QUT Centre for Robotics

A Short Tutorial on Uncertainty in Deep Learning

Dr Dimity Miller

What makes a “good” predictive model in deep learning?

Let’s put **<u>you</u>** to the test!

Not all predictive models are equal.

Beyond accuracy, predictions can also be associated with a “confidence” or “uncertainty”.

There are also different **types** of uncertainty.

Epistemic (knowledge)

Aleatoric (data)

Epistemic (knowledge)

Can be reduced the more knowledge you have.

Aleatoric (data)

Always possible and cannot be reduced.

(1) A model that is 99.9% accurate.

(2) A model that is 99% accurate, AND can predict when it is failing with 99% accuracy.

Credit: Prof. Michael Milford

(1) A model that is 99.9% accurate.

0.1% failure rate

(2) A model that is 99% accurate, AND can predict when it is failing with 99% accuracy.

0.01% failure rate

Credit: Prof. Michael Milford

For robots + autonomous systems…

Robot crushes child's finger in Russian chess match

Science and Technology

Mon 25 Jul 2022

Tesla self-driving car fails to detect truck in fatal crash

By Jessica Castro

Saturday, July 2, 2016

Toyota Paralympics self-driving bus hits disabled athlete

Starship robot 'tries to run over pedestrian'

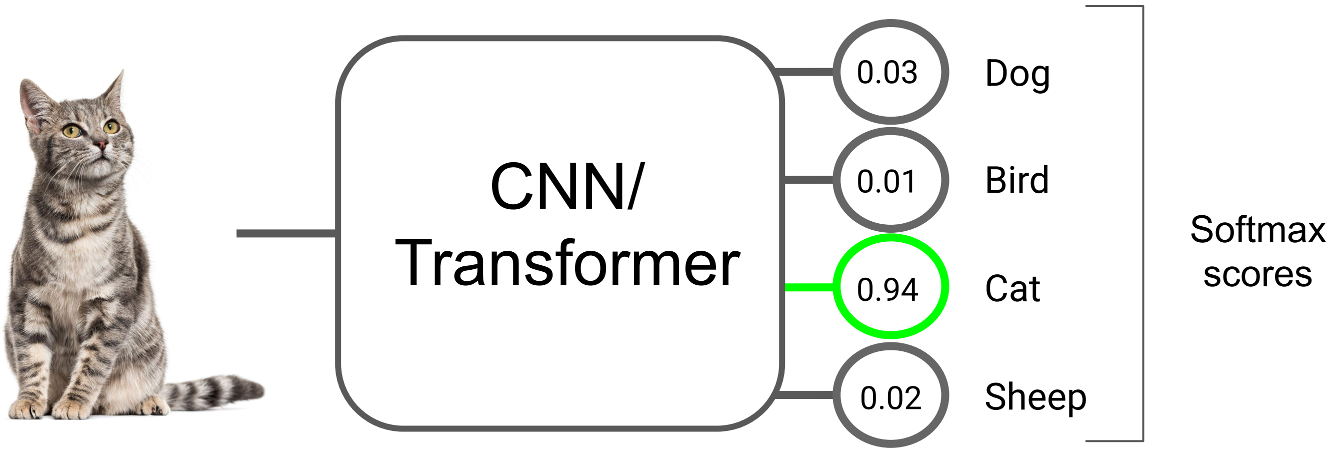
'Worthless' Mater Dei Hospital medicine robots cause mass resignations

What is uncertainty in deep learning?

Predictive Uncertainty in Deep Learning

All predictions returned with an associated confidence or uncertainty.

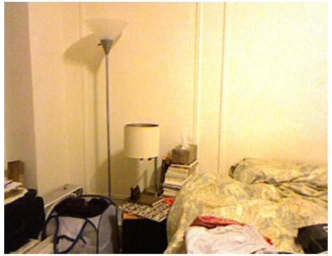
Classification task (e.g. image recognition)

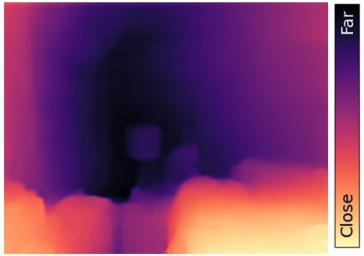


Predictive Uncertainty in Deep Learning

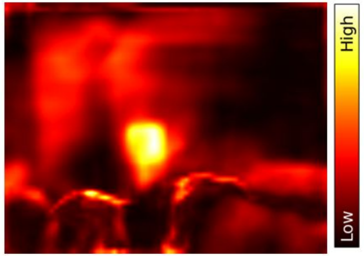
All predictions returned with an associated confidence or uncertainty.

Regression task (e.g. monocular depth estimation)


RGB Image



Depth Prediction



Depth Uncertainty

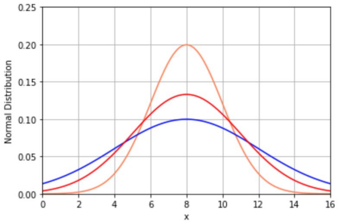
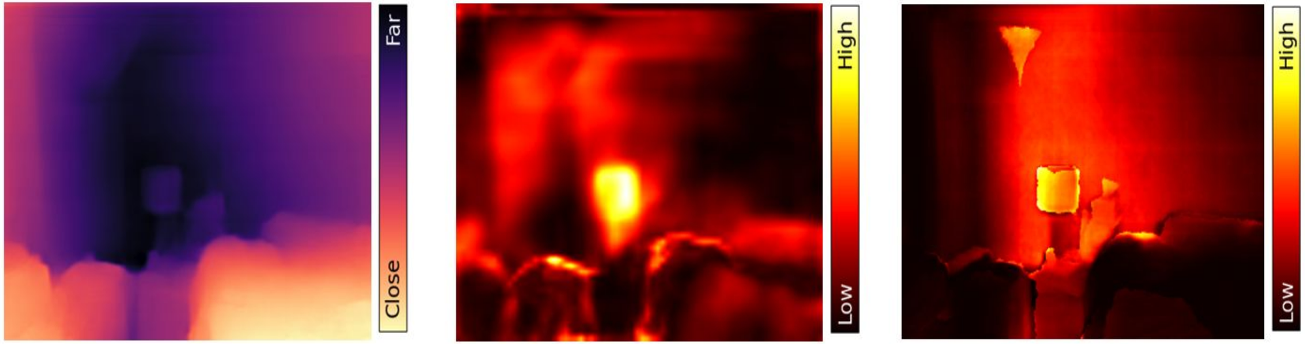


Image credit: Hornauer and Belagiannis

Predictive uncertainty needs to be useful!



Prediction Uncertainty Error

“Good” predictive uncertainty should be related to prediction error.

Image credit: Hornauer and Belagiannis

How can we get predictive uncertainty?

