



## Uncertainty Estimation for I.I.D., Graph, and Sequential Data

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# Abstract

This is the abstract.



# Zusammenfassung

This is the german abstract.



# Acknowledgements

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# **Part I**

## **Introduction**



# 1 Introduction

## 1.1 Motivation

- Practical motivation: trust, security, maintenance, fairness
- Philosophical motivation: Dunning-Kruger effect
- Physics motivation: non deterministic world, nothing is fully observable, uncertainty principle

## 1.2 Contributions

## 1.3 Own Publications

The publications devide in three topics:

- Uncertainty estimation (incl. sparse NN and Energy-based models)
- Structure learning (incl. hierarchical, scikit-network and DAG learning)
- Efficient models (incl. pruning)



## 2 Background

- Desiderata: Epistemic and aleatoric uncertainty (and all their other names), uncertain when it does not know, efficient, architecture-agnostic, robustness.
- Models: Sampling-based (Ensemble, DropOut, BNN) vs Sampling-free (GP, Posterior, Conformal).
- Evaluations: Calibration, OOD detection, OOD generalization, Shifts, Benchmarks.



## **Part II**

# **Uncertainty Estimation for I.I.D. data**





### **3 Uncertainty Estimation for Classification**



## 4 Uncertainty Estimation for Regression



## **5 Robustness of Uncertainty Estimation**



## **Part III**

# **Uncertainty Estimation for non-I.I.D. data**





## 6 Uncertainty Estimation on Graphs



## **7 Uncertainty Estimation on Asynchronous Time Events**



## **8 Uncertainty Estimation for Reinforcement Learning**



## **Part IV**

# **Conclusion**





## 9 Retrospective

- Analysis of optimization, core-architecture, latent space, prior.



# 10 Conclusion

## 10.1 AI alignment/Reliable ML beyond Uncertainty Estimation

- (Adversarial) Robustness
- Interpretable ML
- Green AI

## 10.2 Broader Impact

## 10.3 Open Questions

- Uncertainty Estimation for Active/Online Learning.
- Uncertainty Estimation for Robustness.
- Uncertainty Estimation for Interpretability.
- Uncertainty Estimation and Causality.
- Uncertainty Estimation in the regime of very large data.



## **Bibliography**



## A Additional Stuff

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