Postdoctoral research topic

- Title of the proposed topic: Bayesian Calibration of Computer Models with Applications to Climate Simulations
- Research axis of the 3IA: Axe 1 - Core Elements of AI
- **Supervisor: Maurizio Filippone, EURECOM, maurizio.filippone@eurecom.fr**
- Co-supervisor: Motonobu Kanagawa, EURECOM, motonobu.kanagawa@eurecom.fr
- The laboratory and/or research group: Data Science Department, EURECOM

Apply by sending an email directly to the supervisor.
The application will include:

- Letter of recommendation of the supervisor indicated above
- Curriculum vitæ including the list of the scientific publications
- Motivation letter
- Letter of recommendation of the thesis supervisor

All the requested documents must be gathered and concatenated in a single PDF file named in the following format: LAST NAME of the candidate_Last Name of the supervisor_2021.pdf

---

Description of the topic:
Optimizing parameters of computer models implementing some complex physical phenomenon is a classic problem in Statistics, which finds numerous applications in various fields such as climatology, environmental sciences, biology, and mechanical engineering [1]. This task is usually challenging for a number of computational and statistical reasons. Running the computer model for any given parameters is typically computationally expensive, making it unfeasible to use standard optimization tools. Also, the abstraction provided by the computer model can only be accurate to a certain degree, so that it is difficult to draw meaningful conclusions on the value of the optimal parameters [2].
The framework of Bayesian calibration of computer models offers an established methodology to tackle such limitations [1]. In Bayesian calibration, computational difficulties are bypassed by emulating the response of the computer model with a surrogate statistical model, which is much cheaper to evaluate, and statistical limitations are addressed by explicitly accounting for the discrepancy between the computer model and the real phenomenon of interest. This yields an elegant framework to characterize the uncertainty in model parameters and in the predictions on unseen conditions [1,3].
The modeling assumptions on the surrogate function and the discrepancy become of central importance in Bayesian calibration. In this context, we find two main challenges that require special care when using Bayesian calibration in practice:

(i) when the computer model generates multiple responses, there is a difficulty in modeling the covariance structure of these variables, and this is particularly relevant for applications where such structure is domain knowledge; how can we encode dependencies among these in a meaningful way?
(ii) The introduction of a discrepancy term in the formulation of Bayesian calibration poses some difficulties in being able to draw meaningful conclusions on the values of the parameters; how can we address the lack of identifiability of calibration parameters for these models?

This project aims at advancing the state-of-the-art in these directions, by drawing from the literature on Bayesian deep learning. In particular, we will focus on the connections between Bayesian Deep Neural Networks and Deep Gaussian Processes [3,4], and revisit calibration models in light of recent works on Variational Autoencoders [5]. The project will focus on applications to climate simulations, with the intention of engaging with the Coupled Model Intercomparison Project (CMIP) [6] and/or collaborating with researchers in the network of collaborators of the two supervisors.

References

[1] Kennedy, M. C. and O'Hagan, A. (2001). "Bayesian calibration of computer models." Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63(3): 425–464.

[2] Brynjarsdóttir, J. and O'Hagan, A. (2014). "Learning about physical parameters: The importance of model discrepancy." Inverse Problems, 30(11): 114007.

[3] Marmin, S. and Filippone, M. (2021). "Deep Gaussian Processes for Calibration of Computer Models". Bayesian Analysis, to appear.

[4] Cutajar, K., Bonilla, E. V., Michiardi, P., and Filippone, M. (2017). "Random Feature Expansions for Deep Gaussian Processes." In Precup, D. and Teh, Y. W. (eds.), Proceedings of the 34th International Conference on Machine Learning, volume 70 of Proceedings of Machine Learning Research, 884–893. International Convention Centre, Sydney, Australia: PMLR.

[5] Khemakhem, I., Kingma, D., Monti, R., and Hyvarinen, A. (2020). "Variational Autoencoders and Nonlinear ICA: A Unifying Framework." In Chiappa, S. and Calandra, R. (eds.), Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics, volume 108 of Proceedings of Machine Learning Research, 2207–2217. PMLR. 25

[6] https://www.wcrp-climate.org