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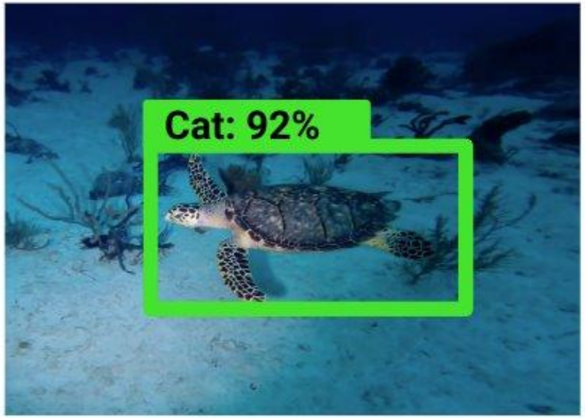
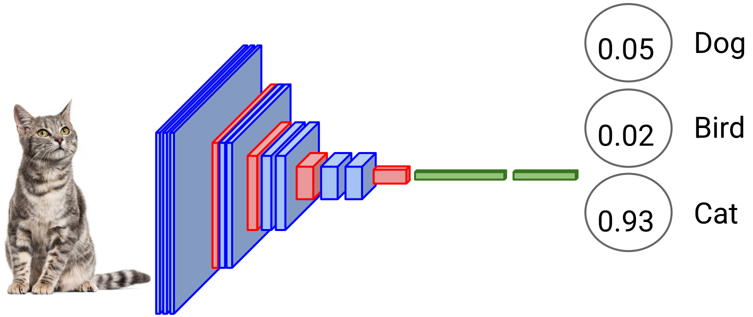
“Let’s use the softmax probability!”

How can we get predictive uncertainty?

"Let's use the softmax probability!"



Why Softmax often is a “bad” measure of uncertainty…



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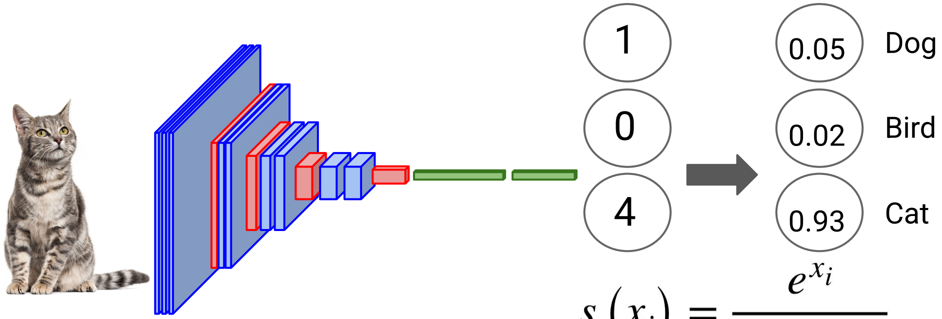
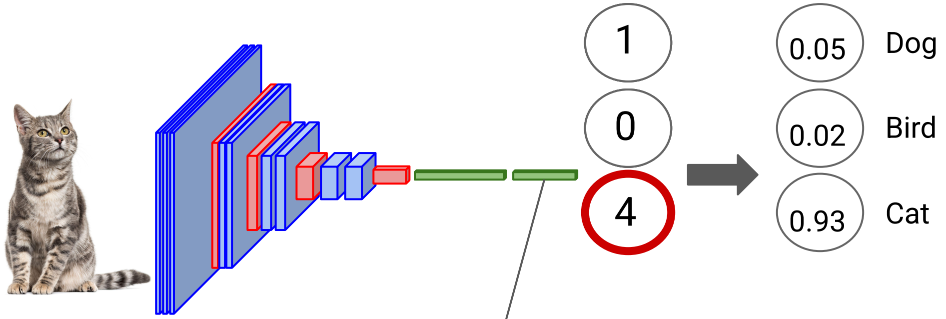
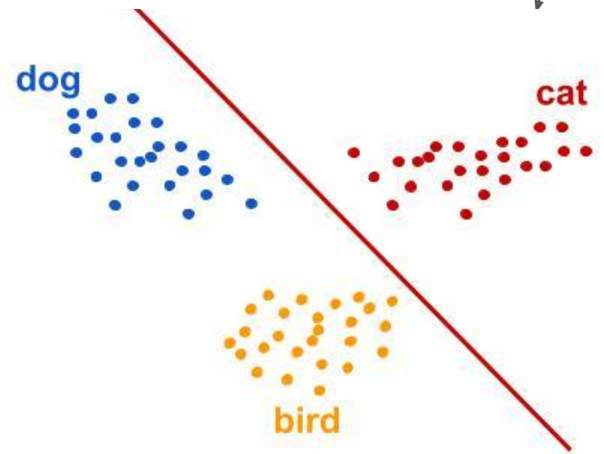


$$s\left(x_i\right) = \frac{e^{x_i}}{\sum_{j=1}^{n} e^{x_j}}$$

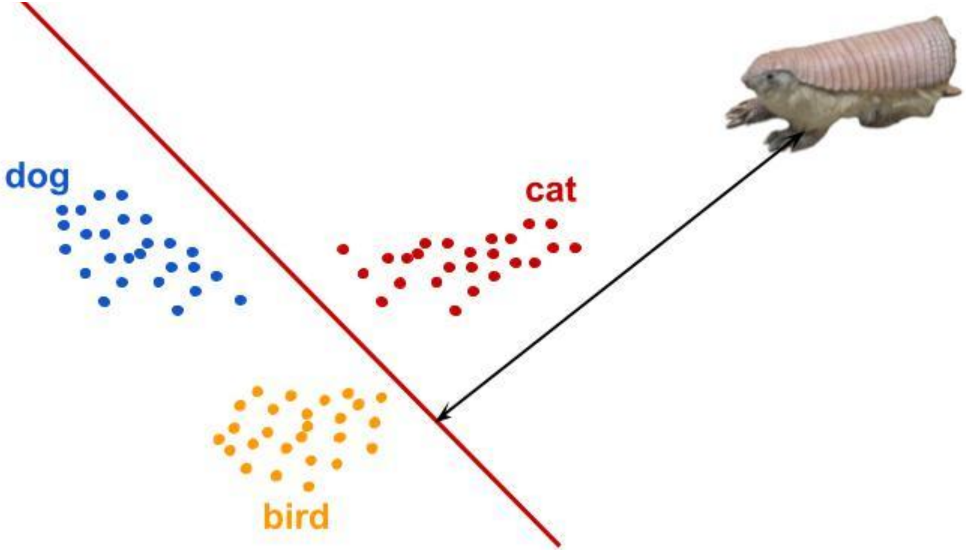
Why Softmax often is a “bad” measure of uncertainty…





Logits are proportional to class-specific linear classifiers.

