Uncertainty Quantification in Deep Learning

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Aalto University
Finland

Vienna Deep Learning Meetup
September 11th, 2024

Outline

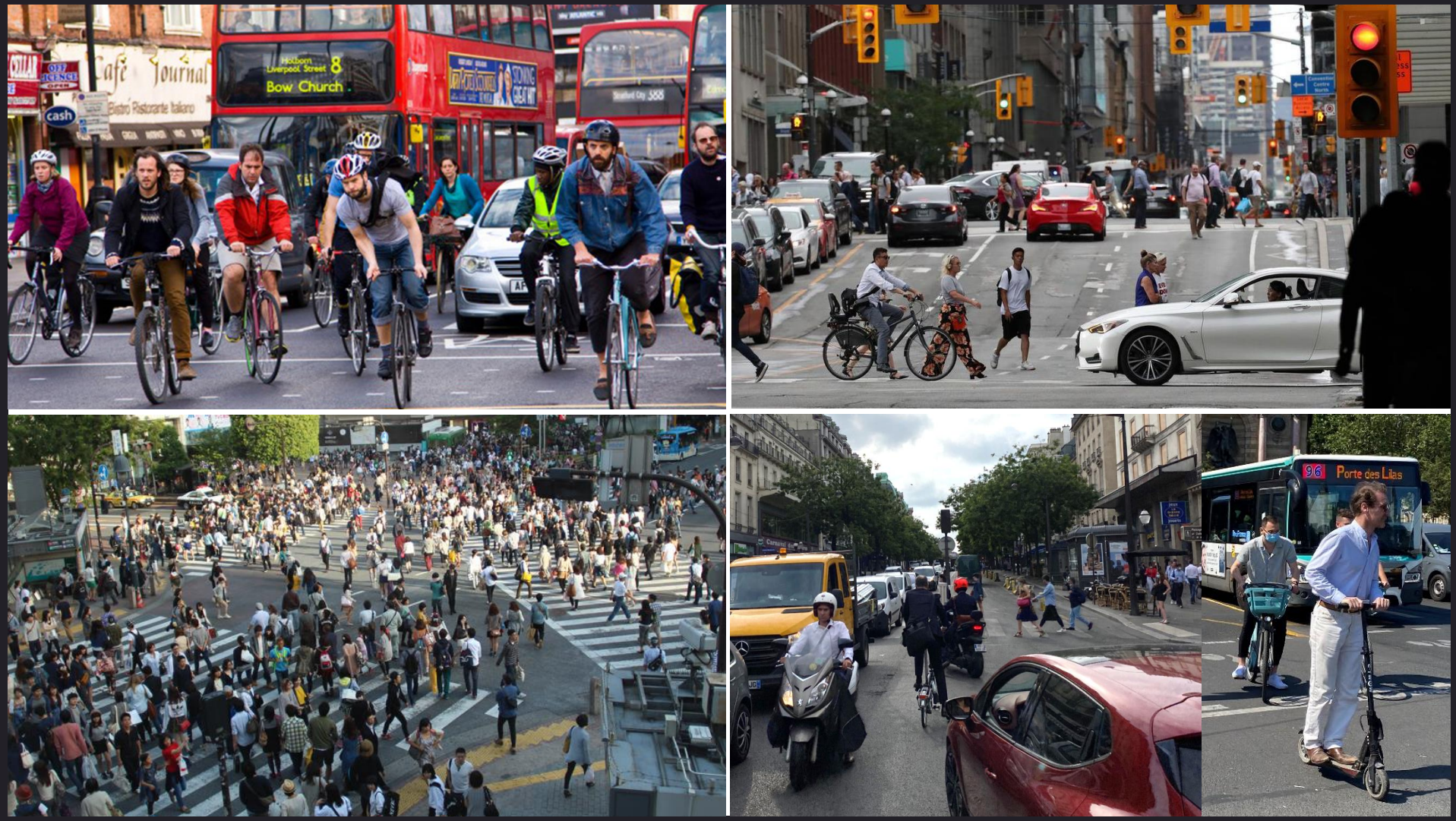
Why … do we need uncertainty quantification?

What … uncertainties are there?

How … can we quantify uncertainties?

Why do we need UQ?

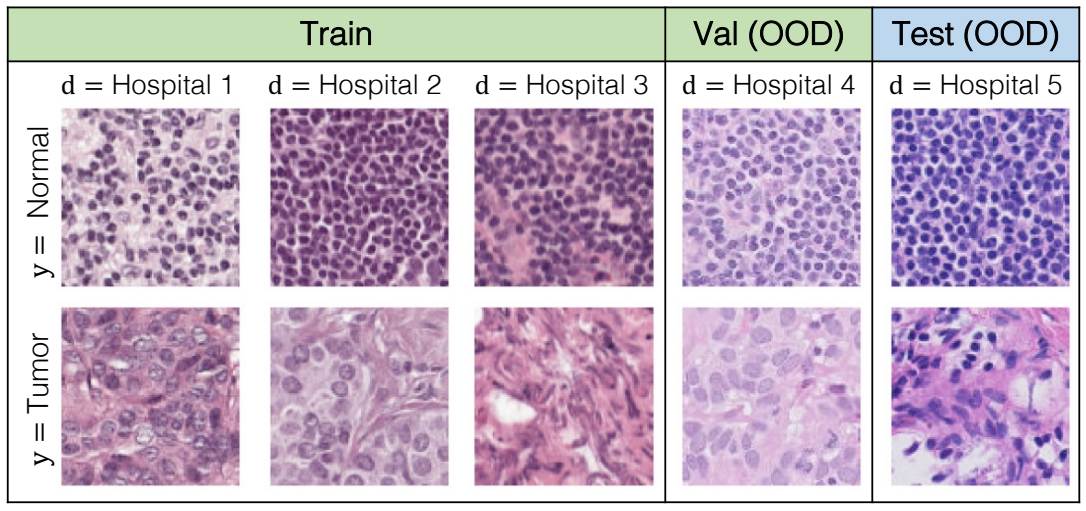
The Real World is Messy



Source: ICCV 2023 Tutorial on *The Many Faces of Reliability of Deep Learning for Real-World Deployment*

The Real World is Messy

Distribution Shifts



Source: P W Koh *et al.* WILDS: A Benchmark of in-the-Wild Distribution Shifts. In ICML, 2021.

Various Sources of Noise

Source: S Sabour *et al.* SpotlessSplats: Ignoring Distractors in 3D Gaussian Splatting. In ICML, 2021.

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Expectations for ML Systems

Our systems/models should be safe and trustworthy.

For this, we require they are:

- Accurate in their predictions
- Robust to input-pertubations (noise, adversarial attacks)
- "Know when they don't know" (recognize out-of-domain data)
- Act if they are uncertain (*e.g.*, active learning, reasoning)

However, ...

- Accurate Predictions
- Sensitive to pertubations
- Don't know when they don't know
- Overconfident in their predictions

Often considered "unreliable"


WELL, WHAT DO
WE DO NOW?
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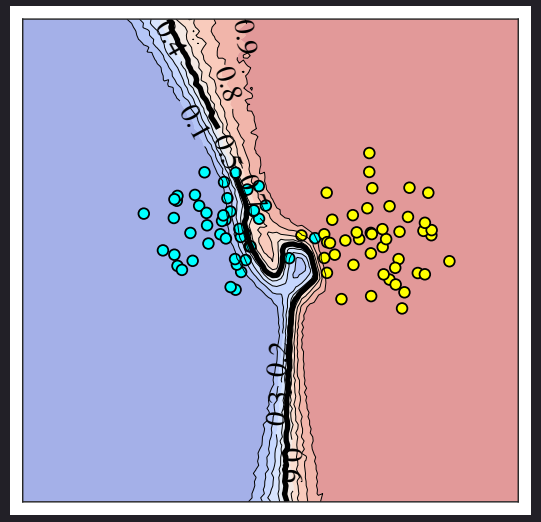
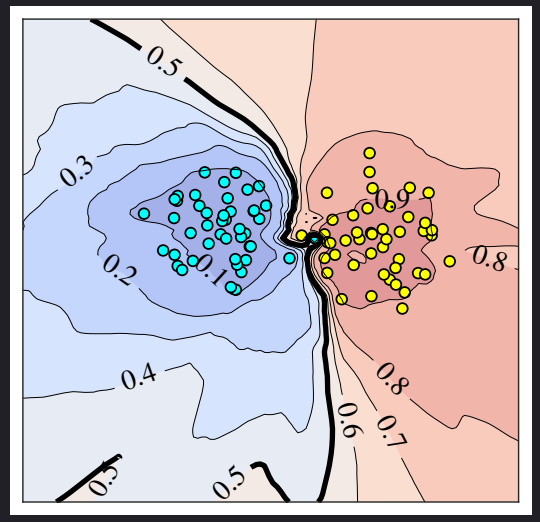
Uncertainty Quantification can Help...

Reduce Overconfidence

NN w/o UQ



NN w UQ



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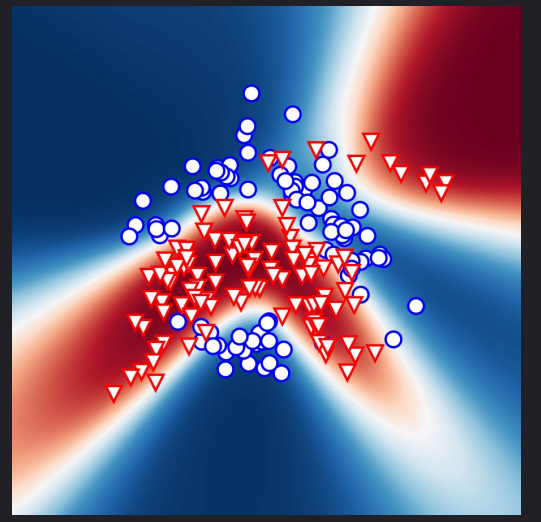
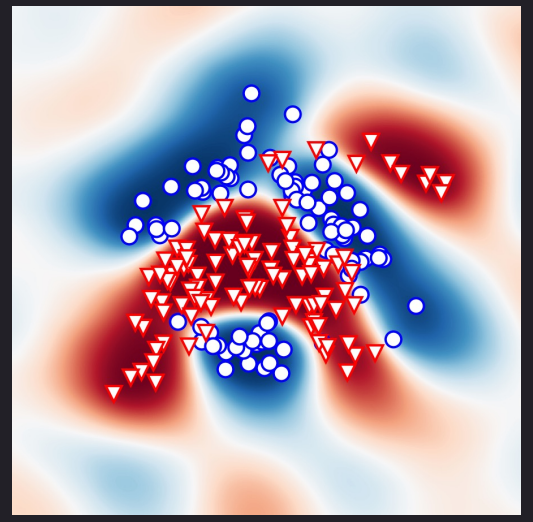
Understand Inductive Biases

