Uncertainty in deep learning versus conventional statistics for applications in medicine

Type: Postdoc or PhD

Principal Investigators

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Background

Reliable uncertainty quantification of deep learning approaches is particular important in medical applications. One source of uncertainty in a prediction of a trained net is the uncertainty of these parameters that remains after training. The huge number of parameters, however, prevents the application of established methods from conventional statistics such as the calculation of a covariance matrix or a full Bayesian inference.

Uncertainty quantification in deep learning is not based on a rigorous application of established methods from conventional statistics but either relies on some sort of approximation (e.g. variational Bayes [1], dropout [2]) or heuristic approaches such as ensemble learning [3]. The relationship of these approaches to methods from conventional statistics in situations where both approaches are applicable has not yet been fully explored nor is the validity of the approximation well understood.

One goal of this project is to explore this relationship for low-dimensional regression problems that can be treated using established methods from statistics as well as regularized deep learning approaches. Furthermore, research connecting deep learning with Gaussian process modeling [4] or non-parametric Bayes [5] shall be deepened. The overall goal is to be enhance the understanding of current uncertainty quantification in deep learning against the background of approaches applied in conventional (Bayesian) statistics. In addition to gaining fundamental insights in uncertainty quantification for deep learning, the results of this project will help in bridging classical uncertainty evaluation in metrology and in deep learning. Another goal is to apply the studied uncertainty methods to a regression problem in mammography image quality assessment.

The goal shall build on PTB-842's work done so far in implementing and testing current uncertainty quantification approaches for deep learning in regression problems and their application in case studies [6], along with PTB's broad experience in Bayesian inference and uncertainty evaluation in metrology [7,8].

Project Aim, Objectives and Program

The goal of the project is to deepen the understanding of the relationship between approaches currently applied for uncertainty quantification in deep learning and conventional Bayesian inference.

Specific objectives are

- Comparison of uncertainty characterization using conventional Bayesian statistics for low-dimensional regression problems with those obtained by current uncertainty approaches for deep learning.
- Deepen the understanding of uncertainty quantification in deep learning from the point of view of non-parametric Bayes and Gaussian process modeling.
- Provide guidance as to the choice of uncertainty quantification method in deep learning from the point of view of its consistency with current uncertainty evaluation standards in metrology.

Work program

- Selection of many (>5) regression scenarios for numerical comparisons including quality assessment for mammography; implementation of current state-of-the-art uncertainty quantification in deep learning; reference treatment of selected benchmark problems using Bayesian inference and different assumptions about available prior knowledge; comparison and assessment of results obtained by the statistical treatment and by deep learning.
- Adaption of deep learning approaches to account for prior knowledge such as physical constraints or prior knowledge about the regression curve. Application to benchmark problems and comparison with reference method (using conventional Bayes).
- Exploration of relationship between current approaches for uncertainty quantification in deep learning with non-parametric Bayes and deep Gaussian process modeling.

Available data

- Virtual mammography phantom data (>40 k, > 1 M possible), already available
- Simulated data for low-dimensional regression problems, readily available

Candidate Requirements

- PhD and/or MSc in statistics or mathematics
- Experience in statistics and, optimally, in deep learning
- Software experience: Python (optimally in PyTorch) and joint development (Git)

References

[1] Bishop, CM. *Pattern recognition and machine learning*. Springer 2006.

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[4] Khan MEE. *Approximate inference turns deep networks into Gaussian processes*. Advances in neural information processing systems. 3091-3104, 2019.

[5] MacEachern, SN. *Nonparametric Bayesian methods: a gentle introduction and overview*. Communications for Statistical Applications and Methods 23 (6): 445-466, 2016.

[6] Hoffmann L, Fortmeier I, Elster C. *Ensemble learning for computational optical form measurement.* Submitted to *Sensor and Measurement Science International 2021*.

[7] Elster C et al. *A guide to Bayesian inference for regression problems*. European Metrology Research Program NEW04, http://www.ptb.de/emrp/new04.html 2015.

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