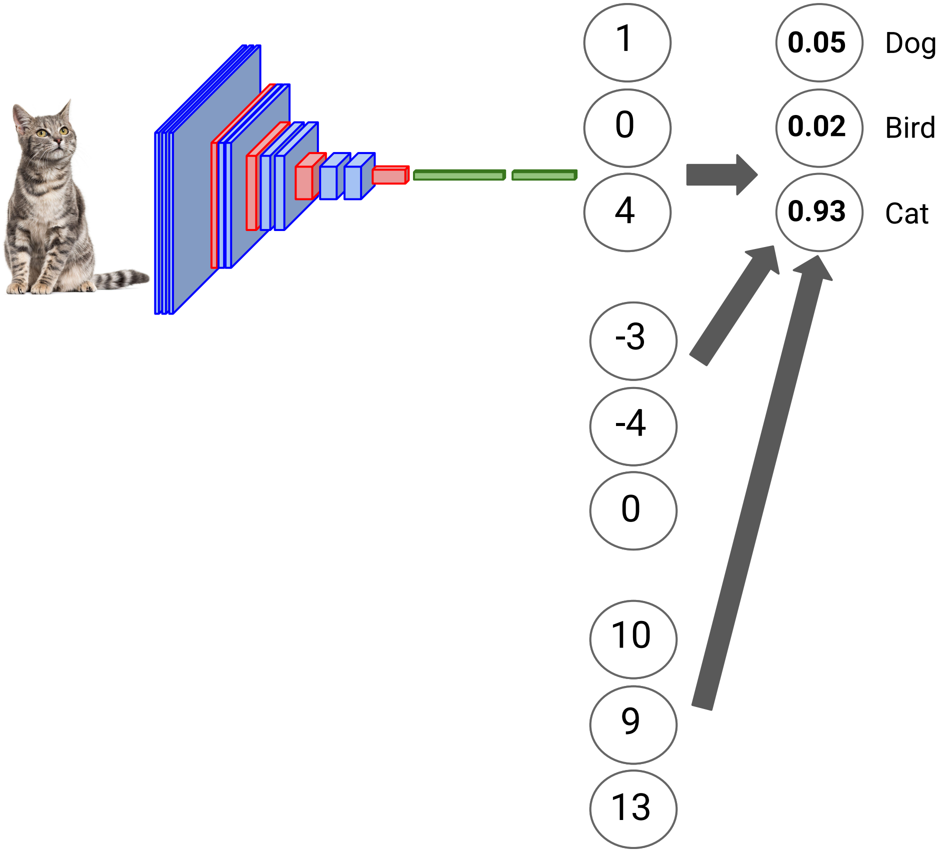
Why Softmax often is a “bad” measure of uncertainty…



Issues:

1. Inputs can get a very high logit even if projected into “unusual” feature regions.

Why Softmax often is a “bad” measure of uncertainty…

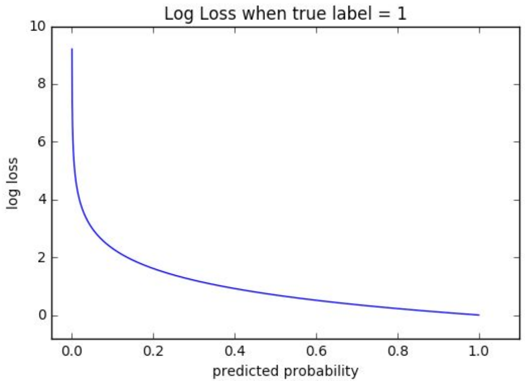


Issues:

1. Inputs can get a very high logit even if projected into “unusual” feature regions.
2. Softmax is a relative function that encourages one-hot behaviour.

$$s\left(x_i\right) = \frac{e^{x_i}}{\sum_{j=1}^{n} e^{x_j}}$$

Why Softmax often is a “bad” measure of uncertainty…



$$\text{Loss} = -\sum_{i=1}^{\substack{\text{output}\\\text{size}}} y_i \cdot \log \hat{y}_i$$

Issues:

1. Softmax is a relative function that encourages one-hot behaviour.
2. Inputs can get a very high logit even if projected into “unusual” feature regions.
3. Cross-entropy loss does not encourage expression of uncertainty

How can we get **good** predictive uncertainty?

Deep Ensembles

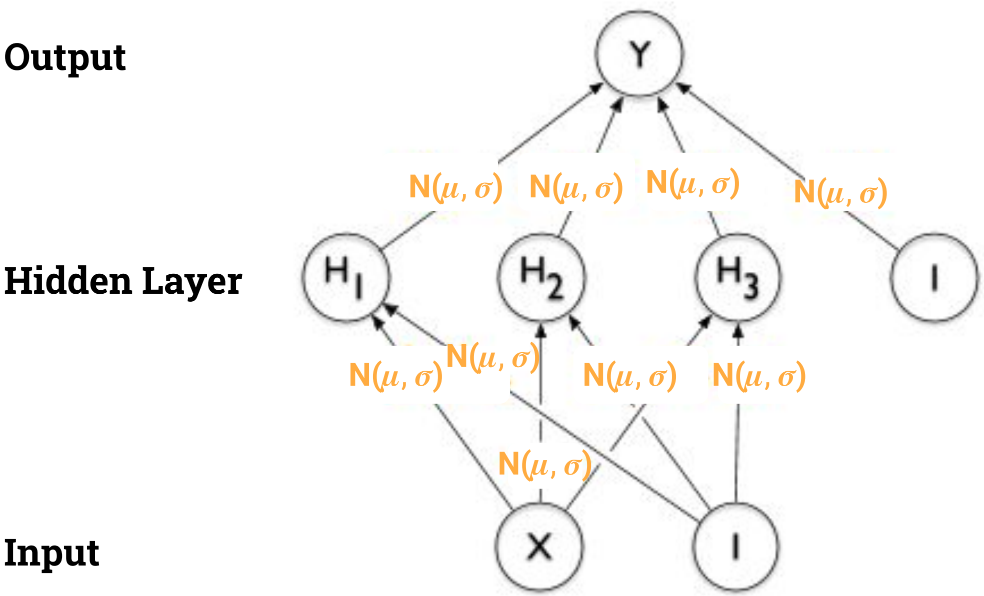
Bayesian Neural Networks

Learnt Uncertainty

Modelling “Normal”

Introspective Methods

Bayesian Neural Networks



Approximate Bayesian Neural Network
Bayesian Neural Network

(Image: Blundell et al., 2015)

Posterior

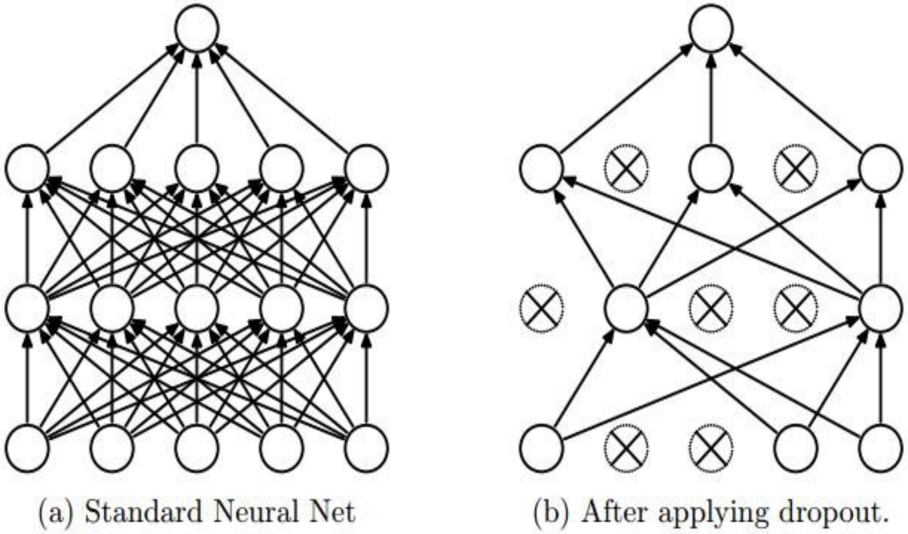
Intractable

$$p(\boldsymbol{\omega}|\mathbf{X},\mathbf{Y}) = \frac{p(\mathbf{Y}|\mathbf{X},\boldsymbol{\omega})p(\boldsymbol{\omega})}{p(\mathbf{Y}|\mathbf{X})}$$

