Bayesian Deep Learning

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Decision-Making

Decision-making is a critical step in several domains [**Norvig and Russell**, **1995**]:

- Policy-making for the environment
- Healthcare
- Society
- ...

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Is Deep Learning effective in assisting decision-making?

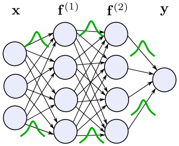
Image prediction: ping-pong ball
Confidence: 99.99%

Illustration: Dianna "Mick" McDougall, Photo: ResNeXtGuesser

Image prediction: pineapple
Confidence: 99.3%

Illustration: Dianna “Mick” McDougall, Photo: ResNeXtGuesser

- Inputs : $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
- Labels : $\mathbf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_N\}$
- Weights : $\mathbf{W} = \{\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}\}$



$\mathbf{w}_i \sim \mathcal{N}(0, \mathbf{I})$

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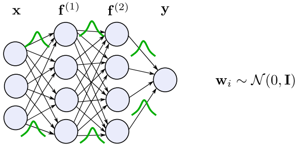
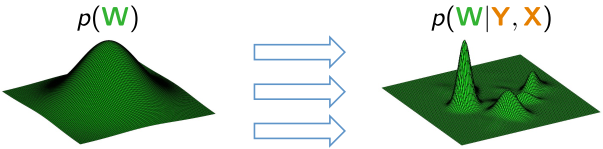
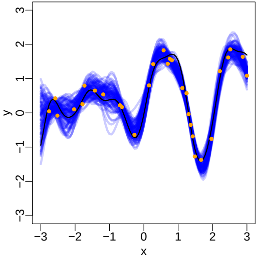


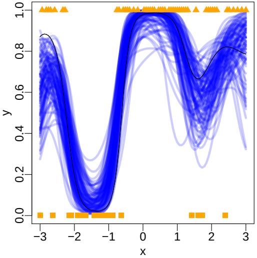


$$p(\mathbf{W}|\mathbf{Y}, \mathbf{X}) = \frac{p(\mathbf{Y}|\mathbf{X}, \mathbf{W})p(\mathbf{W})}{\int p(\mathbf{Y}|\mathbf{X}, \mathbf{W})p(\mathbf{W})d\mathbf{W}}$$

- Predictions consider an infinite number of parameter configurations (e.g., [**Bishop**, **2006**])

$$p(\mathbf{y}^*|\mathbf{x}^*, \mathbf{Y}, \mathbf{X}) = \int p(\mathbf{y}^*|\mathbf{x}^*, \mathbf{W})p(\mathbf{W}|\mathbf{Y}, \mathbf{X})d\mathbf{W}$$





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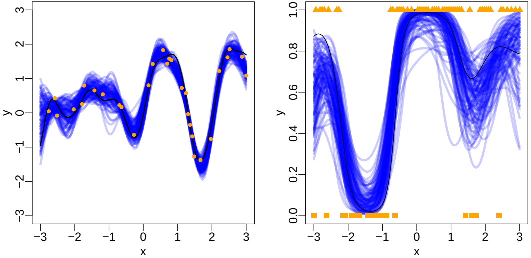

Combining the flexibility of Deep Learning with sound uncertainty quantification!

- The normalization term in Bayes theorem can be used for model selection (e.g., [**Bishop**, **2006**; **Gelman et al.**, **2013**])

$$p(\mathbf{Y}|\mathbf{X}, \mathcal{H}) = \int p(\mathbf{Y}|\mathbf{X}, \mathbf{W}, \mathcal{H}) p(\mathbf{W}|\mathcal{H}) d\mathbf{W}$$

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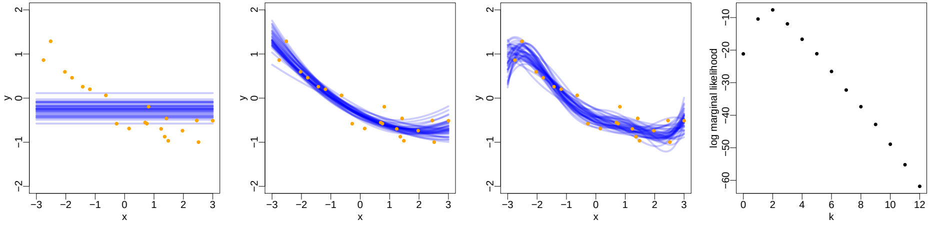
- Illustration of different hypotheses $\mathcal{H}$ for a simple linear model:



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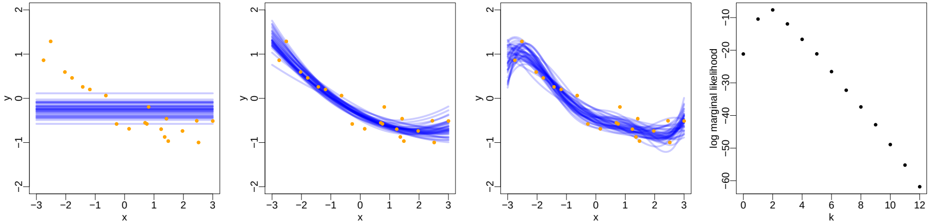

Unfortunately, for Deep Learning models this is intractable!

