g., propellant grain geometry parameters for solid propulsion type and turbine pressure ratio for the liquid rocket engine). Optimization problems involving 'conditional variables' are called 'Conditional Search Space Problem' (CSSP) and require a specific treatment to deal with the tree-structured search space [6].

Recently, new approaches, called Quality-Diversity (QD) [2,3,7,8,9], have been proposed in order to enhance the exploration of the design space through exploring some feature functions that are interesting to assess trade-offs. The result is a set of designs that are optimal with respect to the objective function but also interesting and diversified with respect to the feature functions (e.g., maintenance costs, availability, reliability). It allows to propose to the decision-makers a variety of interesting designs. For instance, for launch vehicle design problem.

When dealing with objective, constraints and feature functions involving complex simulations (e.g. Computational Fluid Dynamics), traditional QD algorithms [2,3] are unaffordable due to computational expensive simulations. Alternatively, approaches based on machine learning such as Bayesian Optimization (BO) techniques [7,8,9] can be used in order to efficiently solve the QD problem while limiting the number of evaluations of the exact intensive functions. BO approaches have been adapted to deal with QD problems with continuous variables. However, in the literature, up to now, such approaches are not adapted to deal with mixed continuous, categorical and conditional variables for CSSP.

In this work, it is proposed to develop a new Quality-Diversity methodology for problems involving mixed continuous, categorical and conditional variables with machine learning approaches (e.g., Bayesian optimization, Gaussian processes). The objective is to propose an approach able to deal with conditional search space problems while limiting the number of exact function evaluations. The performance of the proposed method will be assessed on a benchmark of analytical problems as well as on an industrial design optimization problem dealing with aerospace systems (e.g., reusable launch vehicle). This work will be related to the work of L. Baraton (PhD. student from ONERA/ISAE).

#### Work plan:

- State-of-the-art on Quality-Diversity algorithms, on Conditional Search Space Problem and on machine learning dedicated techniques (Bayesian optimization, Gaussian process)
- Development of a new Quality-Diversity methodology to deal with mixed continuous, categorical and conditional variables
- Application of the proposed approach on a benchmark of analytical problems and on an aerospace design problem

#### References

- [1] M. Balesdent, L. Brevault, B. Paluch, R. Thépot, R. Wuilbercq, N. Subra, S. Defoort, M. Bourgaie, B. Vieille (2023) Multidisciplinary design and optimization of winged architectures for reusable launch vehicles, Acta Astronautica, Elsevier
- [2] Mouret, J. B., & Clune, J. (2015). Illuminating search spaces by mapping elites. arXiv preprint arXiv:1504.04909.
- [3] Fontaine, M. C., Togelius, J., Nikolaidis, S., & Hoover, A. K. (2020, June). Covariance matrix adaptation for the rapid illumination of behavior space. In Proceedings of the 2020 genetic and evolutionary computation conference (pp. 94-102).
- [4] Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E. G., & Guerin, Y. (2019). Efficient global optimization of constrained mixed variable problems. Journal of Global Optimization, 73, 583-613.
- [5] Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2021, July). Constrained Bayesian optimization over mixed categorical variables, with application to aircraft design. In AeroBest 2021.
- [6] Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E. G., & Guerin, Y. (2021). Bayesian optimization of variable-size design space problems. Optimization and Engineering, 22, 387-447.
- [7] Kent, P., Gaier, A., Mouret, J. B., & Branke, J. (2023). BOP-Elites, a Bayesian Optimisation Approach to Quality Diversity Search with Black-Box descriptor functions. arXiv preprint arXiv:2307.09326.
- [8] Hagg, A., Wilde, D., Asteroth, A., & Bäck, T. (2020, August). Designing air flow with surrogate-assisted phenotypic niching. In International Conference on Parallel Problem Solving from Nature (pp. 140-153). Cham: Springer International Publishing.
- [9] Gaier, A., Asteroth, A., & Mouret, J. B. (2018). Data-efficient design exploration through surrogate-assisted illumination. Evolutionary computation, 26(3), 381-410.

Est-il possible d'envisager un travail en binôme ? **Oui**

#### Méthodes à mettre en oeuvre :

- |   |  |
|---|--|
| <input type="checkbox"/> Recherche théorique            | <input type="checkbox"/> Travail de synthèse             |
| <input checked="" type="checkbox"/> Recherche appliquée | <input type="checkbox"/> Travail de documentation        |
| <input type="checkbox"/> Recherche expérimentale        | <input type="checkbox"/> Participation à une réalisation |

Possibilité de prolongation en thèse : **Non**

**Durée du stage :** Minimum : 4 months Maximum :

Période souhaitée : March - August

### PROFIL DU STAGIAIRE

Connaissances et niveau requis :  
Applied mathematics, machine learning  
Knowledges in Python

Ecoles ou établissements souhaités :  
3rd year of engineering school, or Master 2