UNCERTAINTY ESTIMATION FOR DEEP LEARNING IN NEUTRINO PHYSICS

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Outline

I. Motivation: Gedankenexperiment

II. Uncertainty Quantification for Deep Learning

III. Bayesian contra deterministic neural networks

IV. Illustrative case studies, with different algorithms.
A Thought Experiment
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\[ f(x) = \frac{\sin x}{1 + x^2} + \varepsilon \]
A Thought Experiment
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Uncertainty Quantification: Outline

- Science of identifying, estimating and reducing errors & uncertainties and their propagation in models, algorithms, experiments and their predictions.

- How different uncertainties interact and affect the predictions, how they propagate in a model, how to make informed decisions under uncertainty?

Predictive Uncertainty

Epistemic Uncertainty
- Structural

Aleatoric Uncertainty
- Parameter
- Homoscedastic
- Heteroscedastic
UQ Illustration: Weather Forecasts

- Solar+Earth+Atmosphere+Ocean system.
- Aleatoric uncertainty: Location of weather balloons.
  Epistemic uncertainty: Limitations of model to represent radiation, convection, turbulent mixing.
Uncertainty in Neural Network Predictions
Importance of UQ for ML

- Neural networks give *answers*, but no *insight*.
- Akin to Black Boxes.
Importance of UQ for ML

\[
\rho \frac{D \vec{V}}{Dt} = -\nabla p + \rho \vec{g} + \mu \nabla^2 \vec{V}
\]

- Total derivative
- Pressure gradient
- Body force term
- Diffusion term
Importance of UQ for ML

Deterministic Versus Bayesian Neural Networks

Input Layer: $x_1, x_2, x_3, x_4$

Hidden Layer: 3.14, 18.2, 33.7, 1.41, 23.6

Output Layer: 42
Deterministic Versus Bayesian Neural Networks

Gamma Probability Density Function

\( k = 3, \quad q = 9 \)

Normal Probability Density Function

\( \mu = 0, \quad s = 2 \)

Beta Probability Density Function

\( a = 0.5, \quad b = 0.5 \)

Exponential Probability Density Function

\( l = 1 \)

Log-normal Probability Density Function

\( \mu = 5, \quad s = 1 \)
Deterministic Versus Bayesian Neural Networks

Gamma Probability Density Function

Normal Probability Density Function

Beta Probability Density Function

Exponential Probability Density Function

Log-normal Probability Density Function
Deterministic Versus Bayesian Neural Networks

Training Data

Deterministic Neural Network

Bayesian Neural Network
Deterministic Versus Bayesian Neural Networks

Training Data

Deterministic Neural Network

Bayesian Neural Network
Deterministic Versus Bayesian Neural Networks

Training Data

Deterministic Neural Network

Bayesian Neural Network
Illustration Case I

- Classification of particle physics events as background or signal.
- Data projected to 2-dimensions.
- BNN: ADVI [1]

Illustration Case I

*SOFTMAX OUTPUT*

*IS THIS MODEL UNCERTAINTY?*
Illustration Case II

- Proton decay in LArTPC.
- 20000 Images of particle interactions in detector: Background or Signal.
- 10 Layer, Deterministic CNN: 97% Accuracy
- BNN: MC Dropout [2]

Model Ensembling

- Condorcet’s Jury Theorem ➢ Ensemble Methods.
- Dropout.
- Monte Carlo Dropout
Illustration Case II

![Graph showing accuracy vs. MC samples with two lines representing standard dropout accuracy and MC dropout accuracy.]
Summary

• Motivation: Gedankenexperiment

• Uncertainty Quantification for Deep Learning

• Bayesian contra deterministic neural networks

• Illustrative case studies, with different algorithms.