Friedrich-Alexander-Universität
Technische Fakultät

# Advanced Deep Learning

## Bayesian Deep Learning

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# 1. Introduction

## 2. Bayesian Neural Networks

2.1 Bayes by Backprop

2.2 Monte Carlo Dropout

## 3. Ensemble Methods

# Overconfident Networks

Sources:
https://i2.cdn.turner.com/money/dam/assets/160726155524-tesla-truck-crash-780x439.jpg
https://edition.cnn.com/2015/07/02/tech/google-image-recognition-gorillas-tag/index.html

# Overconfident Networks


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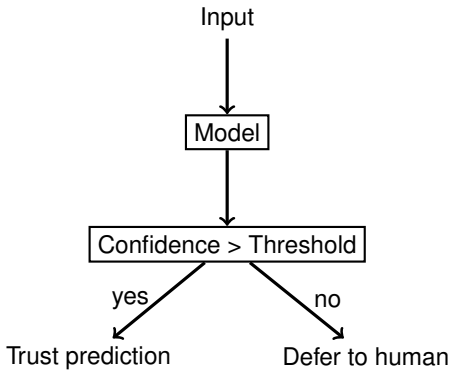
# Why Uncertainty?

## Uncertainty estimation

- Confidence along with prediction
  “the model knows what it doesn’t know”
- Beyond accuracy towards model calibration
- Possible: OOD classification

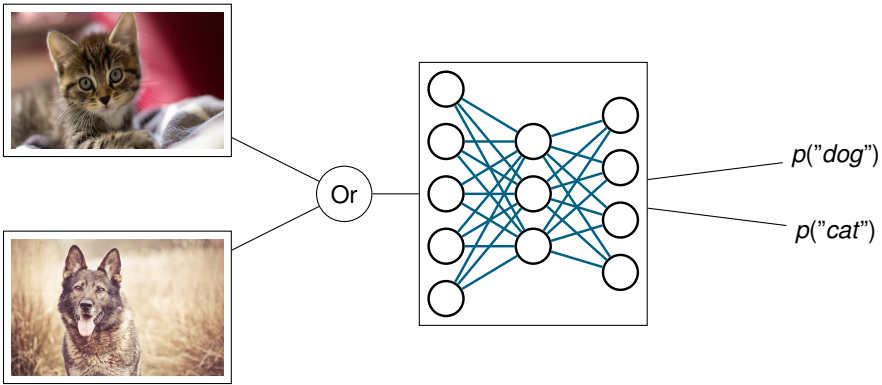
## Applications

- Safety/trustworthy systems
  - Autonomous driving
  - Medical diagnosis
- Active learning, continual learning, reinforcement learning, Bayesian optimization, decision making




Source: https://sonpeter.github.io/slides/Uncertainty&BDL.pdf

# Likelihood vs. Confidence




Source: Cat: https://getwallpapers.com/wallpaper/full/0/d/4/884248-best-cute-kitten-wallpaper-1920x1080-tablet.jpg
Dog: https://wallup.net/animals-dog-tongues/

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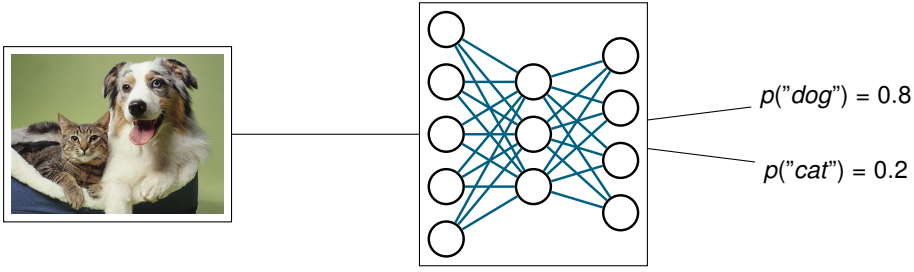


Softmax Layer: p("cat") + p("dog") = 1 !

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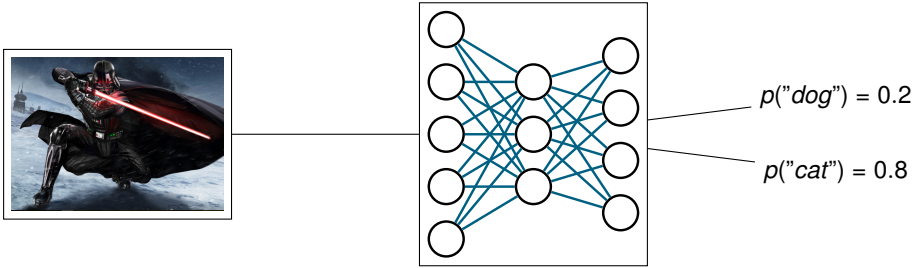


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Source: https://cutewallpaper.org/21/darth-vader-iphone-wallpaper-hd/view-page-21.html