ReLU



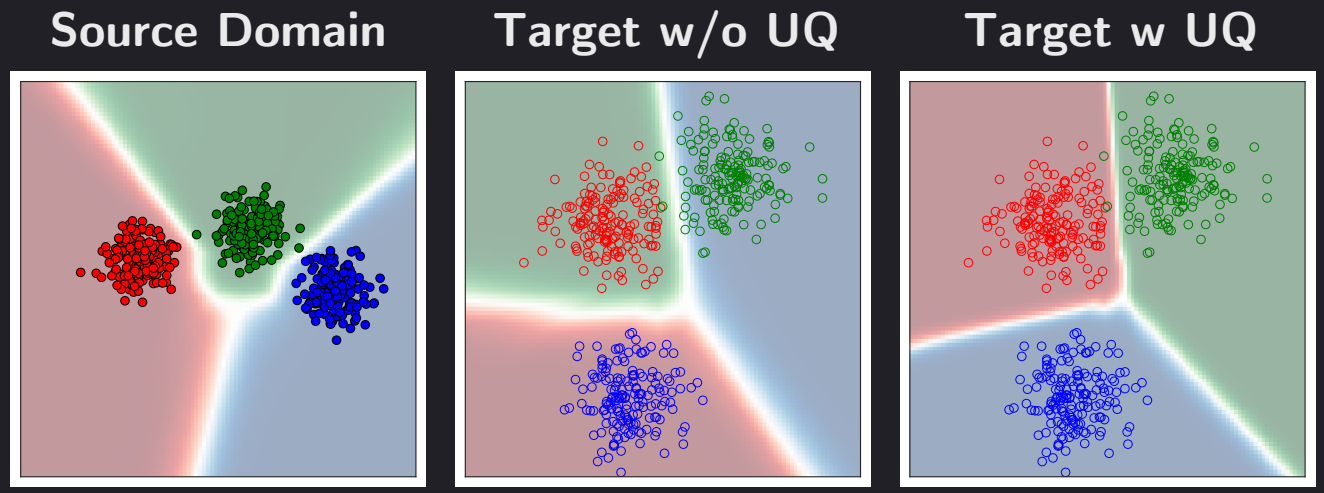
Periodic Function



Source: L Meronen, M Trapp, A Solin. Periodic activation functions induce stationarity. In NeurIPS, 2021.

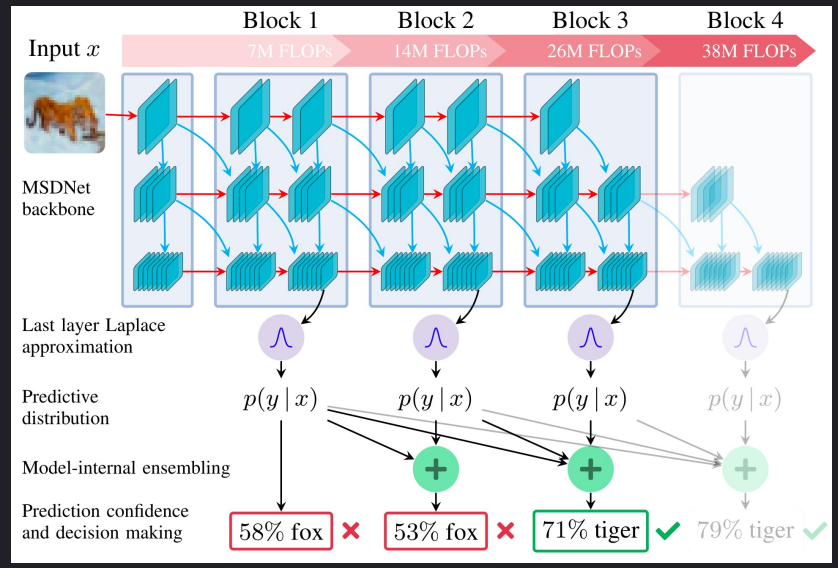
Uncertainty Quantification can Help...

Robustify our Methods



Source: S Roy *et al.* Uncertainty-guided Source-free Domain Adaptation. In ECCV, 2022.

Decide When to Act Differently



Source: L Meronen *et al.* Fixing Overconfidence in Dynamic Neural Networks. In WACV, 2024.

Sources of Uncertainty

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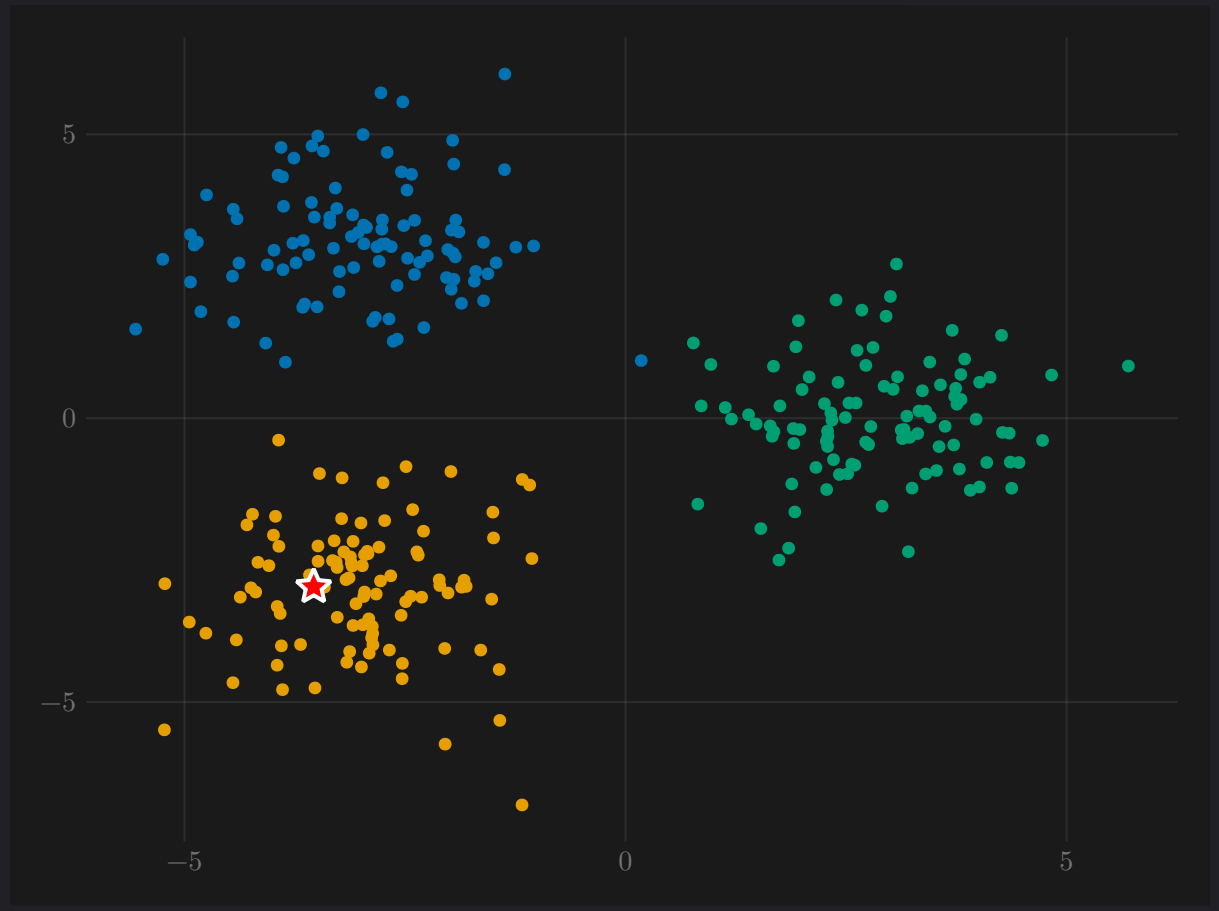
Uncertainty Inherent to the Data



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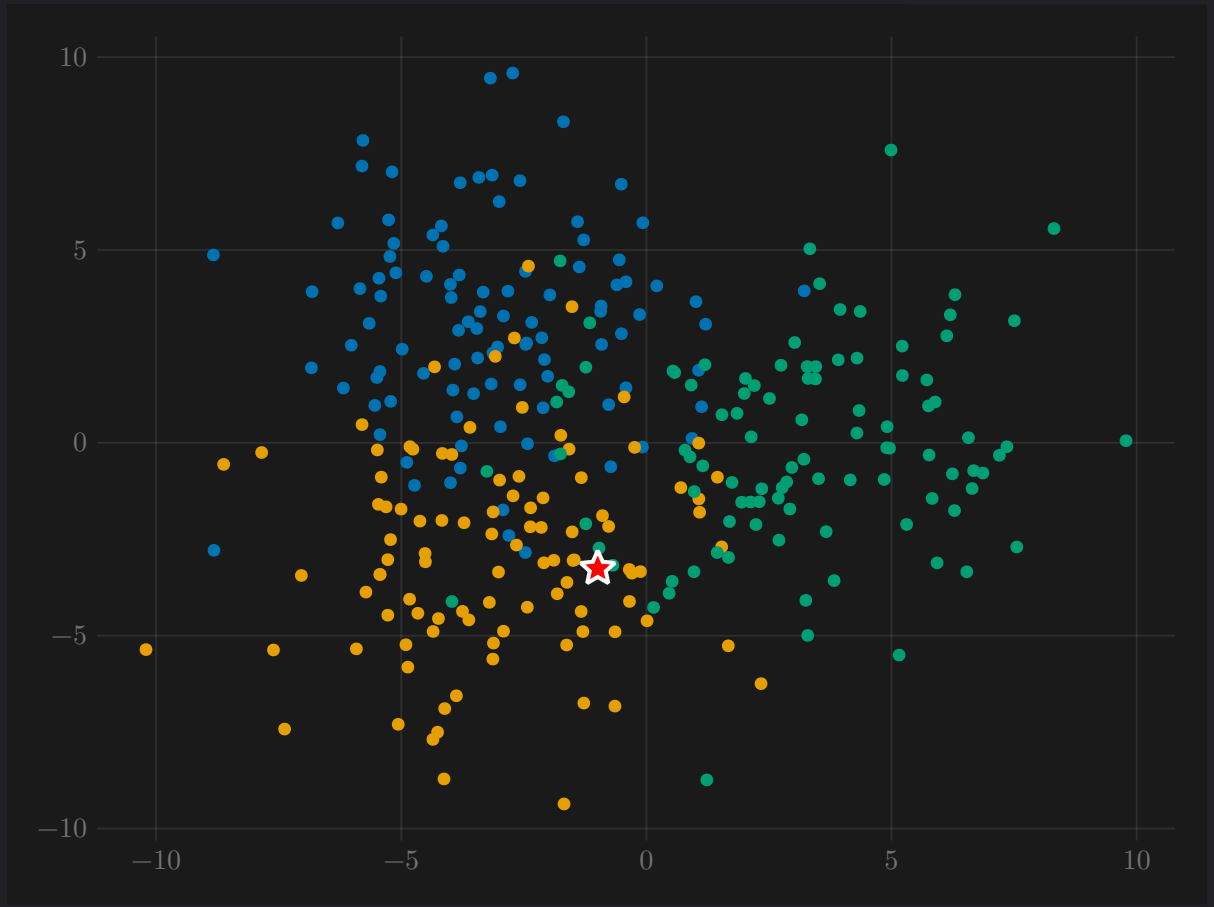

