DÉFINITION DU DOMAINE DE VALIDITÉ EN IA AVEC PRÉDICTION CONFORME : APPLICATION AUX SÉRIES TEMPORELLES À HAUTE FRÉQUENCE

DEFINING DOMAIN OF VALIDITY IN AI WITH CONFORMAL PREDICTION: APPLICATION TO HIGH FREQUENCY TIME SERIES

Etablissement **Université Paris-Saclay GS Mathématiques**

École doctorale **Mathématiques Hadamard**

Spécialité **Mathématiques appliquées**

Unité de recherche **LaMME - Laboratoire de Mathématiques et Modélisation d'Evry**

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Financement Contrats ED : Programme blanc GS-Maths, Programme doctoral en Intelligence artificielle UDOPIA

Le sujet a un financement potentiel 'UDOPIA' par concours.

Le/la candidat.e devra en parallèle candidater à d'autres sources de financement (ex: 'Programme blanc de la GS Math', bourses LMH).

Début de la thèse le **1 octobre 2022**

Mots clés - Keywords

apprentissage automatique, quantification de l'incertitude, données fonctionnelles, séries temporelles, inférence conforme, domaine de validité
machine learning, uncertainty quantification, functional data, time series, conformal inference, domain validity

Profil et compétences recherchées - Profile and skills required

Master en mathématiques appliquées, statistique, données des science ou équivalent.
Expériences en théorie de l'apprentissage, statistiques mathématiques, modélisation et calcul scientifique (eg. Python, R ou matlab).
Familiarité avec les statistiques de grande dimension, les séries temporelles ou l'analyse de données fonctionnelles.
Intérêts pour les applications scientifiques et industrielles des méthodes d'apprentissage automatique.
Master in applied mathematics, statistics, data science or equivalent.
Experiences in learning theory, modelling and scientific computing (eg. Python, R or matlab).
Familiarity with high dimensional statistics, time series or functional data analysis.
Interests in scientific and industrial applications of machine learning methods.

Description de la problématique de recherche - Project description

Les algorithmes d'apprentissage automatique sont couramment utilisés dans les processus décisionnels complexes. Malgré leurs performances impressionnantes dans les tâches prédictives en pratique, on sait peu de choses sur la façcon d'attacher de la confiance à la sortie de ces algorithmes. Ce projet concerne la définition du domaine de validité vers une IA de confiance. Nous proposons de développer des techniques basées sur la prédiction conforme pour évaluer l'impact local des données et identifier la zone de prédiction sûre. Un intérêt particulier est de traiter les données sous la forme de données de séries chronologiques à haute fréquence provenant de capteurs. Le cadre d'inférence conforme a été présenté comme un moyen pratique de mesurer la preuve dans les prédictions, ce qui permet de construire des ensembles de prédiction de confiance avec un taux d'erreur garanti d'une manière sans distribution. Sa simplicité et sa flexibilité ont gagné en popularité ces dernières années et ont démontré la nécessité et le potentiel de telles méthodes. Malgré son succès, la méthode se limite à un paramétrage standard avec des échantillons complets et représentatifs pour une tâche bien définie de problèmes de prédiction, supervisés ou non. Pour résoudre le problème des données dépendantes, irrégulièrement échantillonnées ou contaminées, ce projet propose d'utiliser une représentation alternative des données à haute fréquence en tant que variables à valeur de fonction.
Machine learning algorithms are routinely employed in complex decision-making processes. Despite their impressive performance in predictive tasks in practice, little is known about how to attach confidence to the output of such algorithms. This project concerns with identifying safe prediction zone. A special interest is in dealing with data in the form of high frequency time series data from sensors. The conformal inference framework has been put forward as a practical way to measure the evidence in the predictions, which allows to construct confidence prediction sets with guaranteed error rate in a distribution free manner. Its simplicity and flexibility has gained much popularity in recent years and demonstrated the need and potential of such methods. Despite its success, the method is limited to a standard setting with complete and representative samples for a well defined task of prediction problems, supervised or unsupervised. To

address the problem of dependent data, irregularly sampled or contaminated, this project proposes to utilize an alternative representation of high frequency data as function valued variables.

