Deeply Uncertain: Comparing Methods of Uncertainty Quantification in Deep Learning Algorithms

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Uncertainty Quantification in Deep Learning

Deep learning is used in many applications in the physical sciences.

In those sciences, we are used to having uncertainty on every measurement or prediction.

In last years, many methods put forth for uncertainty quantification:
- Bayesian Neural Networks
- Concrete Dropout
- Deep Ensembles
- ...
**Epistemic and aleatoric, statistical and systematic**

Uncertainty in deep learning is often divided into

| Aleatoric or irreducible: uncertainty related to corruption of input data, such as detector noise | Epistemic or reducible: uncertainty stemming from an imperfect model, goes down with more data |
Epistemic and aleatoric, statistical and systematic

Uncertainty in deep learning is often divided into

| aleatoric or irreducible: uncertainty related to corruption of input data, such as detector noise | epistemic or reducible: uncertainty stemming from an imperfect model, goes down with more data |

Uncertainty in physical sciences is often divided into

| statistical: can be statistically determined from input data | systematic: not statistical |
Epistemic and aleatoric, statistical and systematic

Uncertainty in deep learning is often divided into

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Epistemic is always systematic
Statistical is always aleatoric
No statistical epistemic, but systematic aleatoric do exist
Problem summary: 1. Which uncertainty quantification method to choose
2. How to interpret the results
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2. How to interpret the results

Our contribution: Build simple sandbox with pendulum problem

From \((L, T, m, \theta)\), predict \(g = 4\pi^2 L/T^2\): a problem any physics undergrad is familiar with
Setup

3 hidden layers with 100 nodes each

Image credit: Michael Nielsen
Brief introduction to the UQ methods

For all these methods, optimize \((g, \sigma_g)\) to maximize Gaussian log likelihood of right answer, so loss is

\[
L = \log \sigma_g + \frac{1}{2} \left( \frac{g - g_{\text{true}}}{\sigma_g} \right)^2
\]

\(\sigma_g\) provides an estimate of the aleatoric uncertainty, while the variance between different models' predictions gives epistemic uncertainty.

Deep ensembles: different models  
Concrete dropout: dropping different neurons  
Bayesian NN: each weight is sampled from distribution
How to introduce noise

Statistical (aleatoric): add noise to the T measurements (sample them from a normal distribution)

Systematic (aleatoric): add noise to the single L measurement

Systematic (epistemic): test in different region from training set
Results: how well is aleatoric uncertainty captured?

Plot shows 16, 50, and 84th percentiles.
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Plot shows 16, 50, and 84th percentiles.
Results: out of distribution uncertainties

Several ways to go out of distribution. We train on $g$ in $(5, 15) \text{ m/s}^2$.
Can test on $g$ in $(15, 20) \text{ m/s}^2$:

Terrible results for all methods!
Results: out of distribution uncertainties

An easier test is to let L, T out of training distribution, keeping g in the trained range.

Concrete dropout epistemic uncertainty always very low, as dropout probabilities end up close to zero!

Others starting coming up when we go out-of-distribution.

Plot shows 16, 50, and 84th percentiles.
Results: calibration

Do the uncertainties accurately reflect the error?
Conclusions

- Aleatoric uncertainties are reasonably well-modeled *but* need to make sure to include a large range of uncertainties in the training set. Just like for predictions, but less visible! BNN needs most attention.

- Out of distribution is a hard problem still. CD in particular totally failed us, and all fail when output goes away from the training distribution.

- DE is technically simplest and seems to work well.  
  
  see paper on arXiv for more details!