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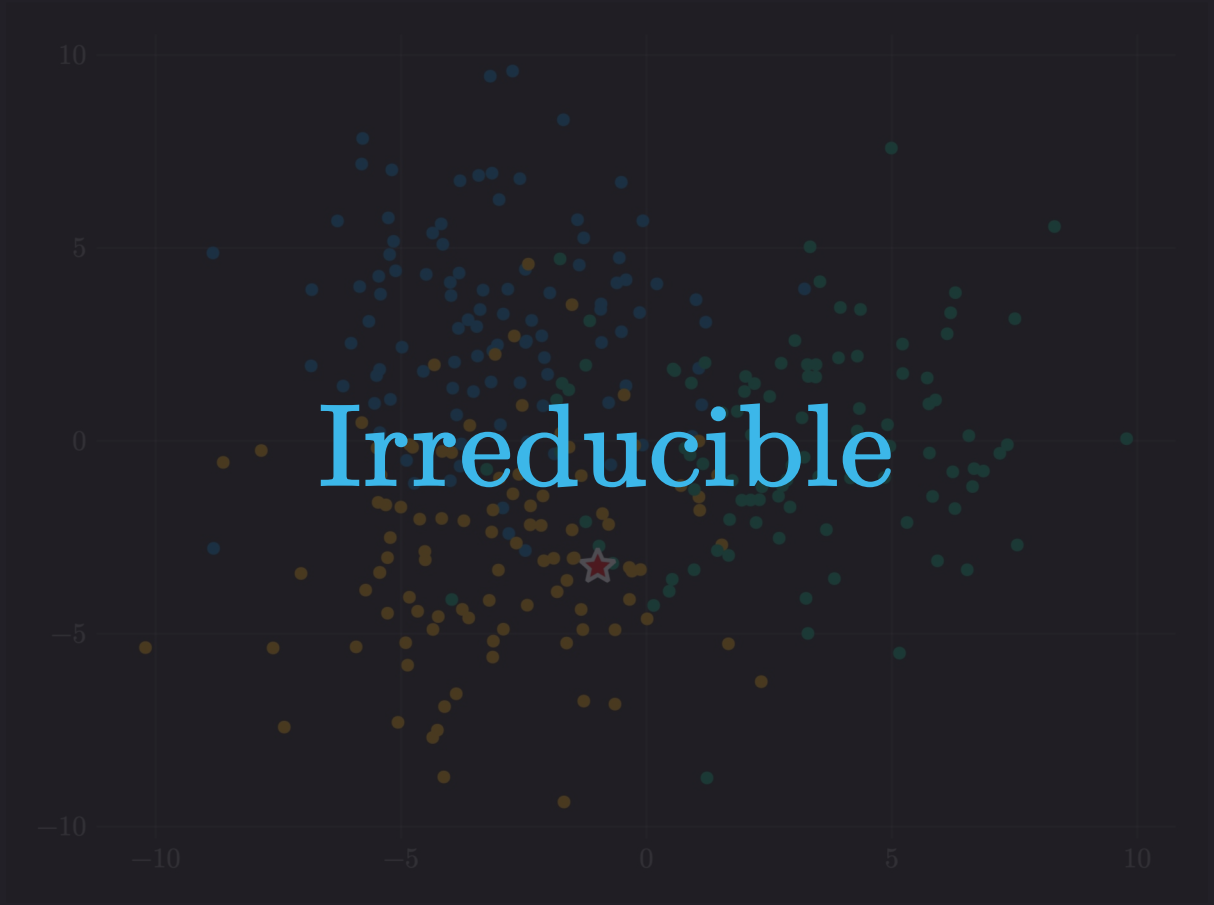
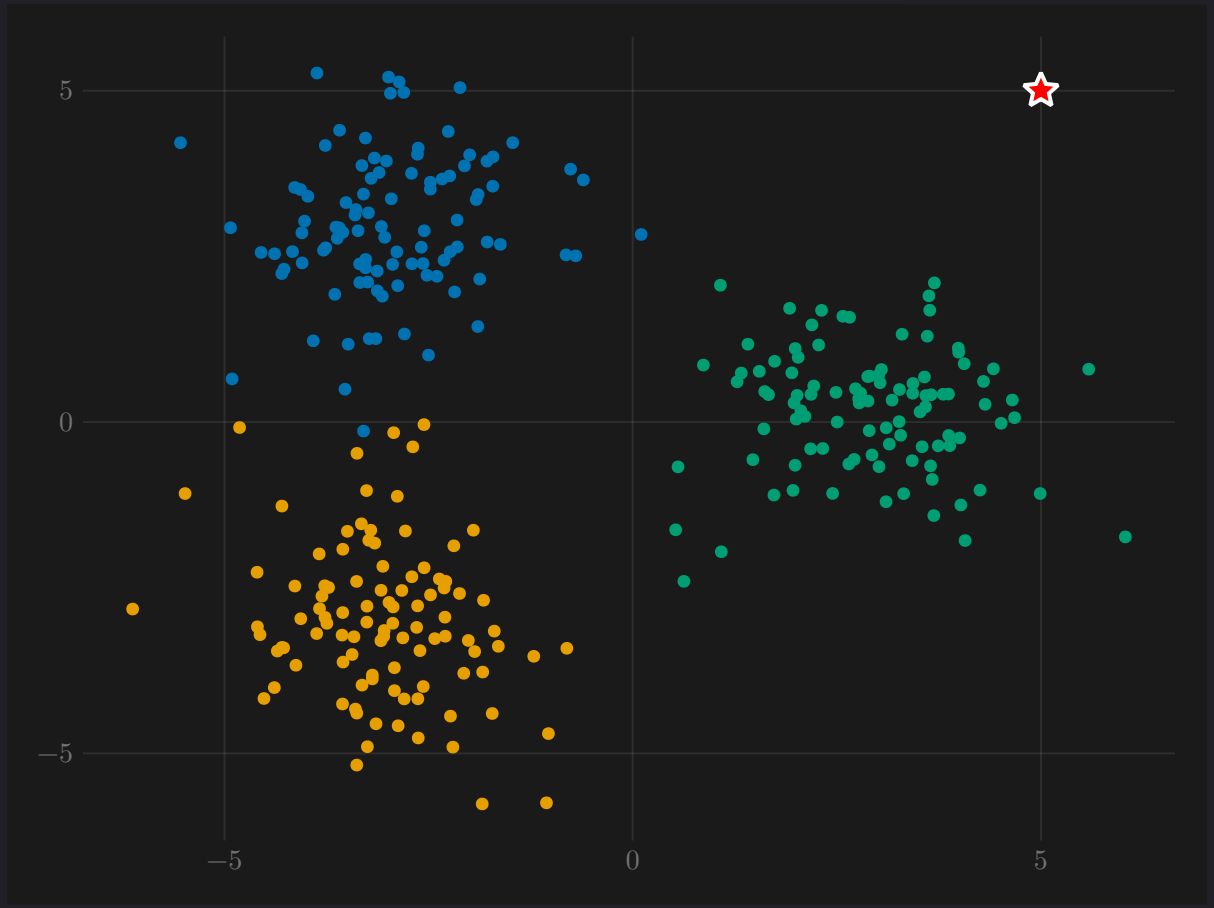