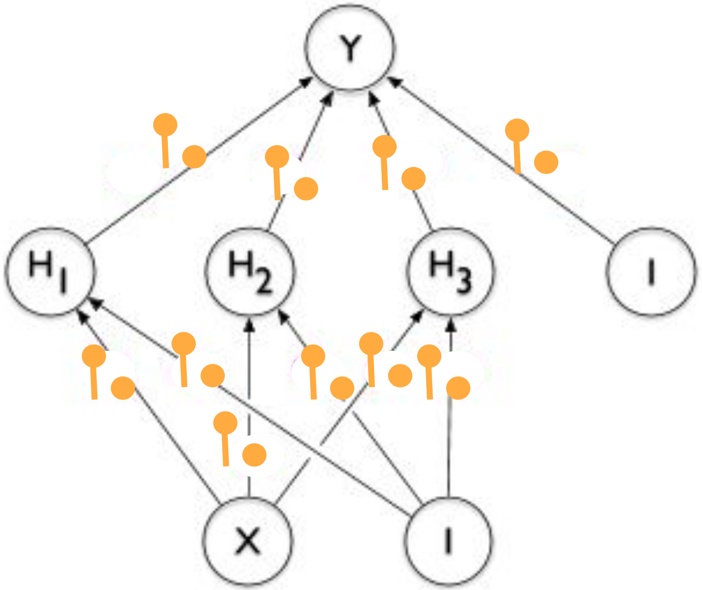
Approximate Posterior

Variational Inference

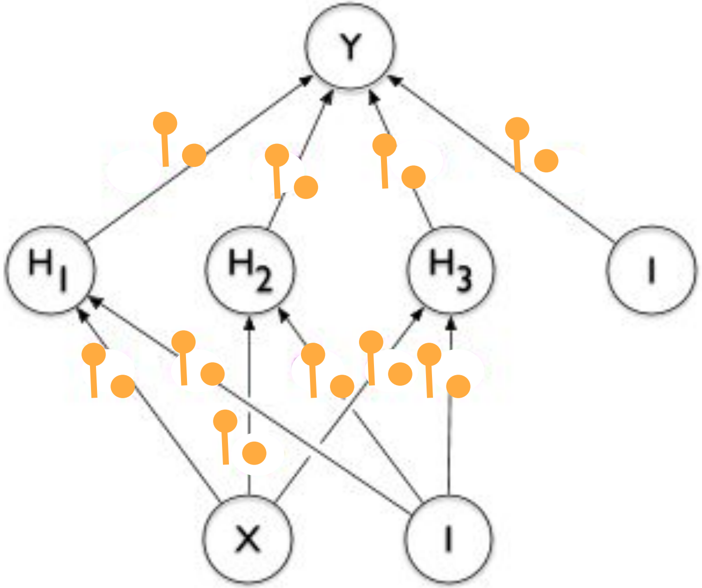
Monte Carlo (MC) Dropout for Bayesian Neural Networks



(Image: Srivastava et al., 2014)



Monte Carlo (MC) Dropout for Bayesian Neural Networks

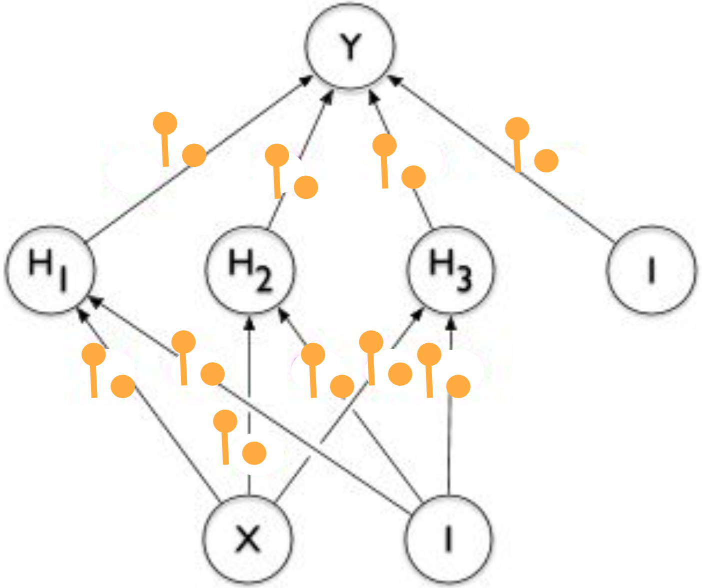


$$\times\, 20 = Y_1, Y_2, Y_3, \ldots, Y_{20}$$

$$\Downarrow$$

$$Y_\mu, Y_\sigma$$

Monte Carlo (MC) Dropout for Bayesian Neural Networks



$$\times 20 = Y_1, Y_2, Y_3, \ldots, Y_{20}$$

$$\Downarrow$$

$$Y_\mu, Y_\sigma$$

See MC Layer Norm for a Transformer-friendly approximate Bayesian inference!

Bayesian Neural Networks

Pros:

