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PDOPT: A Python library for Probabilistic Design space exploration and OPTimisation.

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Software

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Summary

Contemporary engineering systems are characterised by many components and complex interactions between them. The design of such systems entails high uncertainty due to the large number of parameters defining it. An approach to manage it is exploring and evaluating as many alternatives as possible, before committing to a specific solution. The Python package PDOPT aims to provide this capability without the high computational cost associated with the factorial-based design of experiments methods. By exploiting a probabilistic machine learning model, the code identifies the areas of the design space which are most promising for the requirements provided by the user. The result is a large number of feasible design points, aiding the designer in understanding the behaviour of the system under design and selecting the desired configuration for further development.

Statement of need

PDOPT, short for Probabilistic Design and OPTimisation, is a Python package for design space exploration of systems under design. It implements a set-based approach for mapping the requirements of the design space, using a probabilistic surrogate model trained on the provided design model. This procedure enables one to identify the best candidate areas of the design space with the minimum number of assumptions of the design of the system.

The API of PDOPT was designed as a library with class-based interfaces between the components of the framework. This ensures both flexibility and transparency, as the user can inspect the main data structure between the phases of the framework. A full PDOPT test case consists of two phases: the Exploration phase and the Search phase. The first one surveys the design space to identify the areas that are most likely to satisfy the constraints over the quantities of interest of the model. This is carried out by breaking down the design space into a hypercube of parameters's levels (named sets), and rapidly evaluating them with the probabilistic surrogate model. The second phase introduces a multi-objective optimisation problem in each surviving design space area for recovering the individual design points. The result is multiple local Pareto fronts, one for each set. The aggregation of these design points yields the global Pareto front with feasible suboptimal points. Interactive visualisation tools can be used to analyse the results and proceed with design selection. Thanks to the Exploration phase, the computational cost for design space exploration can be reduced by up to 80% (Spinelli, Anderson, et al., 2022).

PDOPT is intended to be used by researchers and engineers alike in developing complex engineering systems. It has been developed within the FutPrint50 project (*FutPrInt50*, 2020) and released as open-source software under the MIT license. The software has been used in several scientific publications regarding the design of hybrid-electric aircraft (Spinelli, Enalou, et al., 2022), and the effects of operating conditions (Spinelli, Krupa, Kipouros, Berseneff, et al., 2023) and technological uncertainty (Spinelli, Krupa, & Kipouros, 2023) on the design.

Availability

PDOPT can be found on GitHub (Spinelli, 2023) and is compatible with the latest Python release. The release includes a PDF manual as a user guide and API reference. An example test set-up is also provided in the GitHub repository. Dependencies include the standard Python scientific stack (`numpy`, `scipy`, `pandas`, `matplotlib`) with the addition of the `scikit-learn` machine learning library, the `pymoo` multi-objective optimisation framework, and the `joblib` parallelisation library. As an optional feature, `plotly` can be installed to take advantage of the prototypical decision-making environment packaged with the library.

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References

FutPrInt50. (2020). https://www.futprint50.eu/

Spinelli, A. (2023). PDOPT. In *GitHub Repository*. GitHub. https://github.com/spinjet/pdopt-code

Spinelli, A., Anderson, L., Enalou, H. B., Zaghari, B., Kipouros, T., & Laskaridis, P. (2022). Application of probabilistic principles to set-based design for the optimisation of a hybrid-electric propulsion system. *IOP Conference Series: Materials Science and Engineering*, *1226*(1), 012064. https://doi.org/10.1088/1757-899X/1226/1/012064

Spinelli, A., Enalou, H. B., Zaghari, B., Kipouros, T., & Laskaridis, P. (2022). Application of probabilistic set-based design exploration on the energy management of a hybrid-electric aircraft. *Aerospace*, *9*(3). https://doi.org/10.3390/aerospace9030147

Spinelli, A., Krupa, G. P., & Kipouros, T. (2023). Set-based design space exploration to investigate the effect of energy storage durability on the energy management strategy of a hybrid-electric aircraft. *AIAA SCITECH 2023 Forum*. https://doi.org/10.2514/6.2023-0837

Spinelli, A., Krupa, G. P., Kipouros, T., Berseneff, B., & Fiette, S. (2023). Investigation of the operational flexibility of a regional hybrid-electric aircraft. *Journal of Physics: Conference Series*, *2526*(1), 012021. https://doi.org/10.1088/1742-6596/2526/1/012021