Uncertainty due to Lack of Knowledge

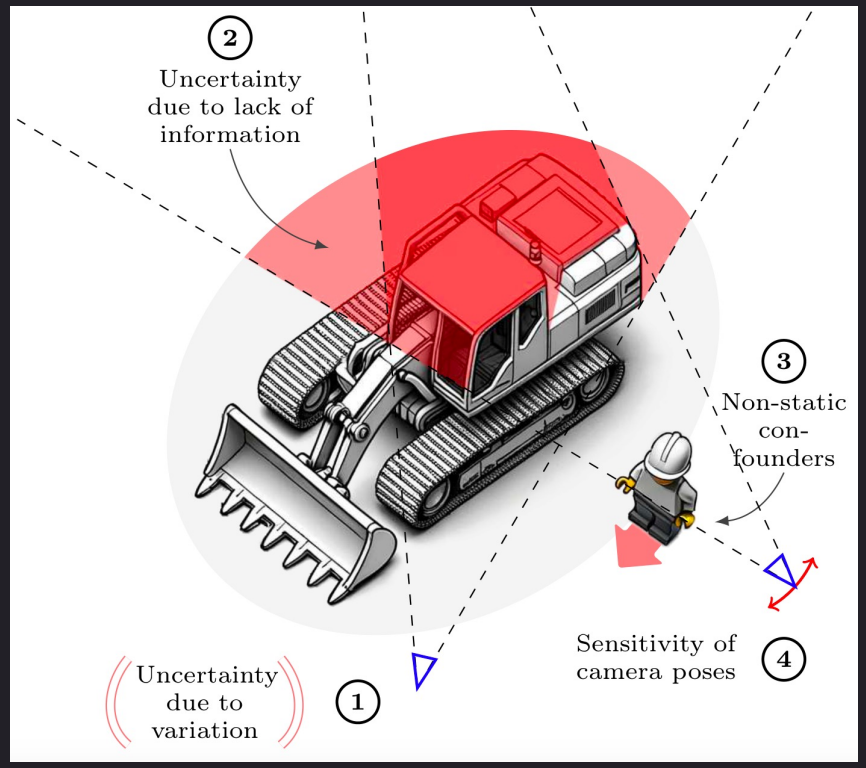


Uncertainty due to Lack of Knowledge

Reducible

Uncertainty due to Lack of Knowledge

Sources vary between Applications



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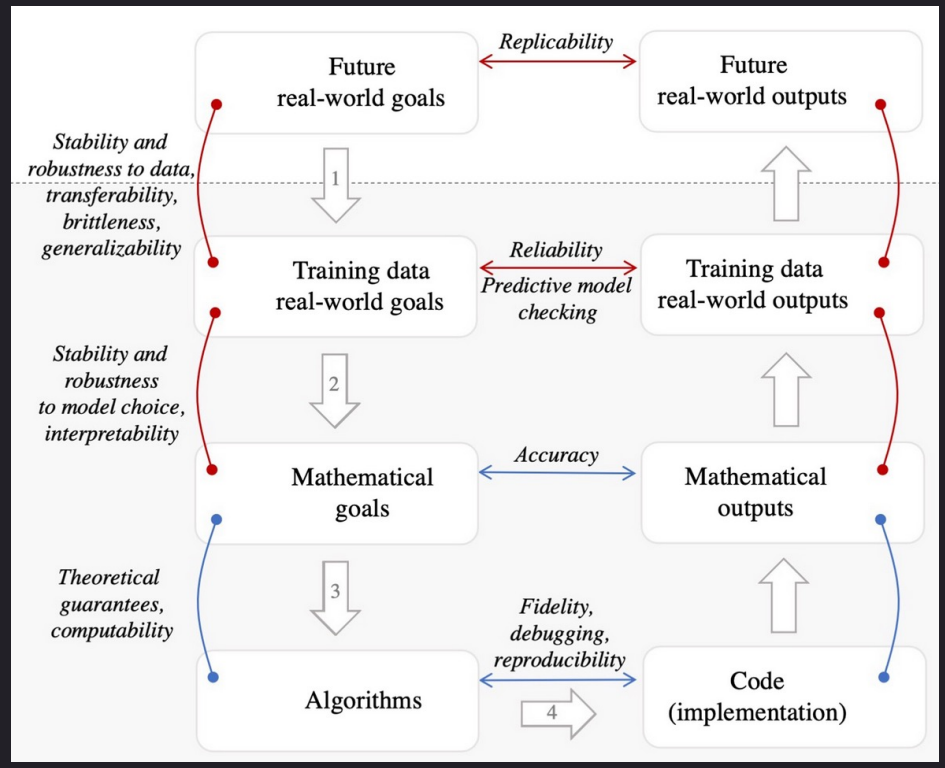
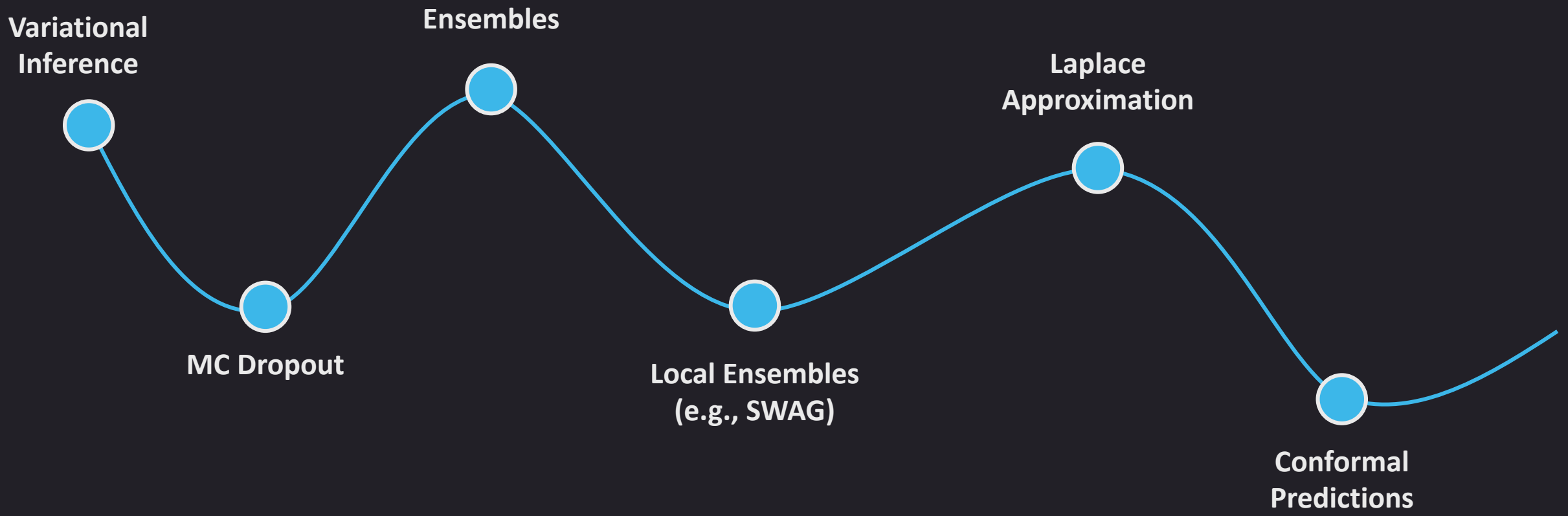


Source: T Broederick *et al.* Toward a Taxonomy of Trust for Probabilistic Machine Learning. Science Advances 9, eabn399, 2023.

Methods for UQ in DL

Methods for Uncertainty Quantification



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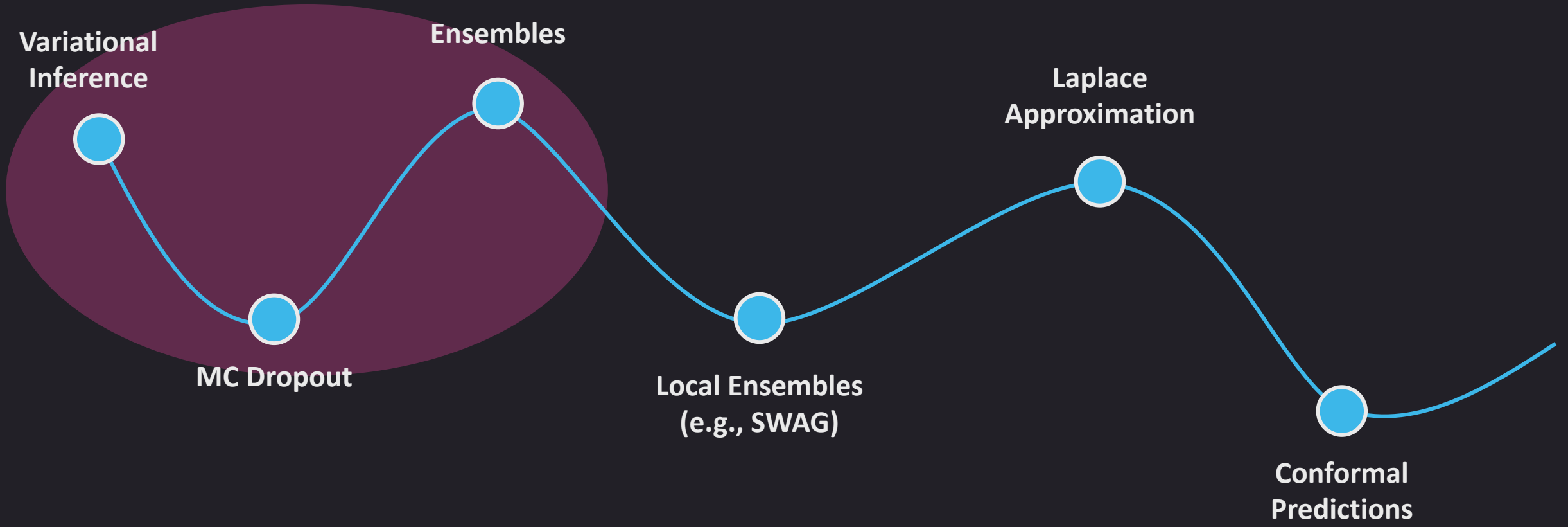
Methods for Uncertainty Quantification



Incorporate UQ into the Training

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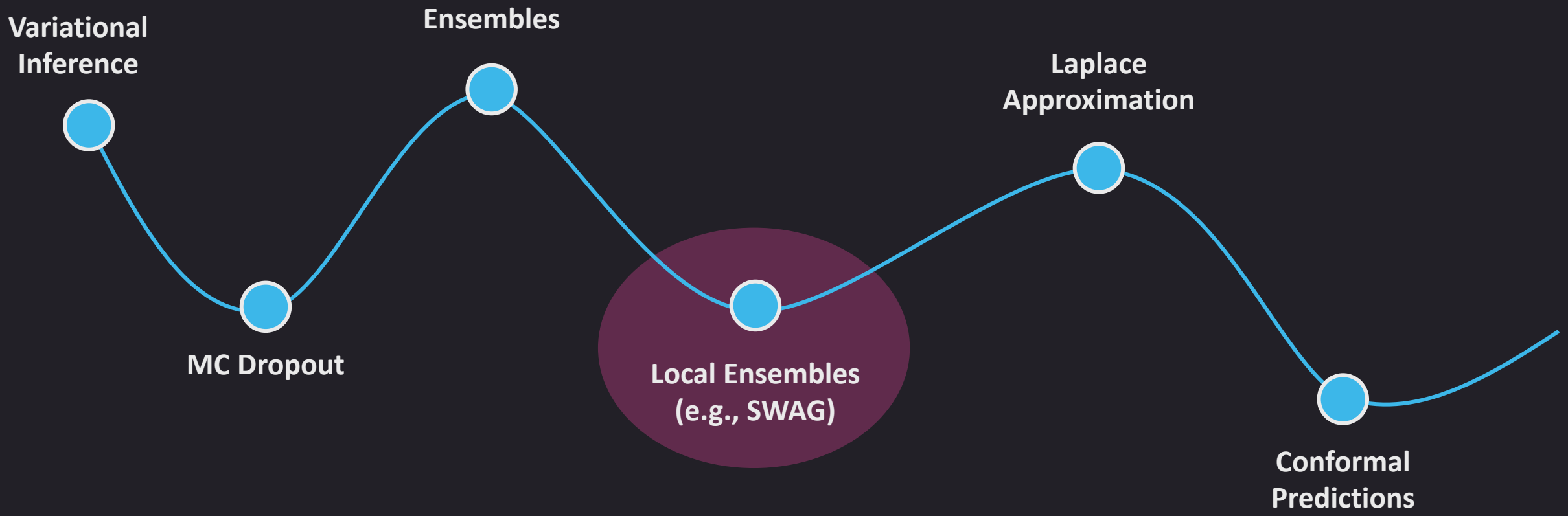
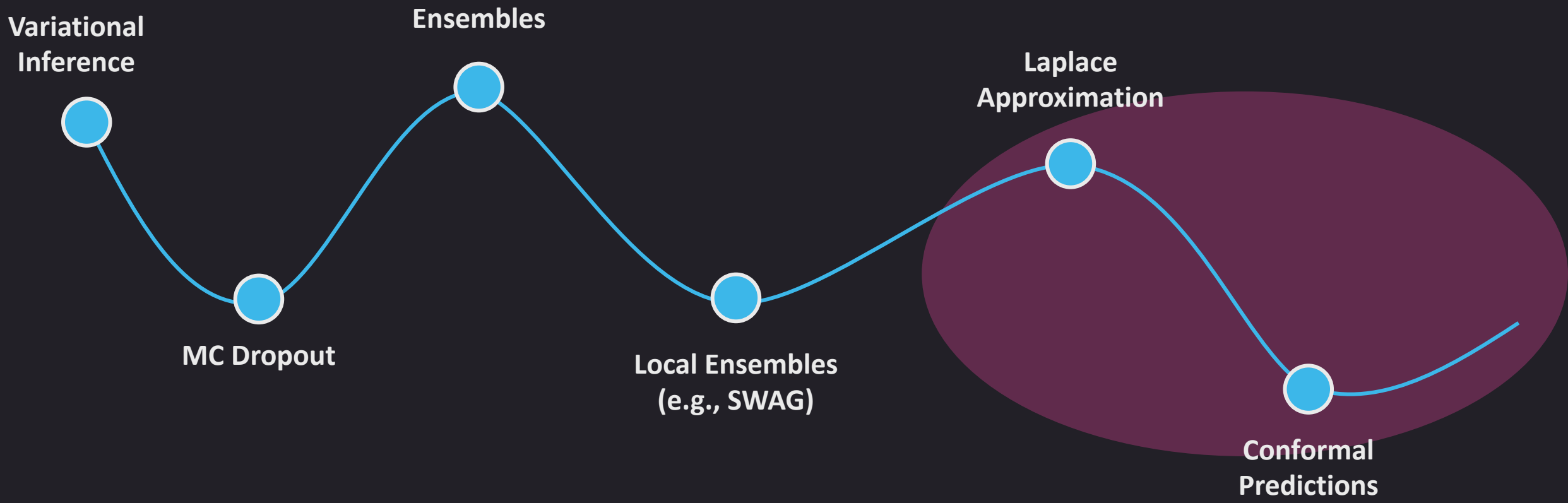
Methods for Uncertainty Quantification