- Strong theoretical underpinnings

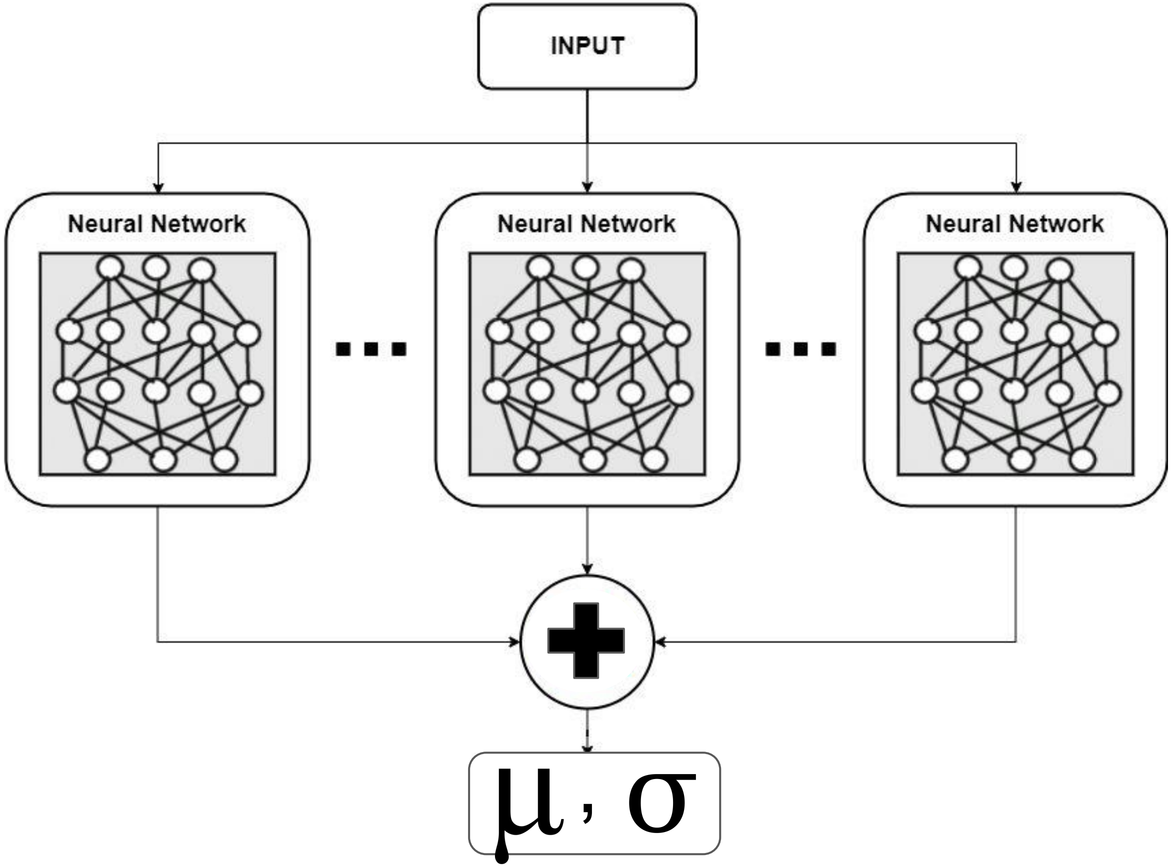
- Generally works well for epistemic uncertainty

Cons:

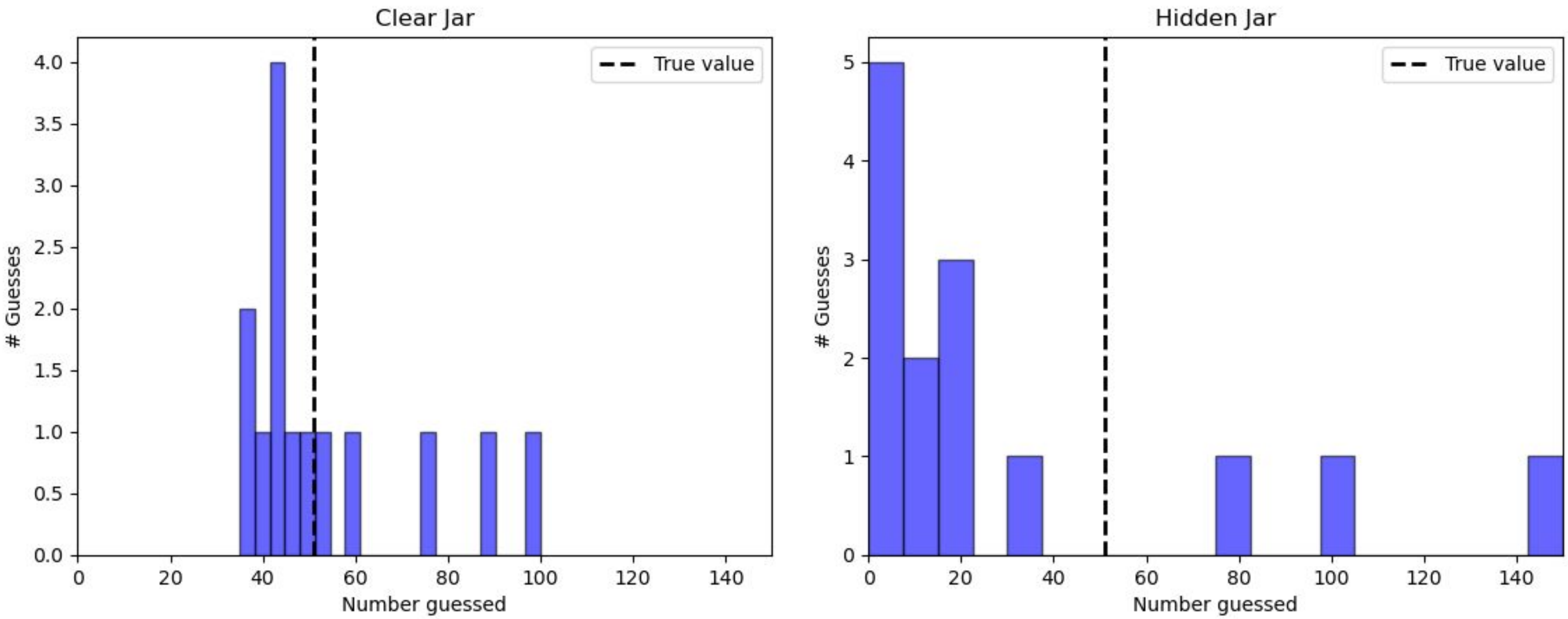
- Especially for large models, computationally expensive in terms of:
  - Number of parameters
  - Multiple forward passes

