Master thesis proposal

Discovering new eco-materials for batteries using Bayesian optimization

Keywords : Surrogate modeling/Bayesian optimization, material database, environnemental impacts, battery

SCIENTIFIC DESCRIPTION :

Including sustainability in a design optimization process is not an easy task as the environnemental choices most often relie on database of discrete properties (Ansys Granta, Ecoinvent etc...). we use Variational AutoEncoders (VAEs) to represent discrete material properties in a continuous latent space, enabling gradient-based multi-objective optimization for material selection that balances mechanical performance with eco-efficiency, such as minimizing CO2 footprint, energy consumption, and waste at fixed topology [1]. It uses a promising differentiable material representation of existing database [2].

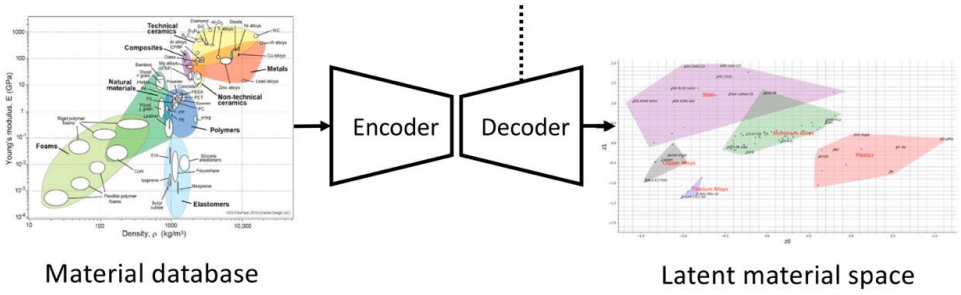

Figure 1: Differentiable material representation using VAE [2]

Recently we use our SMT2.0 framework [3] for predicting crystal structure using Kaggle database [4] as a first experience in material science application (SMT has been applied mainly to Aircraft Fluid/solid mechanics simulation tool). This field offered large database of materials with often different kind of variables. It seems SMT is really suited for this kind of application as it naturally treats mixed type variables (continuous, discrete, categorical, hierarchical) in the BO process.

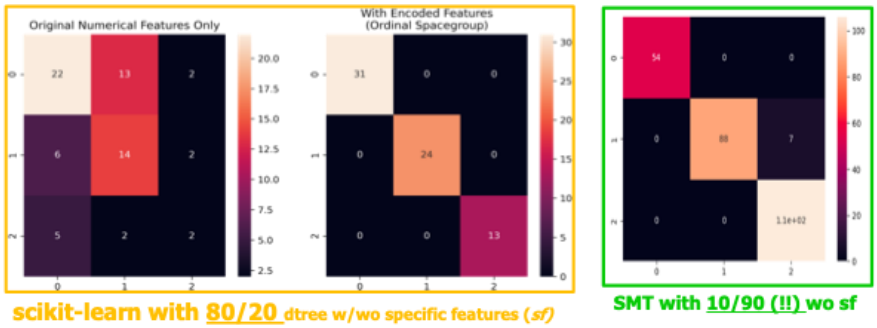

Figure 2: Classical prediction of crystal structure [3] versus mixed variables prediction using SMT 2.O [3]. This result has been presented at GDR I-GAIA 2024.

Master thesis proposal

We target a new application in the field of Discovering new eco-materials for batteries using Bayesian optimization with our in-house python code SEGOMOE [5] based on SMT [3] or a new opensource toolbox [6] also based on SMT.

The final goal will be to develop a prediction tool for new battery material taking into account physical parameters (Young's modulus, density etc…) and environnemental impacts (GWP, CO_2, water consumption etc…) and data coming from the literature [7,8] or database such as ecoinvent.

Techniques/methods in use : AI method so called VAE for Variational Autoencoders, Bayesian optimization with mixed type variables (continuous, discrete, categorical, hierarchical).

References (blue with the PI)

[1] Yepes Llorente, L., Morlier, J., Sridhara, S., & Suresh, K. (2024). A hybrid machine learning and evolutionary approach to material selection and design optimization for eco-friendly structures. Structural and Multidisciplinary Optimization, 67(5), 69.

[2] Chandrasekhar, A., Sridhara, S., & Suresh, K. (2022). Integrating material selection with design optimization via neural networks. Engineering with Computers, 38(5), 4715-4730.

[3] Saves, P., Lafage, R., Bartoli, N., Diouane, Y., Bussemaker, J., Lefebvre, T., ... & Martins, J. R. (2024). SMT 2.0: A Surrogate Modeling Toolbox with a focus on hierarchical and mixed variables Gaussian processes. Advances in Engineering Software, 188, 103571.

[4] Agrawal, D., Crystal System Properties for Li-ion batteries, Properties of Li-ion silicate to predict the crystal system class of the battery, Kaggle, March 2020.

[5] Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., ... & Morlier, J. (2019). Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and technology, 90, 85-102.

[6] Lafage, R. (2022). egobox, a Rust toolbox for efficient global optimization. Journal of Open Source Software, 7(78), 4737.

[7] Barke, A., Thies, C., Popien, J. L., Melo, S. P., Cerdas, F., Herrmann, C., & Spengler, T. S. (2021). Life cycle sustainability assessment of potential battery systems for electric aircraft. Procedia CIRP, 98, 660-665.

[8] Villacis, S., Rahn, A., Brand-Daniels, U., & Vogt, T. (2025). Towards Sustainable Aviation: End-of-Life Scenarios for Lithium-Ion Batteries used in Hybrid Electric Aircraft. Procedia CIRP, 135, 1252-1258.

Budget description and use : Internship salary for 5 months

Applicant skills : Python Programing, material sciences and strength of materials.

Industrial partnership : AIRBUS in the framework of the PhD CIFRE thesis of Shantanu SAPRE

Internship supervisor(s) : Morlier Joseph, joseph.morlier@isae-supaero.fr

Saves Paul, paul.saves@ut-capitole.fr

Internship location : ISAE-SUPAERO, 10 avenue Marc Pellegrin, 31400 Toulouse

Possibility for a Doctoral thesis : Yes