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Topic **- The Effect of Architecture Selection on Prediction Uncertainty**

- **Task Description:**

  Imagine designing a rocket. The materials and structure you choose will determine not just how high it can fly but also how reliably it can withstand turbulence. In machine learning, architectures are the blueprints, shaping not only what a model predicts but also how confident it is in those predictions.

  As machine learning expands into critical domains like autonomous driving and medical diagnostics, prediction uncertainty has emerged as a measure of reliability. But how does the choice of architecture—from traditional CNNs to cutting-edge Vision Transformers—affect prediction uncertainty? This study investigates the relationship between architecture and uncertainty, aiming to provide practitioners with the insights they need to pick the right one for the downstream task.

- **The objectives of this study are as follows:**

  1**. *Compare Architectural Families*** We begin by conducting a thorough review to identify link between architecture choice and uncertainty [1]. This includes architectures—ranging from CNNs to Vision Transformers (ViTs).

  2. ***Establish a Methodology for Quantifying Uncertainty Sensitivity***: Building upon existing uncertainty quantification methods [2,3,4], this thesis will outline a framework for systematically evaluating the sensitivity of prediction uncertainty to each architecture. We will focus on key uncertainty metrics such as prediction entropy, variance in predictions (especially under dropout or ensemble methods).

  3. ***Conduct Experiments Across Challenging Scenarios***: Based on the previous step we want to observe how different architectures respond to real-world scenarios e.g., noisy inputs, covariate shifts, and out-of-distribution (OOD) data.

  4. ***Propose Guidelines for Practitioners***: Deliver insights into the trade-offs between architecture complexity, accuracy, and reliability, tailored for practical applications.

The anticipated outcome of this thesis will highlight how different architectures influence uncertainty quantification, equipping practitioners with the tools to make informed decisions in building reliable, confident AI systems.

Recommended skills

1. Deep learning foundational background (Training/Evaluating DL models, general information related to CNNs and Vision transformers).
2. Good understanding of statistics and probability theory is essential, as uncertainty quantification involves probabilistic concepts and statistical methods.

Tools

- PyTorch is highly recommended.

References

[1] Hüllermeier, Eyke, and Willem Waegeman. "Aleatoric and epistemic uncertainty in machine learning: An introduction to concepts and methods." *Machine learning* 110.3 (2021): 457-506.

[2] Lakshminarayanan, Balaji, Alexander Pritzel, and Charles Blundell. "Simple and scalable predictive uncertainty estimation using deep ensembles." *Advances in neural information processing systems* 30 (2017).

[3] Gal, Yarin, and Zoubin Ghahramani. "Dropout as a bayesian approximation: Representing model uncertainty in deep learning." *international conference on machine learning*. PMLR, 2016.

[4] Angelopoulos, Anastasios N., and Stephen Bates. "A gentle introduction to conformal prediction and distribution-free uncertainty quantification." *arXiv preprint arXiv:2107.07511* (2021).

Gentle Introduction: How to handle Uncertainty in Deep Learning #1.1

Looking forward to hear from you!