- Sometimes so many assumptions/approximations, doesn't actually work that well

Deep Ensembles



Deep Ensembles: Human Edition



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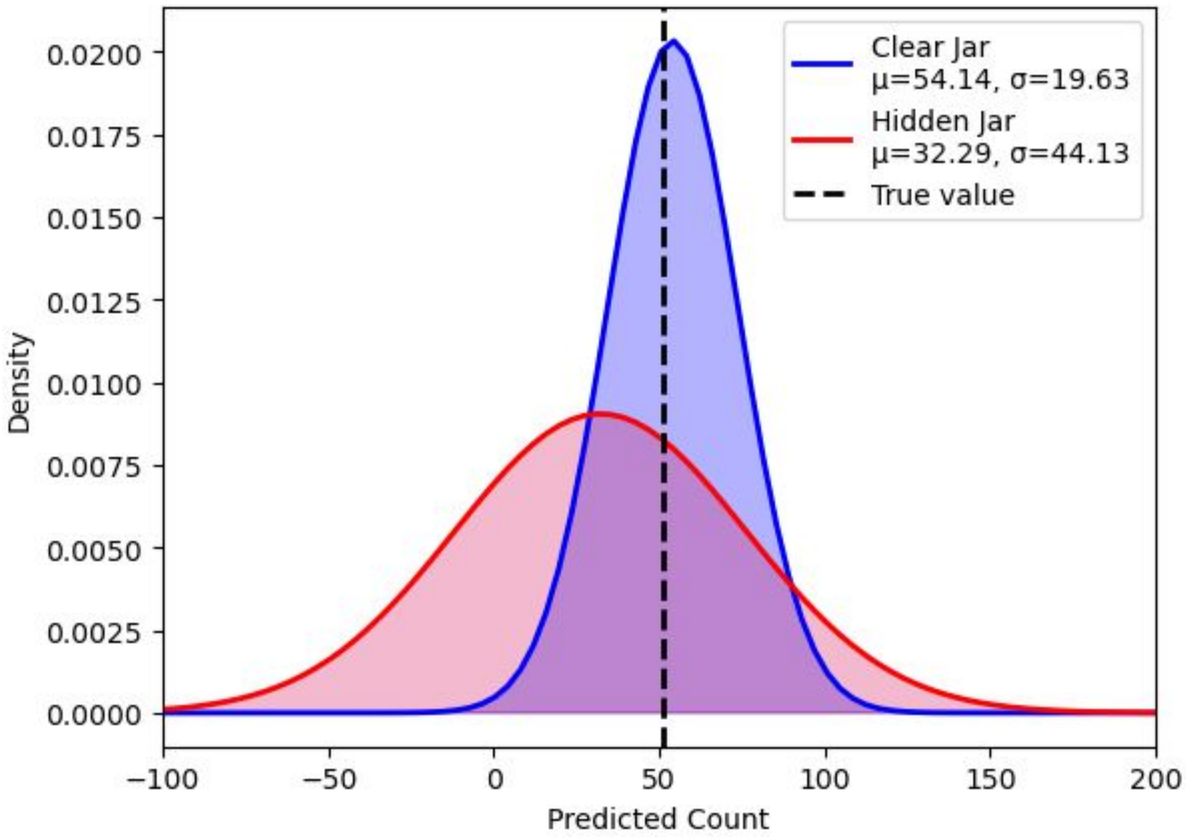


Deep Ensembles

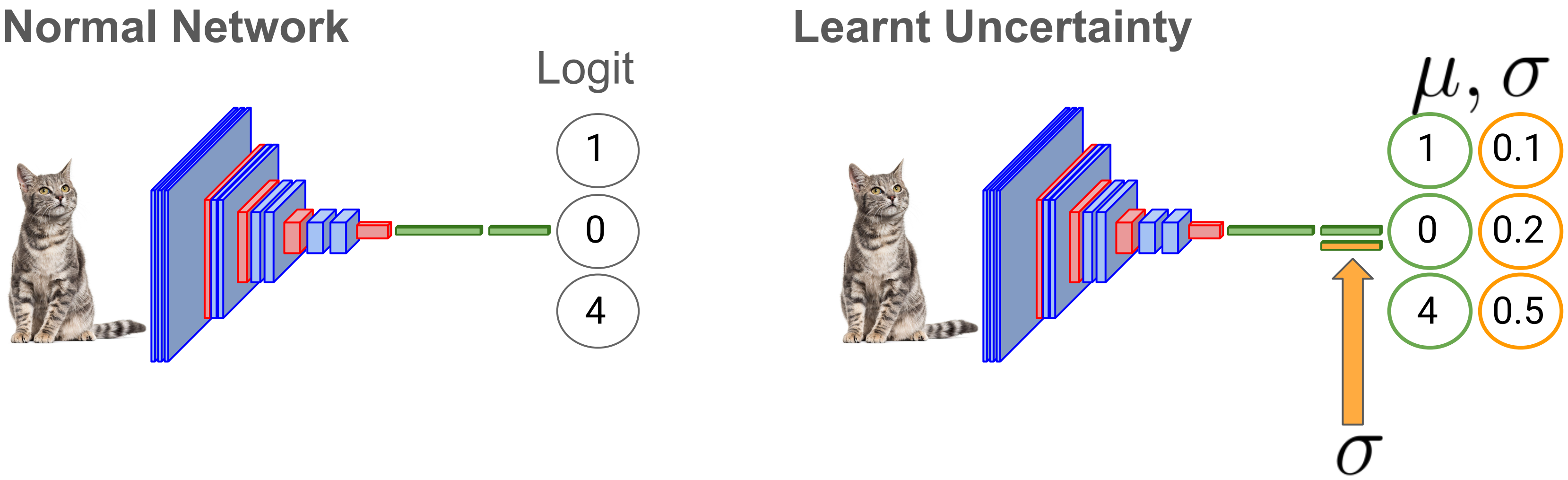
Pros:

- Generally a strong baseline that "just works"
- Easy to implement
- Can capture epistemic and aleatoric uncertainty

Cons:

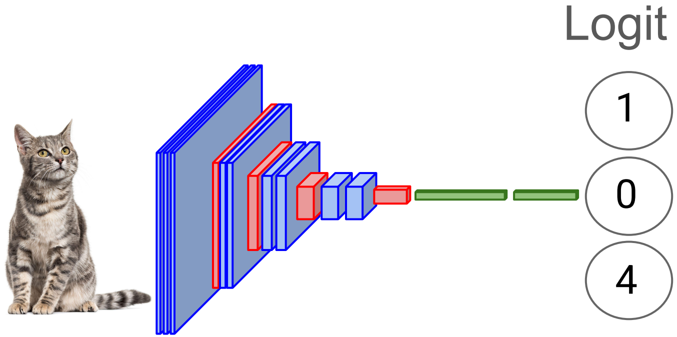
- Computationally expensive to
  - train multiple models
  - test an input through multiple models

