Open-source Development of Frequency Correlation Kernels for Metamodels and Bayesian Optimization Applied to Aerostructure Calculations

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Dates: March 11 to July 15: 4 to 6 months, ~670€/month
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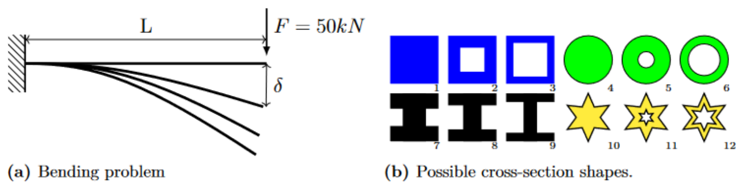
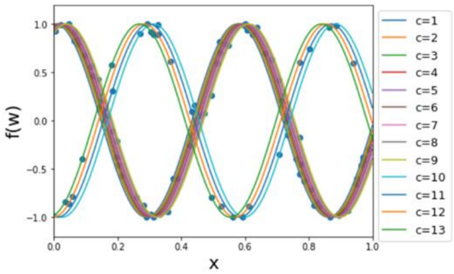


The Cantilever beam bending problem featuring categorical choice



Experimental results of Roustant testcase From SMT and f(d) = -theta_1 sin^2(theta_2d)

As part of several research projects in partnership with industry, ISAE-SUPAERO and ONERA are developing innovative methods for designing and optimizing aircraft and other coupled systems using metamodels in the preliminary design phase. This internship aims to contribute to this approach by focusing on the development of frequency correlation kernels for metamodels, with particular application to Bayesian optimization in mechanics and time-frequency analysis [1-3]. Several works have focused on modeling mixed correlation kernels, such as [4], but these kernels are limited to exponential formulations and should be extended to classes of kernels such as Matern or Exponential Squared Sine. In the field of mechanics, frequency is a crucial parameter, particularly in the context of vibration analysis. Moreover, the high dimensionality of the problems poses a challenge in the choice and application of kernels. The extension of Matérn kernels to handle high dimensionality will be discussed, enabling better adaptation to problems involving a large number of parameters.

Skills

- Mastering of Scientific Computing, Python programming
- Basics of Mechanics, Modeling and Statistics
- Knowledge in Multidisciplinary optimization or Operations research
- Interest for Ecological or Aerospace Engineering

Scientific challenges

These kernels will be applied to classical test cases such as a mixed cosine problem or the cantilever beam problem to evaluate their performance [5-6]. An interesting extension concerns aeroelasticity, particularly for high aspect ratio wings. The use of SHARPy as a reference tool will enable us to explore how frequency correlation kernels can be applied in this specific domain [7]. Other applications will be considered for the prediction of greenhouse gas concentrations and for air traffic management as part of broader ecological projects. The integration of these developments into the Surrogate Modeling Toolbox (SMT) will be a major component of the internship. The aim is to enable access to kernels via handles and to allow the use of user-defined kernels, thus contributing to the improvement of the toolbox [8]. SMT 2.0 is an open-source software package featuring numerous substitution models, including mixed-variable Gaussian processes and gradient-enhanced models developed by ISAE-SUPAERO, ONERA, ICA, NASA, University of California at San Diego, University of Michigan and Polytechnique Montréal (https://smt.readthedocs.io/en/latest/). The technical aspects of the internship will include the implementation of gradient-based likelihood optimization methods, with an emphasis on automatic differentiation. In addition, the use of evolutionary algorithms to optimize kernel likelihood within the framework of Bayesian optimization will be explored [9]. Finally, integer mixed modeling and latent variables will be considered to extend the capabilities of metamodels to handle complex, frequency and discrete variable problems.

External/Internal references

1) Wilson, A., and Adams, R. "Gaussian process kernels for pattern discovery and extrapolation." International Conference on Machine Learning. PMLR, 2013.
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Saves, P., Diouane, Y., Bartoli, N., Lefebvre, T., and Morlier, J. (2023). "A mixed-categorical correlation kernel for Gaussian process." Neurocomputing, 126472.
4) Roustant, O., Padonou, E., Deville, Y., Clément, A., Perrin, G., Giorla J., and Wynn, H.. "Group kernels for Gaussian process metamodels with categorical inputs." SIAM/ASA Journal on Uncertainty Quantification8.2 (2020): 775-806.
5) Cheng, G. H., Younis, A., Hajikolaei, K. H., and Wang, G. G. (2015), 'Trust region based mode pursuing sampling method for global optimization of high dimensional design problems', Journal of Mechanical Design 137, 021407.
6) Michele, C., Morlier, J., and Bauerheim, M. "Prediction of Gust Aeroelastic performance of HALE using Graph Neural Networks." AIAA SCITECH 2023 Forum. 2023.
7) Saves, P., Lafage, R., Bartoli, N., Diouane, Y., Bussemaker, J., Lefebvre, T., Hwang, J. T., Morlier, J. and Martins, J. "SMT 2.0: A Surrogate Modeling Toolbox with a focus on hierarchical and mixed variables Gaussian processes." Advances in Engineering Software 188 (2024): 103571.
8) Gamot, J., Balesdent, M., Tremolet, A., Wuilbercq, R., Melab, N., and Talbi, E. G. (2023). Hidden-variables genetic algorithm for variable-size design space optimal layout problems with application to aerospace vehicles. Engineering Applications of Artificial Intelligence, 121, 105941.