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Topic.1 - **Exploring the Sensitivity of Model Uncertainty to Hyperparameter Variations: A Systematic Analysis**

- **Task Description**:

  Imagine this: you've trained a deep learning model that predicts traffic patterns. It seems perfect on the test set—accurate, efficient, and ready to deploy. But can you trust it to handle rare, unpredictable scenarios, like a sudden traffic jam caused by an accident?

  This is where uncertainty estimation steps in, acting like a reliability score for machine learning models. In critical applications like healthcare, autonomous driving, and financial forecasting, knowing not just ***what*** a model predicts but ***how*** *certain* it is can make all the difference between success and failure.

  But here's the twist: the reliability of uncertainty estimation isn't set in stone. It's shaped by our choices we make during model training—like how fast we let the model learn (learning rate) or how often we drop connections (dropout rate).

  This study explores a simple but profound question: ***How do these hyperparameters influence model uncertainty****?* By uncovering the hidden relationships between hyperparameters and uncertainty metrics, this thesis aims to guide practitioners toward building models that are not only accurate but also confident.

- **The main objective is "*Cracking the Hyperparameters effects*", in details:**

  1**.** ***Identify Key Hyperparameters Influencing Uncertainty***: We begin by conducting a thorough review to identify hyperparameters commonly linked to model uncertainty [1]. This includes parameters like learning rate, batch size, dropout rate, regularization terms, and architecture-specific parameters such as the number of layers or units. These parameters will be systematically varied to observe their individual and combined effects on model uncertainty.

  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 model uncertainty to each hyperparameter. We will focus on key uncertainty metrics such as prediction entropy, variance in predictions (especially under dropout or ensemble methods), and confidence interval widths. A combination of statistical methods and sensitivity analysis techniques will be employed to quantify the impact of hyperparameter changes.

  3. ***Conduct Experiments Across Diverse Datasets and Models***: To ensure the findings are generalizable, experiments will be conducted across DND-SB [6] dataset for multiclass classification tasks. with varying characteristics and different model architectures (e.g., CNNs, and Vision transformers (ViTs), etc.). This approach allows us to assess whether certain hyperparameters consistently affect uncertainty across domains or if their impact is dataset- and model-dependent.

  4. ***Analyze Trade-offs Between Model Performance and Uncertainty Calibration***: A crucial part of this research is to investigate how optimizing for accuracy alone may impact uncertainty estimation and whether there are trade-offs involved.

  5. ***Propose Guidelines for Practitioners***: Based on the experimental findings, the thesis will outline practical recommendations for practitioners on how to tune

hyperparameters to achieve both high performance and reliable uncertainty estimation. This section will include guidelines for various model types, such as deep learning models, ensemble methods, and Bayesian neural networks, tailored to specific application needs.

The anticipated outcome of this thesis is a set of actionable insights and empirical results that demonstrate how hyperparameters can be strategically adjusted to control model uncertainty, thus enhancing the trustworthiness and safety of machine learning models deployed in critical applications. This work seeks to bridge a gap in understanding between hyperparameter tuning and uncertainty quantification, ultimately aiding in the development of robust and reliable machine learning 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).

[5] Kierdorf, Jana, et al. "GrowliFlower: An image time-series dataset for GROWth analysis of cauLIFLOWER." *Journal of Field Robotics* 40.2 (2023): 173-192.

[6] Yi J, Krusenbaum L, Unger P, Hüging H, Seidel SJ, Schaaf G, Gall J. Deep Learning for Non-Invasive Diagnosis of Nutrient Deficiencies in Sugar Beet Using RGB Images. Sensors (Basel). 2020 Oct 18;20(20):5893. doi: 10.3390/s20205893. PMID: 33080979; PMCID: PMC7589690.

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

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Looking forward to hear from you!