Learnt Uncertainty

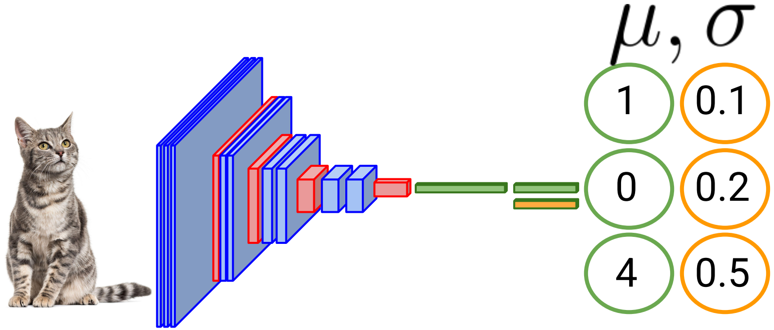


Learnt Uncertainty

Normal Network



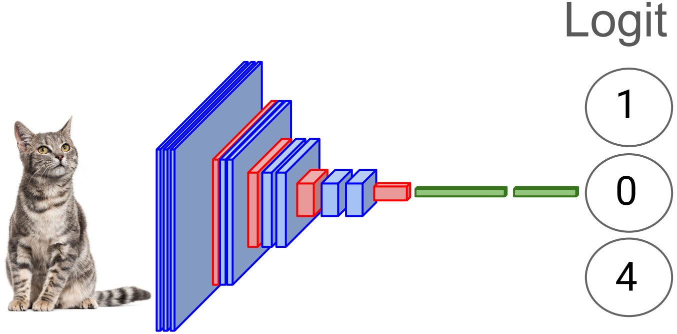
Learnt Uncertainty



$$\mathcal{L} = \frac{||y - \mu||^2}{2\sigma^2} + \frac{1}{2}\log(\sigma^2)$$

Learnt Uncertainty

Normal Network



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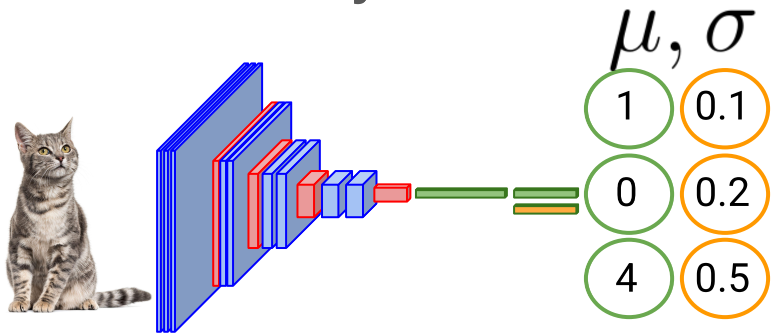
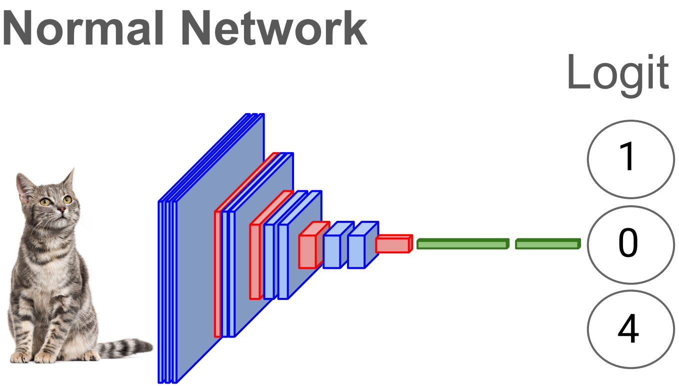
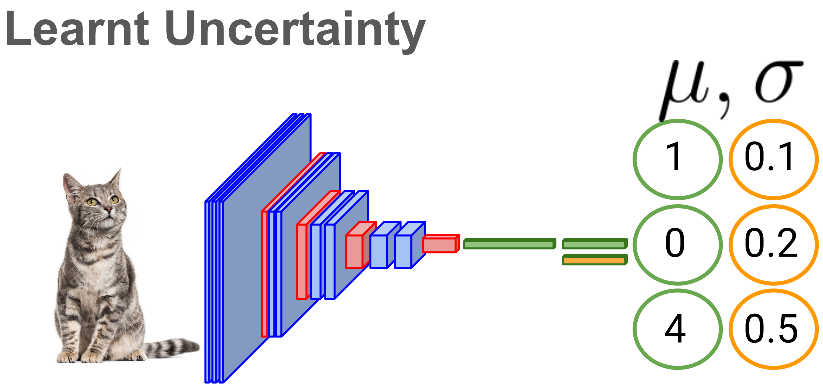


$$\mathcal{L} = \frac{\overbrace{||y - \mu||^2}^{\text{error in prediction}}}{2\sigma^2} + \frac{1}{2}\log(\sigma^2)$$

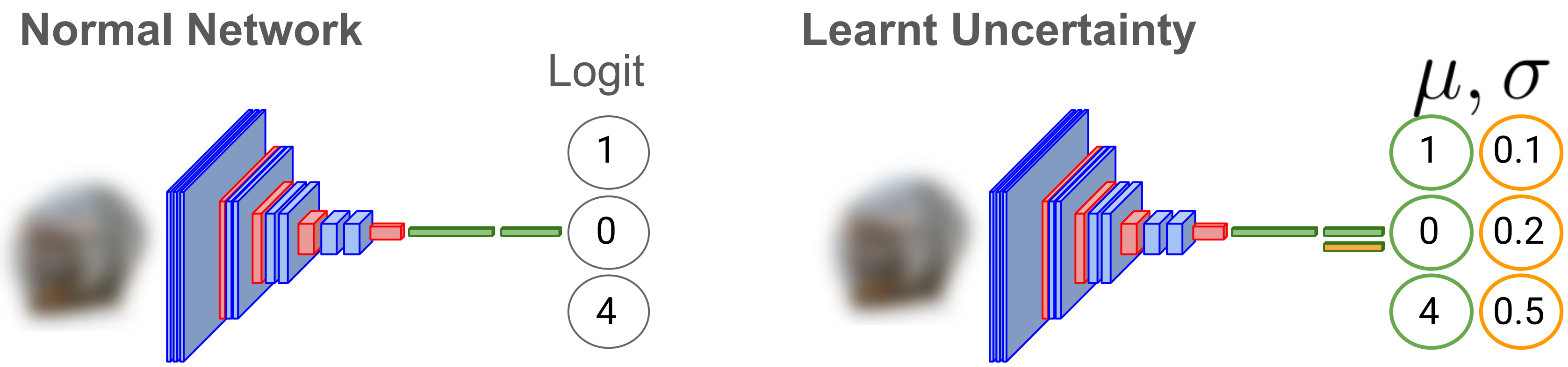
Learnt Uncertainty





$$\mathcal{L} = \overbrace{\underbrace{\frac{||y-\mu||^2}{2\sigma^2}}_{\text{reduce error}}}^{\text{error in prediction}} + \underbrace{\frac{1}{2}\log(\sigma^2)}_{\text{uncertainty penalty}}$$

Learnt Uncertainty



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Learnt Uncertainty

Pros:

- Quick - single forward pass
- Can apply post-hoc to pre-trained network**
- Associated with aleatoric uncertainty

Cons:

- **Performs best when network is trained alongside uncertainty head
- Sometimes doesn’t reach same task performance – network can “opt out” of learning hard data by having high uncertainty

Modelling “Normal”

Statistically model the expected distribution of the network outputs.
At test time, flag abnormal network outputs.