Moved toward post-hoc Methods

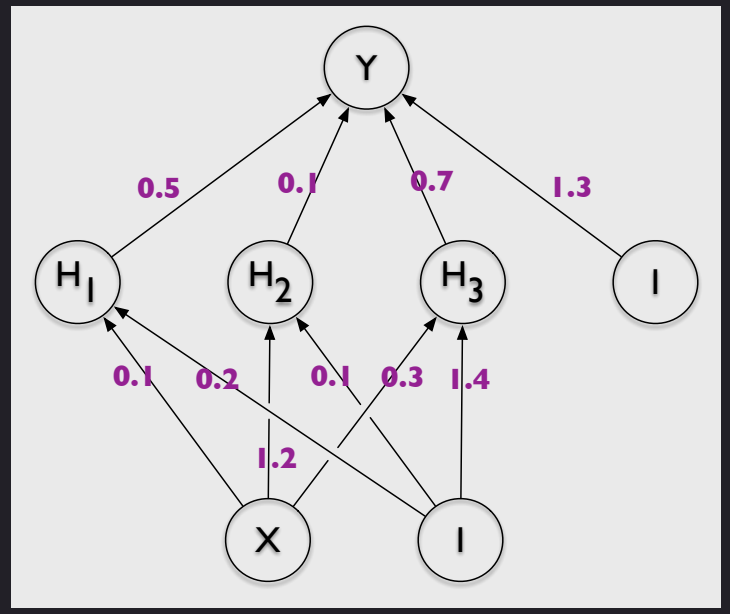
Methods for Uncertainty Quantification



Aera of post-hoc Methods

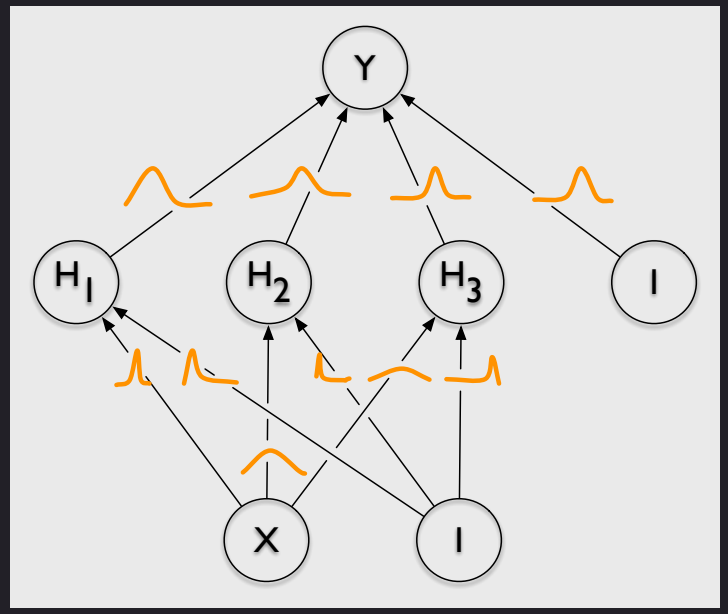
Bayesian Deep Learning

Standard NN



- Weights are learnable parameters
- Output is deterministically given for any input

Bayesian NN



- Weights are represented by probability distributions
- Parameters of probability distributions are learnable
- Output is a distribution and not a single value

Source: C Blundell *et al.* Weight Uncertainty in Neural Networks, In ICML 2015.

Bayesian Deep Learning

Unfortunately, inference in Bayesian Neural Networks (BNNs) is notoriously hard!

In BNNs we need to perform Bayesian inference (conditioning):

Prior on the weights

Training Data

Likelihood function

Posterior (conditional) Distribution over the Weights

$$p(\boldsymbol{w} \mid \mathcal{D}) = \frac{p(\boldsymbol{w})p(\mathcal{D} \mid \boldsymbol{w})}{\int_{\boldsymbol{w}} p(\mathcal{D} \mid \boldsymbol{w}) \mathrm{d}\boldsymbol{w}}$$

We cannot compute this!


WELL, WHAT DO
WE DO NOW?
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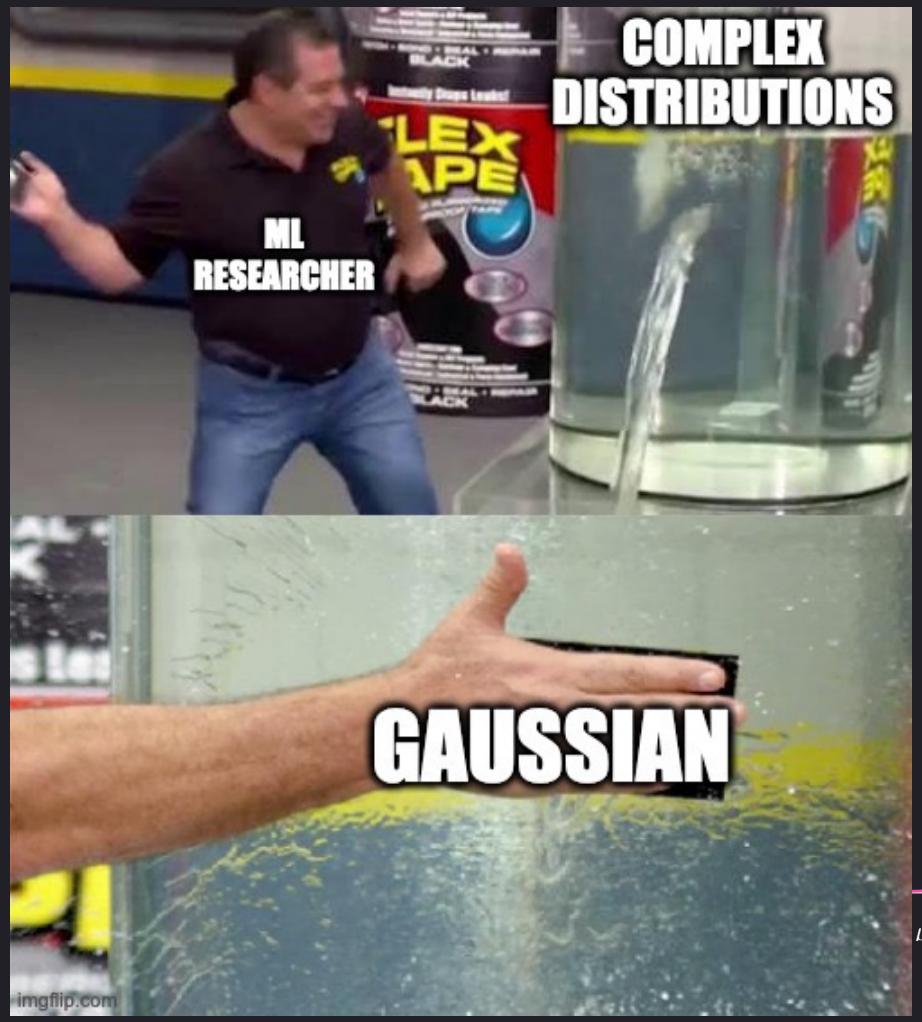
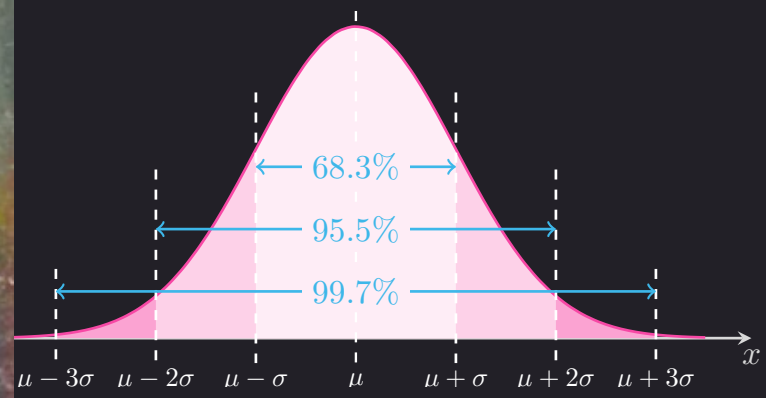
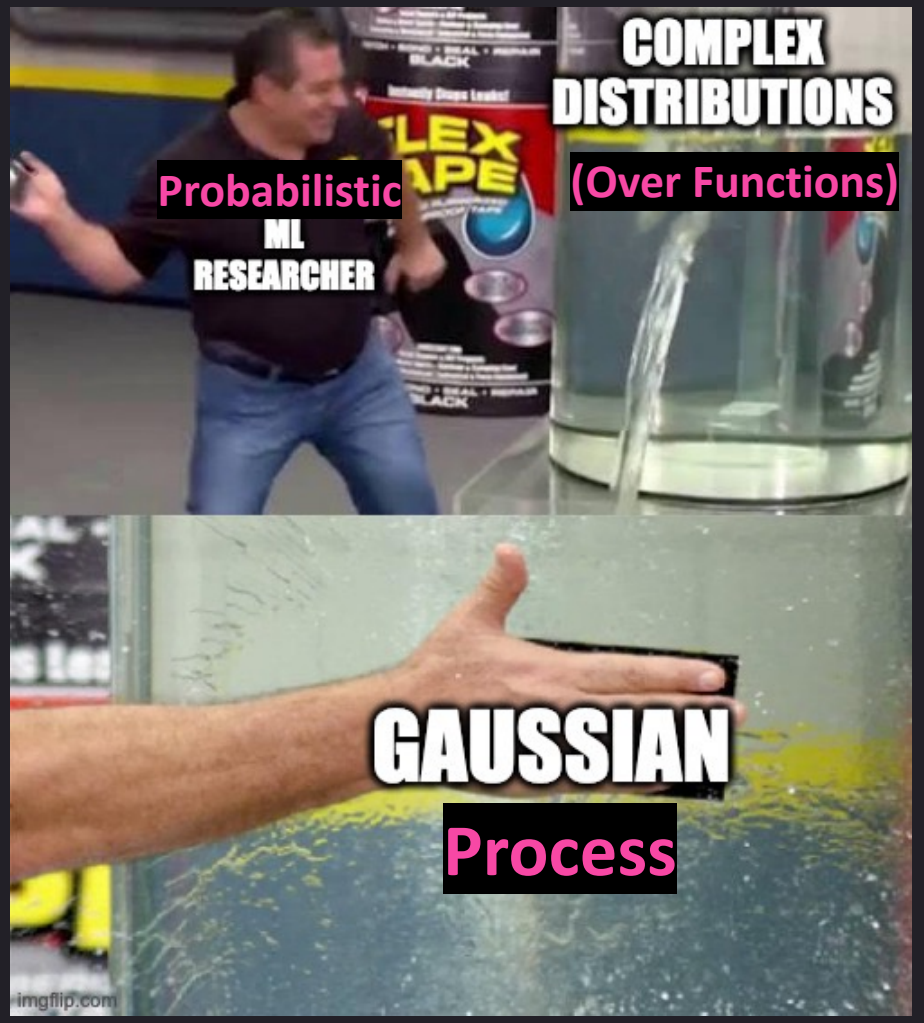
Laplace Approximation