# Empirical uncertainty estimation

Activations: 2.2e-12, 4e-11

Activations: 0.745, 0.435

- Low softmax activation $\rightarrow$ High uncertainty
- Rejection class

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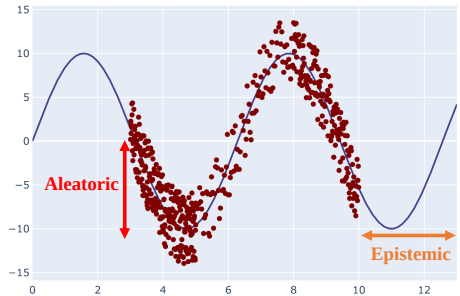
# Sources of Uncertainty

## Data and Model Uncertainty

### Data uncertainty (aleotoric uncertainty)

- Captures noise inherent in the data
- Caused by inherent noise, ambiguous/missing data, human bias
- **Irreducible** with more data – reducible by better data




Source: Abdar et al. 2021 [2]

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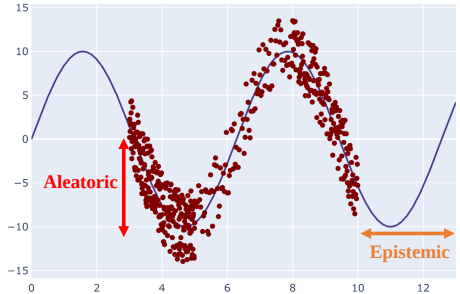
### Model uncertainty (epistemic uncertainty)

- Prediction confidence
- Captures ignorance which model generated our collected data
- Incurred by lack of training data, imbalanced/sparse data, out-of-distribution data
- **Reducible** with more data

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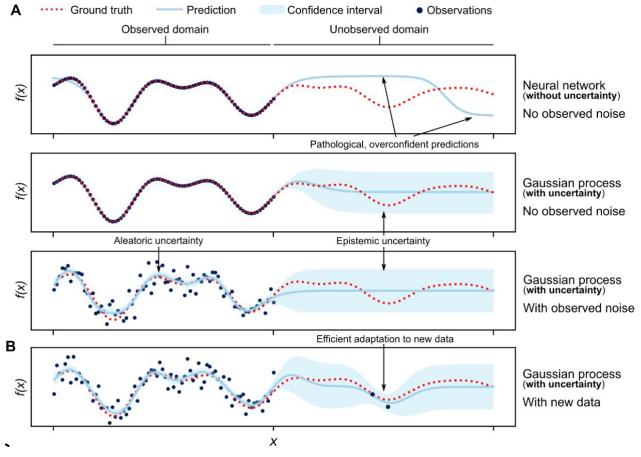


Source: Hie et al. 2020 [3]

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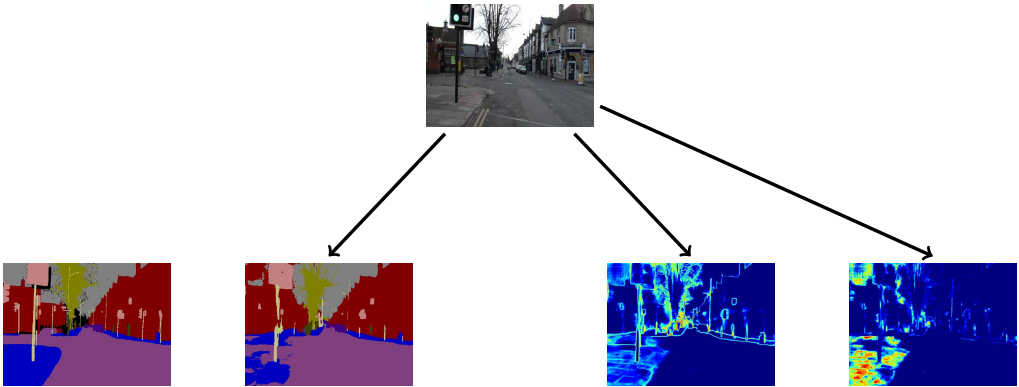


Source: Kendall and Gal 2017 [1]

# Bayesian Learning

Given: observed dataset $\mathcal{D} = \{x_i, y_i | i = 1, \ldots, N\}$ and model $\mathcal{M}$ with weights $\boldsymbol{\theta}$

## Frequentists

- Maximize likelihood $p(\mathcal{D}|\boldsymbol{\theta})$
- Learning: Find optimal $\boldsymbol{\theta}$ using optimization through differentiation

