PhD Position: "Conformal Prediction and Physics-Informed Machine Learning"

1 Research Project

1.1 Context

Conformal Prediction (CP) (Vovk et al., 2005; Lei et al., 2018) has recently emerged as one of the most widely used technique for uncertainty quantification in the prediction of supervised machine learning models. The core idea is relatively simple: instead of predicting a single value (such as a label class in classification or a scalar in regression), it uses a non-conformity score function to construct a prediction set that contains the true target value Y with a probability greater than a specified coverage level $1 - \alpha$.

During this PhD we aim to develop CP methods in the context of Physics-informed Machine Learning (PiML) (Karniadakis et al., 2021; Hao et al., 2023). PiML has recently emerged as a promising way to learn efficient surrogate solvers for Partial Differential Equations (PDEs) and to learn prediction models using both real-data and the physical knowledge brought by a PDE. However, despite indisputable advances, PiML remains an emerging topic that raises many open problems.

In this context, several research directions emerge. Regarding CP alone, a lot has been done in the construction of prediction sets for a univariate target variable Y. However, far less research has been made when Y is a structured multivariate output, such as a spatio-temporal one (Sun, 2022; Dheur et al., 2025). This specific setting indeed brings the question of taking into account the correlation structure between the dimensions of Y. Another important research direction is also to develop CP for the problem of model selection and uncertainty minimization when several prediction models are available. These two challenges are particularly relevant in the context of PiML, where the target data are naturally spatio-temporal and where multiple physical knowledge can lead to several potential models. In this case, open questions notably include: can CP be used to measure the uncertainty of PiML models? how can CP be refined to take into account the spatio-temporal nature of the data induced by physical applications? given a family of pretrained PiML, how can we construct a valid prediction set while selecting the model that minimizes the width of the set?

1.2 Research Objectives

This research project will consider the different challenges and questions mentioned above, with a particular focus on the problem of CP with multivariate and spatio-temporal output data, so as CP with different models and sources of uncertainty.

A first possible research direction is to extend the work of Le Bars and Humbert (2025) to multivariate output data, including spatio-temporal ones. The objective will be to learn a non-conformity CP score function, that notably takes into account the correlation structure of Y, in order to reduce the size of the prediction set and the uncertainty. In the context of PiML, the objective will be to include the knowledge brought by the PDE in the learning of the score function.

More generally for conformal PiML, we will aim at designing CP frameworks that are tailored to PiML models, whether we are dealing with a PDE surrogate solver (Podina et al., 2024), or a prediction model learned with real data and an PDE-based regularizer (Doumèche et al., 2024). In both cases, we expect that the physical knowledge brought by the PDE should be included in the design of the CP method (see e.g. Xu et al. (2024)). In particular, an interesting lead is to quantify the uncertainty of a surrogate solver to the initial conditions.

In a second time, the recruited PhD student will investigate the problem of performing conformal prediction with several models or sources of uncertainty. Among the questions that we would like to investigate, there is the one of model selection or model aggregation based on conformal prediction. In other words, given a family of models, how to select the model that minimizes the width of the CP set? In this context, simply choosing the model with the smallest empirical set breaks the statistical validity of CP methods. This issue is a well-known phenomenon in multiple testing and transductive CP, necessitating the correction of the sets to maintain validity. While this question has started to be investigated in (Yang and Kuchibhotla, 2025; Liang et al., 2024), it remains to make a proper link with more classical cross-validation techniques for model selection in ML (Arlot and Celisse, 2010). More specifically to PiML, the objective would be to study several strategies for combining multiple PiML models related to different variants of PDEs and to quantify the uncertainty of the resulting combined model. Several key questions will be investigated, such as how to construct a valid prediction set by combining the prediction sets given by each PiML models (as in Humbert et al. (2023) or Gasparin and Ramdas (2024) for instance) and how to detect and use the potential relationships between the different PDEs to minimize the size of the final prediction set.

1.3 Timeline

The tentative work-plan for this PhD is as follows:

1. M1-M6: Review the existing literature on Conformal Prediction and Physics-informed Machine Learning. Explore the different ways of performing CP for PiML. Apply the standard baselines for the models cited in MELISSA (e.g. Swift-Hohenberg)

2. M4-M16: Develop a theoretical Conformal Prediction framework adapted to multivariate or spatio-temporal data. Extend the work of Le Bars and Humbert (2025) to this setting, taking into account the physical knowledge brought by a PDE. Apply this to a neural network being a surrogate solver of a PDE, or to a ML model, learned with a physical prior regularization or not.