Laplace Approximation



Laplace Approximation

$$p(\boldsymbol{w} \mid \mathcal{D}) = \frac{p(\boldsymbol{w})p(\mathcal{D} \mid \boldsymbol{w})}{\int_{\boldsymbol{w}} p(\mathcal{D} \mid \boldsymbol{w})\mathrm{d}\boldsymbol{w}}$$

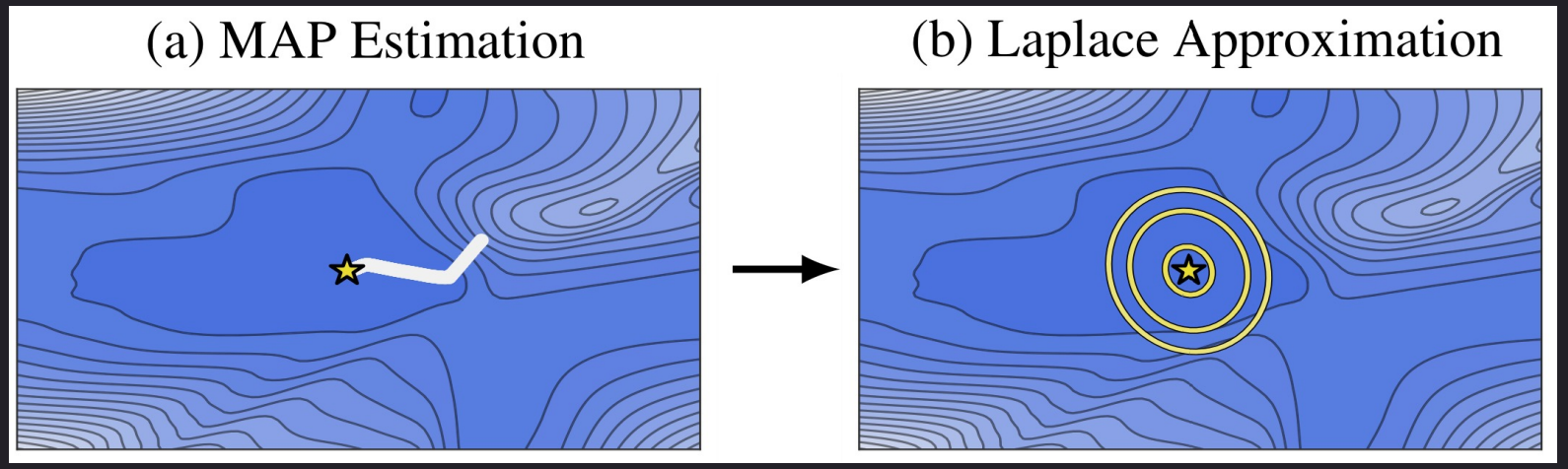
$$\log p(\boldsymbol{w} \mid \mathcal{D}) = \overbrace{\underbrace{\log p(\boldsymbol{w})}_{\text{L2 regularization}} + \underbrace{\log p(\mathcal{D} \mid \boldsymbol{w})}_{\text{Cross-Entropy}}}^{\text{Negated Loss}} - \underbrace{C}_{\text{Unknown}}$$

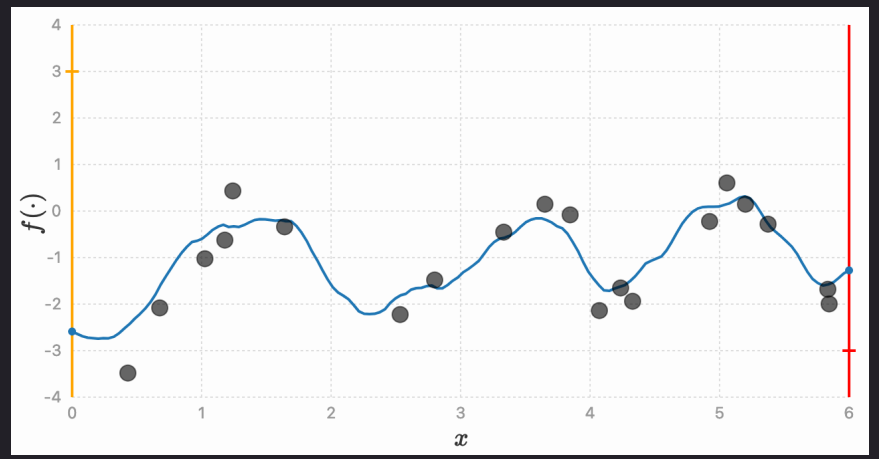
$$\underbrace{\log p(\boldsymbol{w}) + \log p(\mathcal{D} \mid \boldsymbol{w})}_{\ell(\boldsymbol{w})} \approx \ell(\boldsymbol{w}^*) + \boldsymbol{J}_{\ell|_{\boldsymbol{w}=\boldsymbol{w}^*}}(\boldsymbol{w} - \boldsymbol{w}^*) - \frac{1}{2}\boldsymbol{H}_{\ell|_{\boldsymbol{w}=\boldsymbol{w}^*}}(\boldsymbol{w} - \boldsymbol{w}^*)^2$$

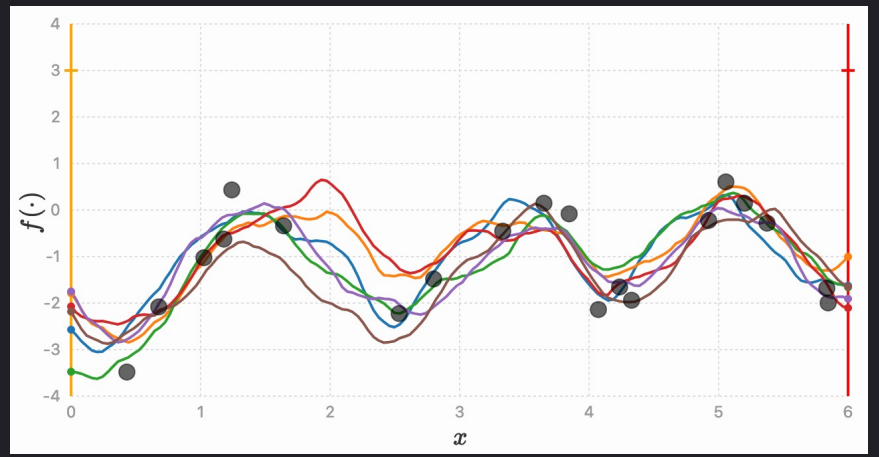
$$= \ell(\boldsymbol{w}^*) - \frac{1}{2}\boldsymbol{H}_{\ell|_{\boldsymbol{w}=\boldsymbol{w}^*}}(\boldsymbol{w} - \boldsymbol{w}^*)^2$$

$$\propto \log \mathcal{N}(\boldsymbol{w}^*, \boldsymbol{H}^{-1}_{\ell|_{\boldsymbol{w}=\boldsymbol{w}^*}})$$