Introspective Methods

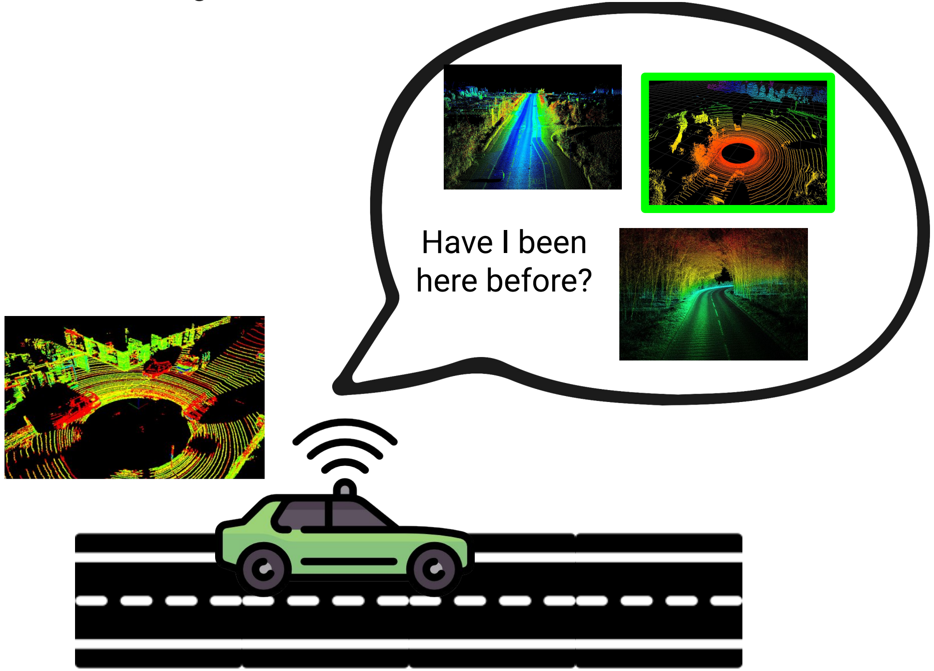
Monitor intermediate values **inside** the model
(NOT just by observing outputs).

Which uncertainty technique is the best?

Some lessons learnt…

LiDAR Place Recognition

Keita Mason, Joshua Knights, Milad Ramezani, Peyman Moghadam, and Dimity Miller. “Uncertainty-aware lidar place recognition in novel environments”. In *2023 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS).*



MC Dropout

Learnt Uncertainty

Deep Ensembles

Slide credit: Keita Mason

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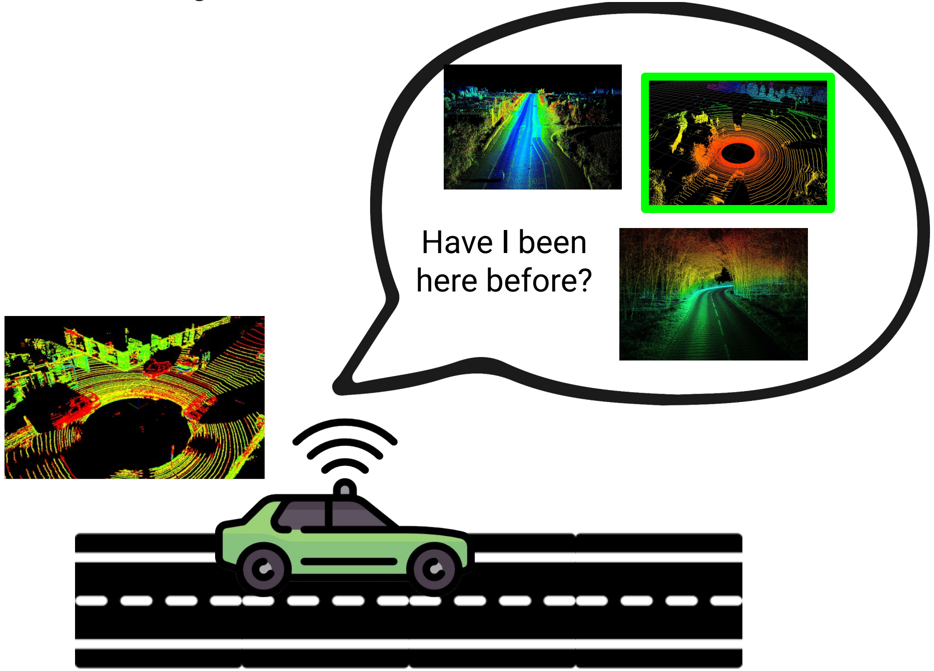

MC Dropout ✗

Learnt Uncertainty ✗ ✓

Deep Ensembles ✓

Slide credit: Keita Mason

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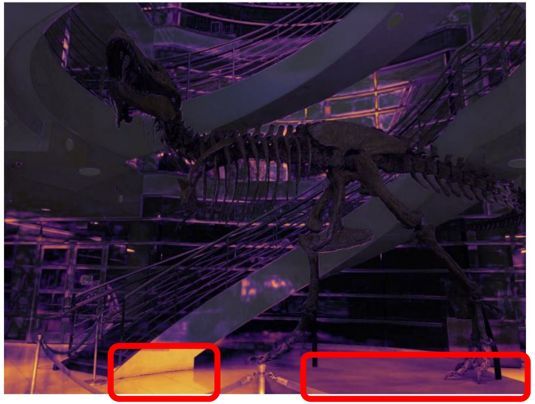
NeRFs

Niko Suenderhauf, Jad Abou-Chakra, and Dimity Miller. “Density-aware NeRF Ensembles: Quantifying Predictive Uncertainty in Neural Radiance Fields”. In *2023 IEEE International Conference on Robotics and Automation (ICRA).*

Prediction

Error



Uncertainty

Deep Ensembles

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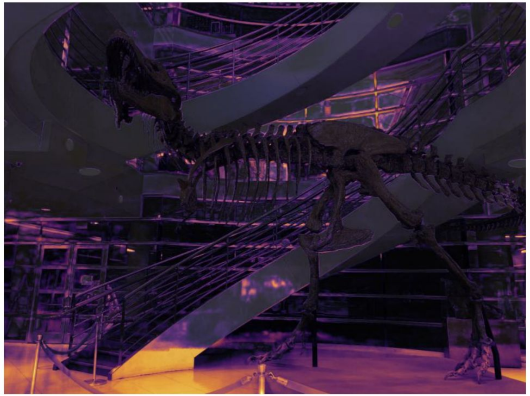

Uncertainty

Deep Ensembles

+

Introspection (Ours)

Object detection with novel objects

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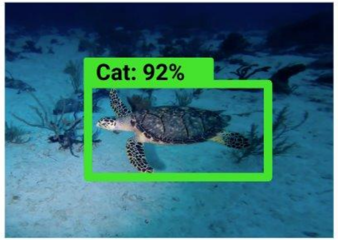
Dimity Miller, Niko Suenderhauf, Michael Milford and Feras Dayoub. “Uncertainty for Identifying Open-Set Errors in Visual Object Detection”. In *IEEE Robotics and Automation Letters (RA-L), 2022.*

Trained on:

Tested on:



MC Dropout, 2.8fps

Deep Ensembles, 4.6fps

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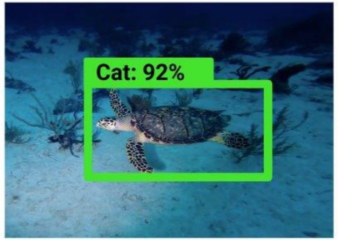

MC Dropout ✓ , 2.8fps

Deep Ensembles ✓ , 4.6fps

Modelling “Normal” (Ours)

✓ ✓ , 19.7fps

Key take-aways:

1. Uncertainty is important, especially for robotics
2. There are different types of uncertainty
3. Softmax is NOT a probability and often not a useful estimate of uncertainty
4. The “best” uncertainty technique depends on the type of uncertainty AND characteristics of your problem