Thématique / Domaine / Contexte

uncertainty quantification, trusted AI, complex data, applications in mobility, transportation and energy

machine learning, statistics, data science, statistical learning

We contribute to trusted AI as it is now a major challenge for the development of AI in our society. The unprecedented progress in performance and scalability of Machine Learning models has permitted to address and solve impressively difficult problems. There is no doubt on the role of AI in the industry or for improving the society, nevertheless one of the major hurdles to mass adoption lies in the identification of high-risk use cases that needs reliable AI solutions. The EU has presented in April 2021 its regulation law project based on a risk analysis of AI use-cases: medical applications, loan granting, autonomous vehicles etc. (https://digital-strategy.ec.europa.eu/en/policies/european-approach-artificial-intelligence)
Trustworthy AI is now a vivid scientific that aims at studying and controlling some specific properties of models: Transparency, Uncertainty and Robustness.
Quite remarkably, Uncertainty quantification is poorly addressed in machine learning in a generic way. We are particularly concerned with the recent scientific stream ``Distribution Free and Uncertainty Quantification', its interaction with explainable AI and reliability.

In this project, we focus on uncertainty in the regression. In a standard setting where the training data are independent and identically distributed (i.i.d.) from unknown distribution, the solution for uncertainty quantification is well known. The conformal prediction framework allows us to construct a prediction set that contains the new response variable with high probability. It does so by introducing a conformity score function, which is a function of training data and the new observations. This property is known as marginal validity and does not vary over the feature space. A more relevant concept for understanding the effect of the features would be the conditional validity. However, it is known to be impossible to achieve the conditional validity in a meaningful sense. Instead a weaker form of local validity is proposed, which amounts to partitioning the feature space into subsets and construct the prediction set locally.
Although valid for any choice of the score function, efficiency measured by the volume of the sets depends on the choice of scoring method, that is, a poor choice of the scoring function can create a prediction set with too large volume. The algorithm is computationally intensive and is difficult to scale up to high dimensional problems. For computational efficiency, inductive or splitting conformal method is generally adopted. A more efficient variant of jackknife method based on residuals is also available.
There is limited research in the non-standard setting where the data are not i.i.d. which is the focus of this project.

Objectifs

We aim at developing uncertainty quantification techniques based on Conformal Prediction (CP) in order to give insight into the domain of validity of the model. In particular, we aim at evaluating the usage of uncertainty in building the domain of validity.
The domain of validity is not yet uniquely defined. In particular, we are interested in computing confidence intervals for identifying the domain of validity based on a measure of precision of the prediction. In addition, the domain of validity is also the domain where the decisions of the models are easily understood, i.e intelligible.
We propose to focus on the construction of CP with conditional coverage in order to
(i) have local confidence intervals of various lengths that help locate safe prediction zones
(ii) complement local explainable approaches such as Same Decision Probabilities (SDP, Amoukou and Brunel, 2021). In that case, we select subsets of locally important variables by looking for variables that inflate significantly the confidence intervals when they are missing.

This domain of validity should be defined in realistic settings, with possible missing data, anomalies or outliers.

Méthode

We consider the problem of uncertainty quantification and domain validity in the regression with dependent data, such as high frequency time series responses. We approach this problem by transforming the time series responses to function valued variables. We develop the conformal inference framework for functional regression. It is not trivial to identify or parametrize the class of regression models with functional responses, with potentially scalar, vector or functional covariates. We will consider the class of nonparametric models utilizing the metric space approach for function valued variables.

Résultats attendus - Expected results

New methodology contributing to uncertainty quantification with dependent data, relation to domain validity, including its validation and implementation.

Précisions sur l'encadrement - Details on the thesis supervision

It will follow the standard protocol in EDMH. There will be regular meetings between supervisors and the student (normally once a week). The student will have an opportunity to attend and present at topic specific research coures and conferences for further research training. A research committee will be formed to follow up the progress of the study.

Conditions scientifiques matérielles et financières du projet de recherche

financement potentiel 'UDOPIA'

Objectifs de valorisation des travaux de recherche du doctorant : diffusion, publication et confidentialité, droit à la propriété intellectuelle,...

The main outcome of the project will be several articles, expected to be submitted to high-quality peer-reviewed journals.
As the project is geared toward developing implementable methods for analysing real data, an important aspect of the dissemination of this work will be the writing of software, based on a publicly available programming language such as Python.

Références bibliographiques

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