Laplace Approximation

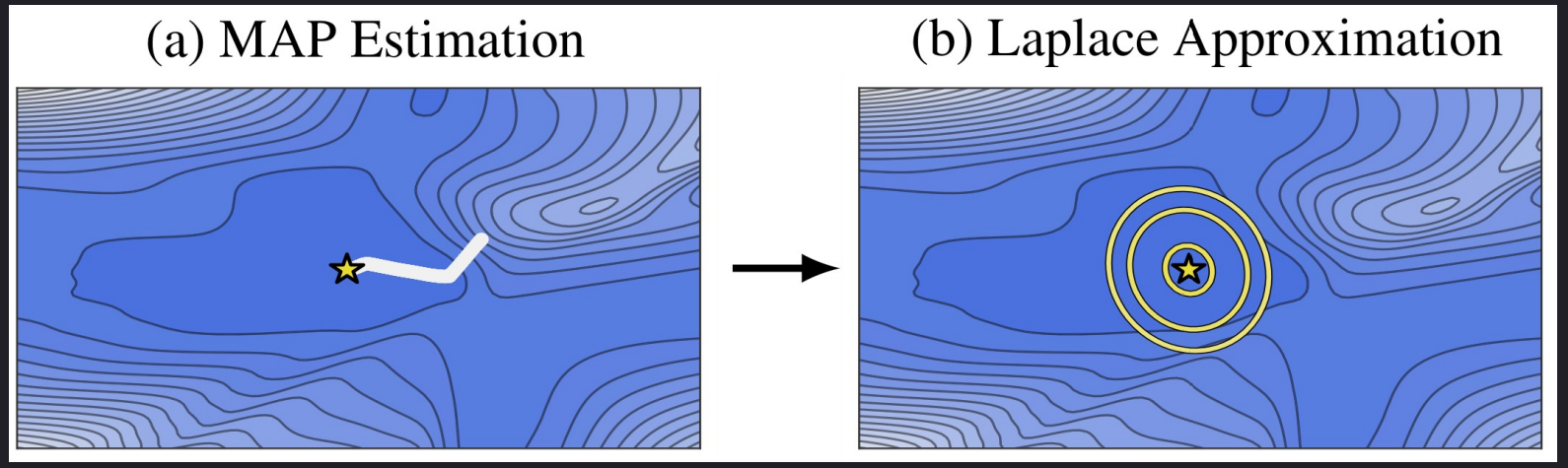


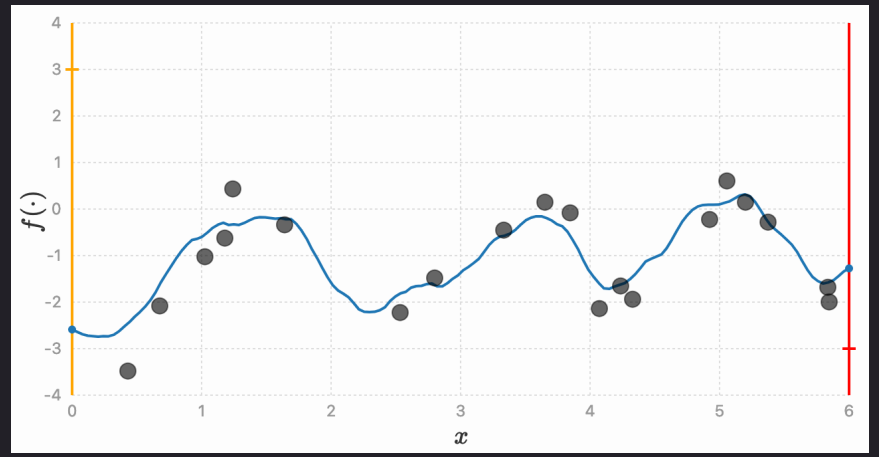


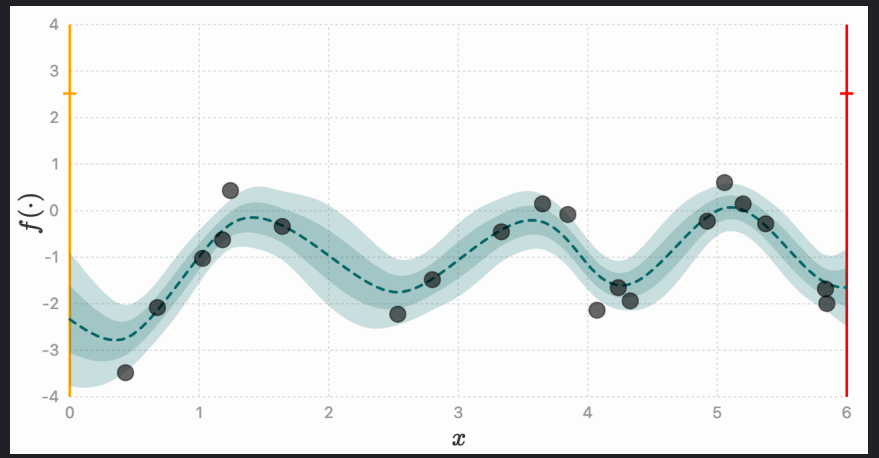


Source: E Daxberger *et al.* Laplace Redux - Effortless Bayesian Deep Learning. In NeurIPS 2021.
Source: Interactive Gaussian Process Visualization by Ti John (http://www.infinitecuriosity.org/vizgp/)

Laplace Approximation







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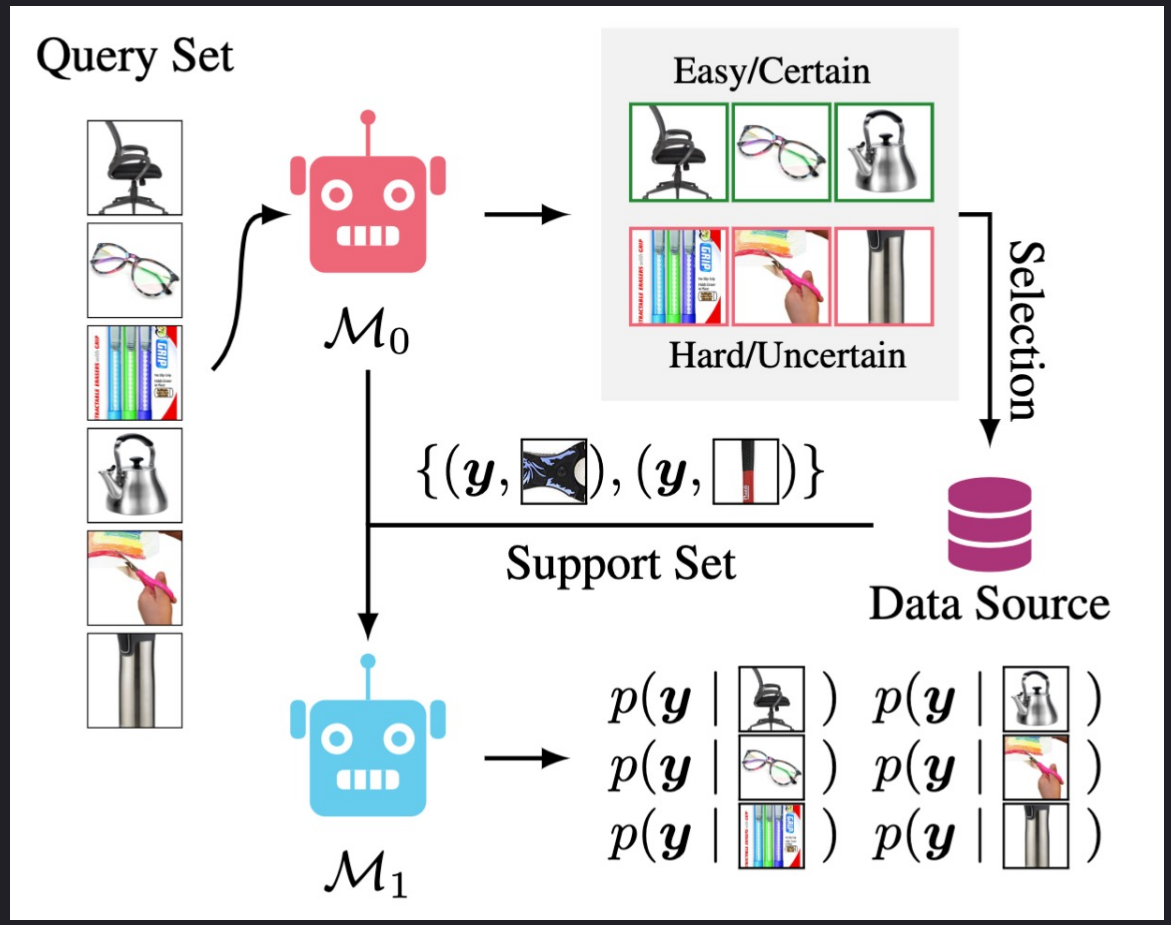
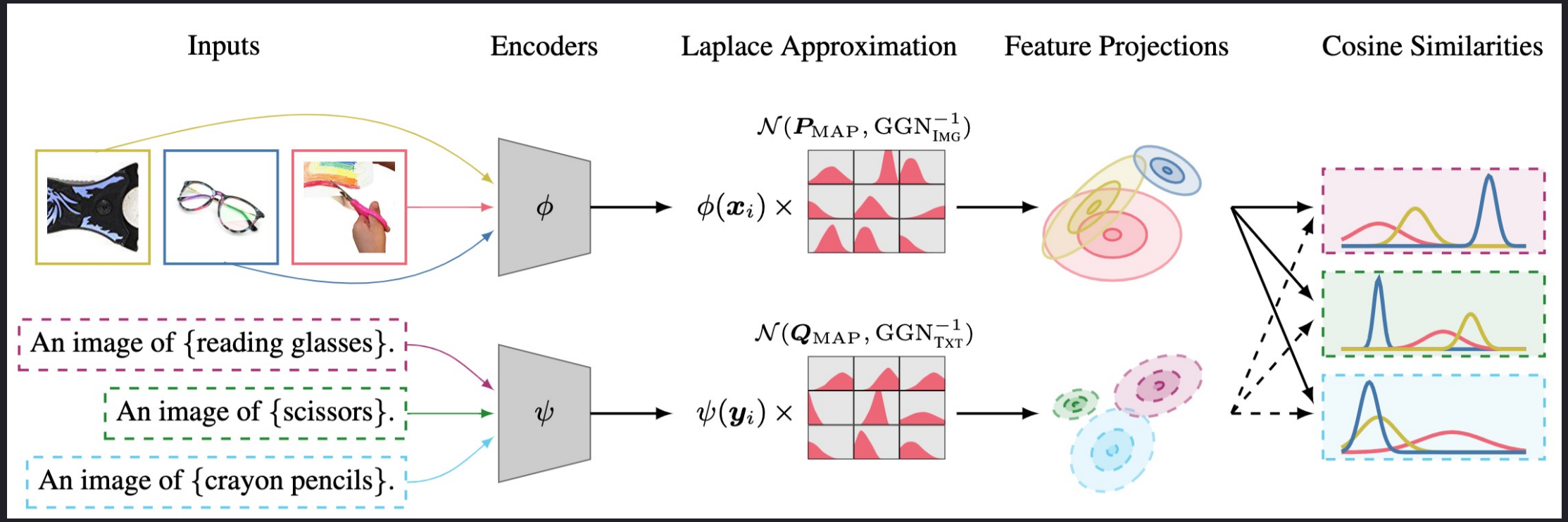
Probabilistic Active Learning in VLMs



Source: A Baumann *et al.* Probabilistic Active Few-Shot Learning in Vision-Language Models. Under review.

Probabilistic Active Learning in VLMs



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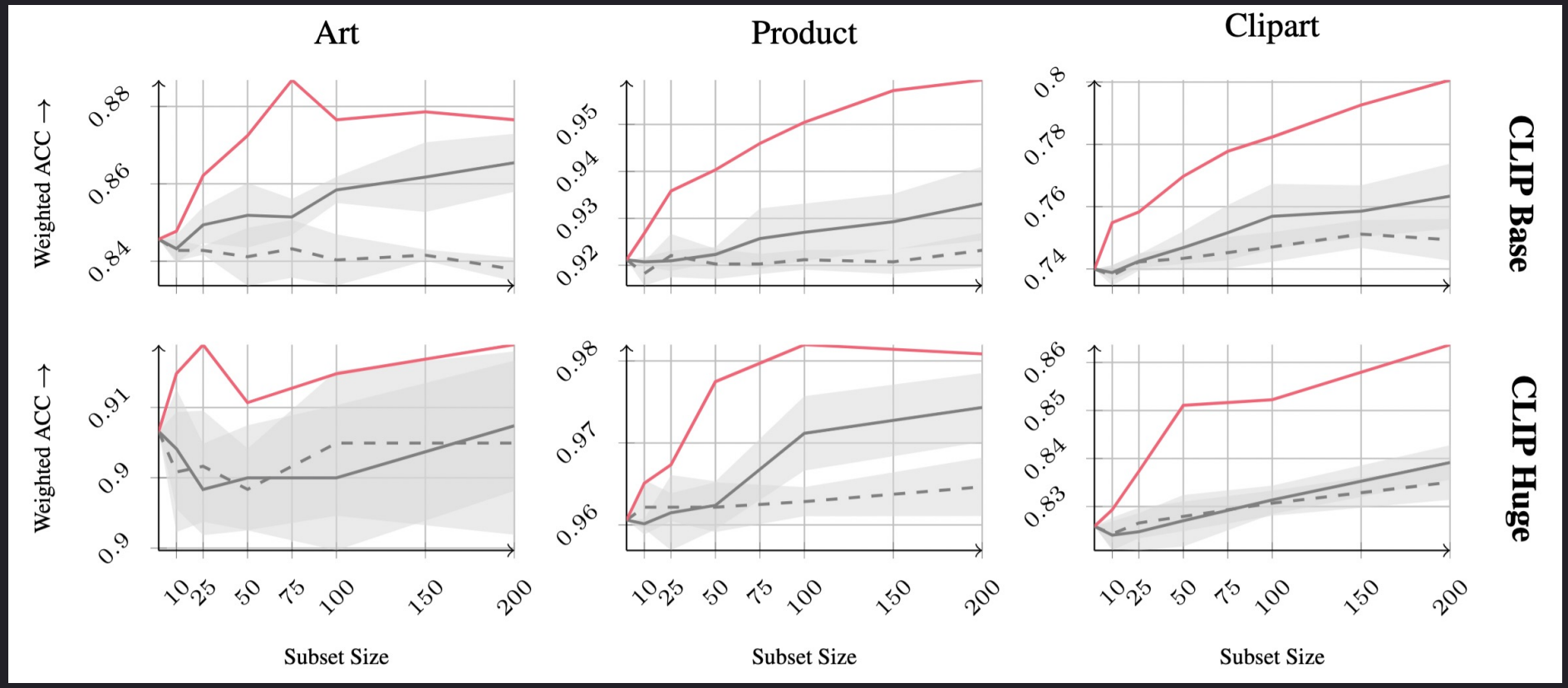
Probabilistic Active Learning in VLMs



selection informed by uncertainties

uninformed random/informed random selection

Source: A Baumann *et al.* Probabilistic Active Few-Shot Learning in Vision-Language Models. Under review.