3. M12-M30: Consider the setting with performing CP with multiple models, and propose new methods for model selection using conformal prediction. Extend this to the PiML problem where we have access to several PDEs being uncertain.

4. M24-M32: Show the relevance of the proposed approaches on real-world data coming from the MELISSA applications (see the following section).

5. M30-M36: Write the thesis manuscript and prepare for the defense

1.4 Expected skills

The applicant is expected to have studied machine learning and/or statistics, and to have good mathematical skills. Some knowledge in optimization and physics, so as a broad interest for the topic of Physics-informed ML is a plus.

2 Research environment

This research project is funded by the ANR project MELISSA (MEthodological contributions in statistical Learning InSpired by SurfAce engineering). In MELISSA, members are conducting research in statistical machine learning, following the constraints, the physical background knowledge and the observations of physical phenomena involved in repeated laser impacts on surfaces.

The hired PhD student will be based in the Inria Magnet team (Lille, France) and will be jointly supervised by Marc Tommasi, Batiste Le Bars and Pierre Humbert (CNRS, LaMME, Evry, France). Together, they gather a world-leading expertise in Machine Learning and Conformal Prediction. This project will stimulate existing and emerging collaborations with other research groups on themes at the intersection between machine learning, statistics and physics. For instance, there will be opportunities to collaborate with other members of the MELISSA project in Saint-Étienne (Laboratoire Hubert Curien, Teams MALICE, Data Intelligence and Laser-Matter interaction) and Sorbonne University (Laboratoire ISIR, MLIA Team).

References

Arlot, S. and Celisse, A. (2010). A survey of cross-validation procedures for model selection.

Dheur, V., Fontana, M., Estievenart, Y., Desobry, N., and Taieb, S. B. (2025). A unified comparative study with generalized conformity scores for multi-output conformal regression. In *Forty-second International Conference on Machine Learning*.

Doumèche, N., Bach, F., Biau, G., and Boyer, C. (2024). Physics-informed machine learning as a kernel method. In *The Thirty Seventh Annual Conference on Learning Theory*, pages 1399–1450. PMLR.

Gasparin, M. and Ramdas, A. (2024). Merging uncertainty sets via majority vote. *arXiv preprint arXiv:2401.09379*.

Hao, Z., Liu, S., Zhang, Y., Ying, C., Feng, Y., Su, H., and Zhu, J. (2023). Physics-informed machine learning: A survey on problems, methods and applications.

Humbert, P., Le Bars, B., Bellet, A., and Arlot, S. (2023). One-shot federated conformal prediction. In *International Conference on Machine Learning*, pages 14153–14177. PMLR.

Karniadakis, G. E., Kevrekidis, I. G., Lu, L., Perdikaris, P., Wang, S., and Yang, L. (2021). Physics-informed machine learning. *Nature Reviews Physics*, 3(6).

Le Bars, B. and Humbert, P. (2025). On volume minimization in conformal regression. In *Forty-second International Conference on Machine Learning*.

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. J., and Wasserman, L. (2018). Distribution-free predictive inference for regression. *Journal of the American Statistical Association*, 113(523):1094–1111.

Liang, R., Zhu, W., and Barber, R. F. (2024). Conformal prediction after efficiency-oriented model selection. *arXiv preprint arXiv:2408.07066*.

Podina, L., Rad, M. T., and Kohandel, M. (2024). Conformalized physics-informed neural networks. *arXiv preprint arXiv:2405.08111*.

Sun, S. (2022). Conformal methods for quantifying uncertainty in spatiotemporal data: A survey. *arXiv preprint arXiv:2209.03580*.

Vovk, V., Gammerman, A., and Shafer, G. (2005). *Algorithmic learning in a random world*. Springer.

Xu, R., Sun, Y., Chen, C., Venkitasubramaniam, P., and Xie, S. (2024). Robust conformal prediction under distribution shift via physics-informed structural causal model. *arXiv preprint arXiv:2403.15025*.

Yang, Y. and Kuchibhotla, A. K. (2025). Selection and aggregation of conformal prediction sets. *Journal of the American Statistical Association*, 120(549):435–447.