Uncertainty in Machine Learning

Introduction to the Course

Dr. Matias Valdenegro

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About your Lecturer

- Assistant Professor for Machine Learning, since February 2022.
- Previously Researcher at German Research Center for Artificial Intelligence in Bremen, Germany.
- PhD from Heriot-Watt University, MSc from Hochschule Bonn-Rhein-Sieg,
- Expertise in Uncertainty Quantification, Deep Learning, Computer Vision, Reinforcement Learning.
- Likes Japanese Food, Traveling, Movies, PS5 Gaming, Swimming, Talking, Photography, Carpentry.
- Can cook many Japanese Dishes (Okonomiyaki, Oyakodon, Onigiri, Onigirazu, learning about Ramen)

About the Course

- This course is about machine learning models that output a prediction and an associated confidence or uncertainty.
- First time I teach this course, I have previously taught short courses on uncertainty.
- By completing the course you will learn a lot of techniques for uncertainty quantification, the basic concepts of uncertainty, how to evaluate, and which applications benefit from it.
- We will also have programming exercises so you can see how these models are trained in practice.

Course Description

Standard neural networks and machine learning models are popular, but they only produce point-wise predictions, without proper calibrated confidence values. This limits its usefulness as the model limits are unclear.

In contrast, Bayesian neural networks and models with uncertainty are able to output a probability distribution, which contains uncertainty information, allowing the model to communicate its level of certainty to the end user and other systems.

Course Description

Uncertainty and confidence is important for real-world applications of machine learning, such as autonomous driving, computer vision, and natural language processing.

Throughout this course we will see how these models are trained, their difficulties and limitations, how to evaluate them, and how to use them in several real-world applications.

Learning Outcomes

1. Explain the basic concepts of Uncertainty Quantification in the context of ML and AI.
2. Implement, train and evaluate Bayesian Neural Networks and models with uncertainty.
3. Perform out of distribution detection for complex tasks.
4. Evaluate quality of uncertainty through calibration and other metrics.
5. Know the principal research challenges involving uncertainty quantification in machine learning.

Requirements

The basic requirements of this course are:

- Basic machine learning knowledge (training formulation, overfitting, classification, regression).
- Basic neural networks knowledge.

And recommended is to have a good statistics background. We will have a refresher on statistical concepts during the next lecture.

Lecture Planning

- 20.4 Refresher on Statistics and Probability
  Covers concepts of probability distributions, sampling, random number generation.
- 4.5 Introduction to Uncertainty Quantification
  Main introduction to the topic.
- 11.5 Methods for Uncertainty Quantification I Direct (Ensembles, Dual Head, DUQ, Gradient) and Sampling-based methods (Dropout, DropConnect, Test Time Augmentation). Gaussian Processes.

Lecture Planning

18.5 Methods for Uncertainty Quantification II
Bayesian Neural Networks, Variational Inference, Bayes by Backprop, Flipout. Disentanglement.

25.5 Evaluation of Uncertainty
Metrics, losses, evaluation protocols.

1.6 Confidence Calibration
Calibration error and curves. Recalibration methods.

Lecture Planning

8.6 Out of Distribution Detection
Concept of OOD, data distributions, methods for detection. Open Set Recognition.

15.6 Uncertainty in Computer Vision, Robotics, and Reinforcement Learning. Selection of applications and applied models using uncertainty quantification.

Practicals

We will have weekly practicals from the 3rd week, which will be supported by the TAs:

- You can ask questions, work on your homework, and receive help. I will be present in some but not all practicals.
- TAs will be Peter Varga and Cosmin Harsulescu.
- Close to the end of the course, we will hold a special practical with questions for the exam.

Expectations

- There is no point in memorizing, the idea of this and many other courses, is that you learn concepts, and apply them in real-world problems, and you should be able to **generalize**.
- Memorizing equations and concepts does not have a value for you, it is a waste of time. It would not be useful for taking the exam.
- You should be able to explain concepts in your own words.

Expectations

- You can and *should* ask questions during the lecture. If you have questions later when studying, you can ask them in the discussion forum or via email.
- Not asking questions and leaving with doubts is a bad idea. Part of the lecture is dedicated to answering questions and clarifying concepts.
- If nobody asks questions, I might ask questions to you :).
- Leaving with doubts and then consulting internet materials is a worse idea. Problem is that many internet materials might be wrong and you would not be aware of that. Your first source should be the lecturers, we can point you to good resources.

Classrooms

Lectures

In-person at BB 5161.0151. Only in exceptional cases (like sickness) these can be held virtually in Nestor.

Practicals

In-person at LB 5173.0169.

Complete plan is available on Rooster:
`https://rooster.rug.nl/#/nl/2021-2022/schedule/course-WBAI054-05/timeRange=all`

Evaluation & Exam

Homework

We will have three graded homeworks, taking around two weeks each. Each of them will include theoretical/conceptual questions and possibly a simple programming exercise.

Exam

We will have an in-person written exam, lasting two hours. In extreme circumstances due to the pandemic we could replace it with a virtual oral exam or a virtual written exam.

Exam will be on June 21, and resit will be on July 14.

Exam questions will be similar to conceptual questions in homework. I will provide example questions, but no example exam and/or answers. We will discuss some questions in the last practical.

Grading

Each homework assignment will be graded (Three in total).
The average of the three grades will be your homework grade.

The grade for the course is split over two parts:

1. Homework: 40% of the grade.
2. Written Exam: 60% of the grade which will take place on June 21.

In order to pass the course you

- need to score > 5.0 at the final exam
- and have a final average grade ≥ 5.5

Literature

Unfortunately there is no book in this topic. There are two survey papers that we can use as main reference:

- A Survey of Uncertainty in Deep Neural Networks by Gawlikowski et al. 2021.
  Available at `https://arxiv.org/abs/2107.03342`
- A Review of Uncertainty Quantification in Deep Learning: Techniques, Applications and Challenges by Abdar et al. 2020. Available at `https://arxiv.org/abs/2011.06225`

Each lecture will also link to specific papers in the literature. It is not required for you to read these papers, they can be useful as reference, but they are not written specifically for bachelor students. The lectures should be your main source.

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3. What is the Gaussian/Normal Distribution?
4. What is the Central Limit Theorem?
5. What is Maximum Likelihood Estimation?
6. Why does all the above matter?