Streamlining Predictions in BDL

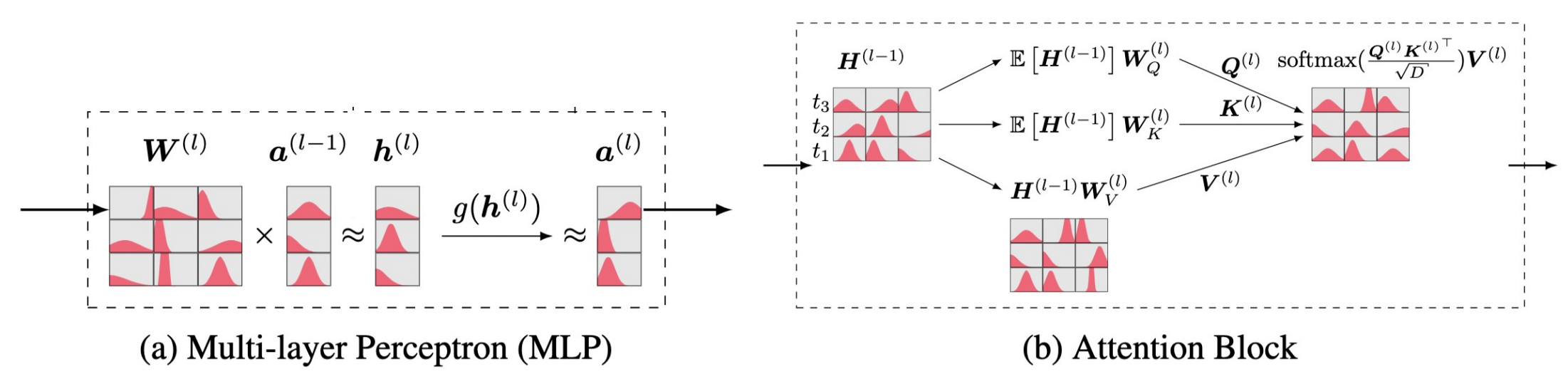
$$p(\boldsymbol{w} \mid \mathcal{D}) = \frac{p(\boldsymbol{w})}{\int}$$

Laplace
Variational Approximation

$$w)\mathrm{d}\boldsymbol{w}$$

$$p(y = c \mid \boldsymbol{x}^*, \mathcal{D}) = \int_{\boldsymbol{w}} p(\boldsymbol{w} \mid \mathcal{D}) p(\boldsymbol{x}^* \mid \boldsymbol{w}) \mathrm{d}\boldsymbol{w}$$

Streamlining Predictions in BDL



(a) Multi-layer Perceptron (MLP)

(b) Attention Block

Source: R Li *et al.* Posterior Inferred, Now What? Streamlining Prediction in Bayesian Deep Learning. Under review.

Challenges

- Laplace approximations are local approximations
- Estimating the Hessian matrix is computational demanding (requires approximations)
- Predictions under the linearized Laplace can be expensive to perform
- Somewhat ad-hoc, requires tuning of the prior variance.
- Unclear, what is a good prior on the weights.

Despite those challenges, current tools can already provide useful estimates in many scenarios.

Ready-Made Libraries

Python (PyTorch)

- Laplace Redux: https://github.com/aleximmer/Laplace

Julia

- LaplaceRedux.jl: https://github.com/JuliaTrustworthyAI/LaplaceRedux.jl

Conclusion

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Conclusion

- To get toward reliable ML, we need to account for uncertainties!
- We need to move away from looking only at accuracy!
- Modern (post-hoc) tools can provide useful estimates.

Various open challenges, but the future looks bright!

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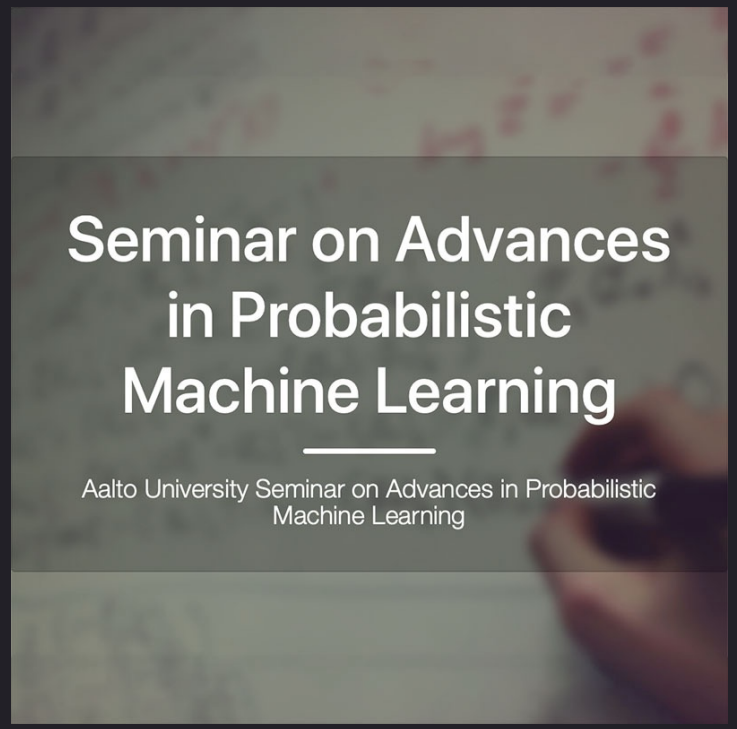
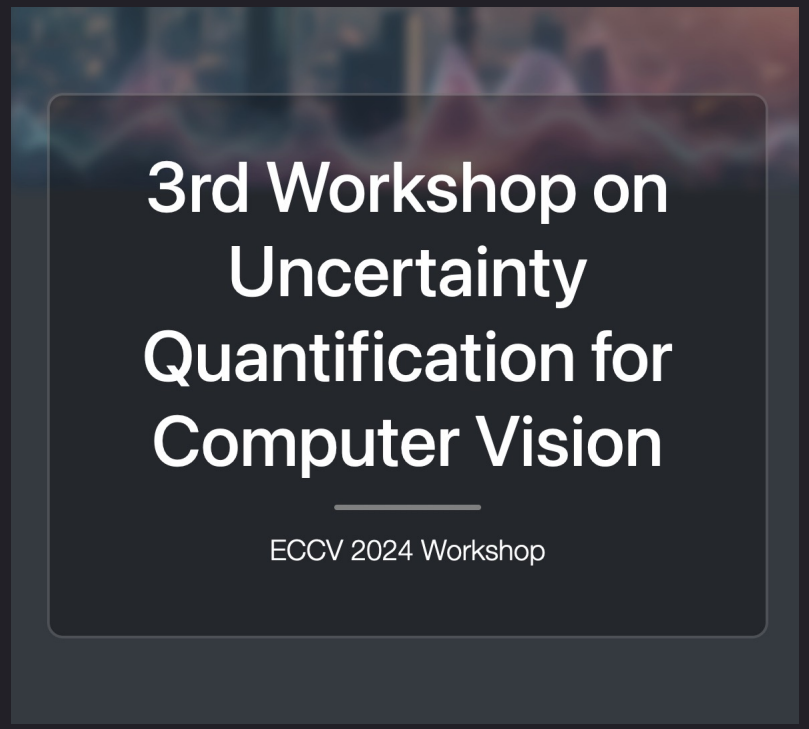
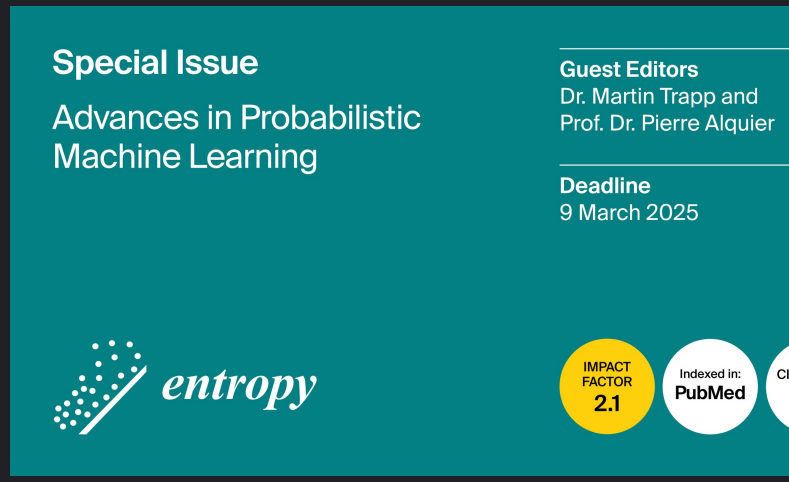
Some Advertisement



https://aaltoml.github.io/apml/



https://uncertainty-cv.github.io



References (order of appearance) 1/2

- P W Koh *et al.* **WILDS: A Benchmark of in-the-Wild Distribution Shifts**. In ICML, 2021. *(https://arxiv.org/abs/2012.07421)*
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- A Kristiadi, M Hein, P Hennig. **Being Bayesian, Even Just a Bit, Fixes Overconfidence in ReLU Networks.** In ICML, 2020. *(https://arxiv.org/abs/2002.10118)*
- L Meronen, M Trapp, A Solin. **Periodic activation functions induce stationarity.** In NeurIPS, 2021. *(https://arxiv.org/abs/2110.13572)*
- S Roy *et al.* **Uncertainty-guided Source-free Domain Adaptation.** In ECCV, 2022. *(https://arxiv.org/abs/2208.07591)*
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