école doctorale **sciences pour l'ingénieur et microtechniques**

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| **PhD title:** Uncertainty quantification for machine and deep learning techniques | |
| **Host laboratory:** FEMTO-ST | |
| **Speciality of PhD:** Engineering science | |
| **Keywords:** Uncertainty quantification, Neural networks, Diagnosis, Breast Cancer. | |

**Job description:**

**Context and motivation:** Most of the real physical system and everyday situations include uncertainty. This is the case for medical diagnosis, weather forecasting, evolution of the stock market and so on. In the literature two types of uncertainty are distinguished: aleatoric uncertainty denotes the one that is inherent to the data, e.g., noise in measurements or natural variability of the inputs, and epistemic uncertainty related to the model and due to lack of knowledge. Measuring the uncertainty is important, so as to support the user in the action to take. For example, when an anomaly is detected, with weak confidence level, another source of information should be added (image, human intervention, etc.) before planning intervention actions. More generally, quantification of the prediction uncertainty allows to trust or not predictions. In fact, incorrect overconfident predictions can be harmful and lead to erroneous decision.

**State of the art:** Uncertainty quantification (UQ) is an open research issue. For Neural Networks (NN), the standard approach has been to train a Bayesian neural network based on the idea of replacing deterministic values of the NN parameters by probability distributions with Gaussian prior and aim at learning the parameters of these distributions. Once trained, the NN outputs can be evaluated multiple times to obtain an empirical output distribution, [1], [2] and [3]. However, these approaches usually consider small NN architectures to avoid prohibitive complexity. In [4], the authors propose a method that can be applied even for complex NN architecture using the dropout. The authors show that using dropout in NN can be interpreted as a Bayesian approximation of a Gaussian process. The dropout is activated in test time, and the NN is evaluated multiple time to get the model uncertainty. On the other hand, a non bayesian approach has been proposed in [5], using the ensemble. The limit is the computational cost since many copies of the NN are trained adversely. As an alternative the Platt scaling method is used to transform the output of the algorithm to probability distribution, initially proposed for classification [6]. An extension to regression has been proposed in [7], by adding a calibrating procedure for any regression algorithm so that the confidence interval includes the true output. The above cited works suppose particular distribution form (independent identically distributed data, Gaussian), which may be limited in some applications. Furthermore, the conformal prediction is a distribution free approach with, to create a rigorous uncertainty sets for the predictions of any model [8]. The idea is to define a score function measuring the model uncertainty to get an interval of confidence for regression, and a set of plausible classes are given for classification. The prediction set can be adaptive to each input, i.e the set is larger when the model is uncertain. Nevertheless, the efficiency is conditioned by good choice of the score function, otherwise the approach is usefulness [9]. In addition, the approach is only valid for exchangeable data and with symmetric algorithm. For deep learning, a review of UQ techniques is given in [10]. UQ is a crucial part in the decision-making process, despite the diversity of the state of the art, many research directions are still opened. For distribution restrictive approaches, studying the coverage proof, and relaxing initial hypothesis (iid data, Gaussian process). Regarding conformal prediction, many questions still be opened related to exchangeability of the data and the coverage properties. Moreover, considering noisy and missing data, that are often encountered, when evaluating uncertainty is also relevant research perspective.

**Goal of the thesis:** The goal of this thesis is to develop a robust method to evaluate uncertainty for machine and deep learning algorithm predictions. Major of works focused on improving the algorithm performance, few works deal with measuring the uncertainty related to the predictions. In particular in this thesis we want to relax some hypothesis in the existing approach related to the distribution of the data and symmetry of the algorithm. This subject is challenging with many theoretical and applicatives difficulties. It is multidisciplinary including competences in probability, statistic and data processing. The two principal goal are:

- First, we aim to measure the impact of uncertainty miss evaluation on the decision.
- The second part is focused on developing new method to quantify uncertainty, that can be applied to different type of data and without restrictive constraint on distribution or the exchangeability.
- The third part, includes generalization of the proposed method when we have noisy and/or missing data.

The second part include study of the theoretical aspects: proof of convergence, complexity issue. In addition to practical aspects: independence from the chosen algorithm, architecture of the NN, implementation... Finally, a validation criterion is defined to attest the performance of the uncertainty measure.

**Application:** In this thesis, the aim is to propose a general approach in the sense to be applied for different machine and deep learning techniques. Moreover, the particular context of breast cancer diagnostic is considered to get proof of concept of the method. This thesis aims to: 1) Quantify the impact of ignoring the uncertainties on the decision. 2) Provide accurate uncertainty measure to get supplementary information to support the decision about the patient score. 3) Deal with noisy and missing data when evaluating uncertainties.

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**Applicant profile:** Master in applied mathematics (or equivalent). Probability, statistic. Good skills in Python programming. Experience in machine learning/deep learning

**Financing Institution:** MESRI

**Application deadline:** 15 June 2023

**Start of contract:** Fall 2023

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