- Leverage statistical connections [**Akaike**, **1973**] between the model selection problem:

$$\arg\max_{\mathcal{H}} \{\log [p(\mathbf{Y}|\mathbf{X}, \mathcal{H})]\}$$

and the minimization of the following Kullback-Leibler divergence [**Tran et al.**, **NeurIPS 2021**]:

$$\arg\min_{\mathcal{H}} \{\mathcal{D}_{\mathrm{KL}}[\pi_{\mathrm{TRUE}}(\mathbf{Y}|\mathbf{X}) \,\|\, p(\mathbf{Y}|\mathbf{X}, \mathcal{H})]\}$$

to obtain simple and tractable objectives for model selection.

Research Project Idea

- Leverage statistical connections [**Akaike**, **1973**] between the model selection problem:

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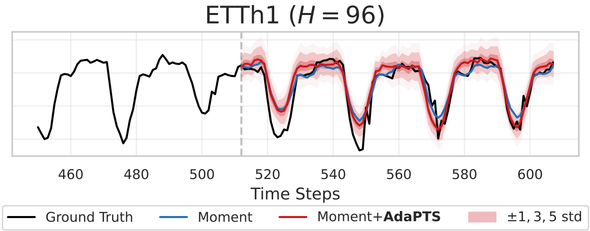
to obtain simple and tractable objectives for model selection.

This can be leveraged for architecture search!

Research Project Idea - Why does it matter?

- Occam's razor [**Solomonoff**, **1964**] for Deep Learning
- Efficient (compute and size) Deep Learning models
- Parsimonious probabilistic foundation models



Research Project Idea - Why KAUST?

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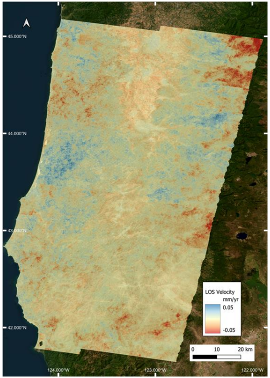
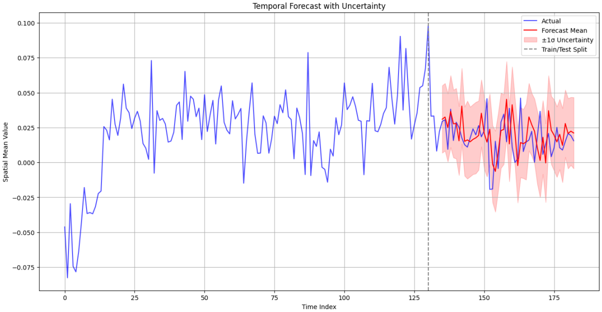
- New foundation models for applications in Statistics





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- Key collaborations in Deep Learning and Statistics worldwide

Position: Bayesian Deep Learning is Needed in the Age of Large-Scale AI

Theodore Papamarkou [1] Maria Skoularidou [2] Konstantina Palla [3] Laurence Aitchison [4] Julyan Arbel [5] David Dunson [6] Maurizio Filippone [7] Vincent Fortuin [8 9 10] Philipp Hennig [11] José Miguel Hernández-Lobato [12] Aliaksandr Hubin [13 14] Alexander Immer [15] Theofanis Karaletsos [16] Mohammad Emtiyaz Khan [17] Agustinus Kristiadi [18] Yingzhen Li [19] Stephan Mandt [20] Christopher Nemeth [21] Michael A. Osborne [22] Tim G. J. Rudner [23] David Rügamer [10 24] Yee Whye Teh [25 26] Max Welling [27] Andrew Gordon Wilson [28] Ruqi Zhang [29]

Abstract

In the current landscape of deep learning research, there is a predominant emphasis on achieving high predictive accuracy in supervised tasks involving large image and language datasets. However, a broader perspective reveals a multitude of over-uncertainty, active and continual learning, and scientific data, that demand attention. Bayesian deep learning (BDL) constitutes a promising avenue, offering advantages across these diverse settings. This paper posits that BDL can elevate the capabilities of deep learning. It revisits the strengths of BDL, acknowledges existing challenges, and

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Spatial Bayesian neural networks

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ABSTRACT

Statistical models for spatial processes play a central role in analyses of spatial data. Yet, it is the simple, interpretable, and well understood models that are routinely employed even though,

- Unique World-class AI and Statistics research environment!
- Vision 2030 drives methodological questions!

Thank you!

Questions?