## Bayesianists

- Instead of point estimation, infer posterior distribution over $\boldsymbol{\theta}$:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{\overbrace{p(\mathcal{D}|\boldsymbol{\theta})}^{\text{likelihood}} \overbrace{p(\boldsymbol{\theta})}^{\text{prior}}}{\underbrace{p(\mathcal{D})}_{\text{evidence}}} = \frac{p(\mathcal{D}|\boldsymbol{\theta})\, p(\boldsymbol{\theta})}{\int p(\mathcal{D}|\boldsymbol{\theta}')p(\boldsymbol{\theta}')\, d\boldsymbol{\theta}'}$$

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$p(\mathcal{D}|\boldsymbol{\theta})$ : encodes data uncertainty
$p(\boldsymbol{\theta}|\mathcal{D})$ : encodes model uncertainty

# Bayesian Learning (cont.)

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})\, p(\boldsymbol{\theta})}{p(\mathcal{D})} = \frac{p(\mathcal{D}|\boldsymbol{\theta})\, p(\boldsymbol{\theta})}{\int p(\mathcal{D}|\boldsymbol{\theta}')p(\boldsymbol{\theta}')\, d\boldsymbol{\theta}'}$$

- Learning: "(Exact) Bayesian inference", finding posterior distribution

☞ For full posterior: marginalize over the whole parameter space → intractable!

→ Main problem of Bayesian learning

- At test time: predictive distribution is approximated via MC sampling:

$$p(y|x, \mathcal{D}) = \int p(y|x, \boldsymbol{\theta}')p(\boldsymbol{\theta}'|\mathcal{D})\, d\boldsymbol{\theta}' = \frac{1}{S}\sum_{s=1}^{S} p\left(y|x, \boldsymbol{\theta}^s\right)$$

# Bayesian Learning

**Goal: posterior distribution $p(\theta|\mathcal{D})$ intractable → approximate inference**

## 1. Gradient-based stochastic approximation

- Energy-based perspective
- Simulate dynamical systems whose stationary distribution is desired target distribution
- True posterior sampling generated via discretizing differential equations describing those dynamics

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### 1. Gradient-based stochastic approximation

- Energy-based perspective
- Simulate dynamical systems whose stationary distribution is desired target distribution
- True posterior sampling generated via discretizing differential equations describing those dynamics
- Methods:
  - Hamiltonian Monte Carlo (HMC): gold standard
  - Stochastic Gradient Hamiltonian Monte Carlo (SGHMC) [4]
  - Stochastic Gradient Langevin Dynamics (SGLD) [5]

\+ high fidelity approximation

– high complexity, many potential biases

**Goal: posterior distribution $p(\theta|\mathcal{D})$ intractable → approximate inference**

## 2. Deterministic approximation: local approximation

- Laplace approximation [6]
- Variational inference: employ parametric variational distribution $q_\phi(\boldsymbol{\theta})$
  → minimize $\mathbb{D}_{\mathrm{KL}}(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$
  → equivalent to maximizing variational lower bound (ELBO):

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi(\boldsymbol{\theta})} \log p(\mathcal{D}|\boldsymbol{\theta}) - \mathbb{D}_{\mathrm{KL}}(q_\phi(\boldsymbol{\theta})||p(\boldsymbol{\theta}))$$

  - Mean-field VI: $q_\phi(\boldsymbol{\theta})$ is factorized distribution (e.g. diagonal Gaussian), examples: Bayes by backprop
  - Dropout inference: Monte-Carlo Dropout

# Bayes by Backprop

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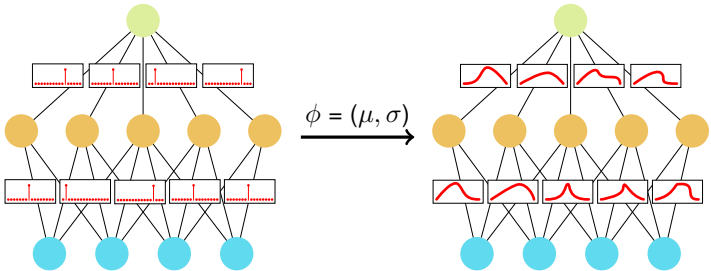
## Weight Uncertainty in Neural Network [7]




Source: Jospin et al. 2022 [8]

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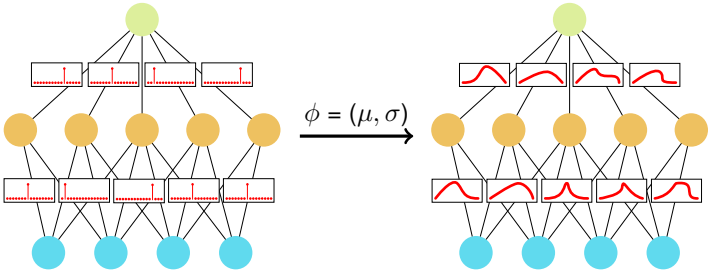


In practice: use re-parametrization trick!

- $w_i = \mu_i + \sigma_i * \epsilon$ with $\epsilon \sim \mathcal{N}(0, \mathbf{I})$
- NN with 2x #parameters

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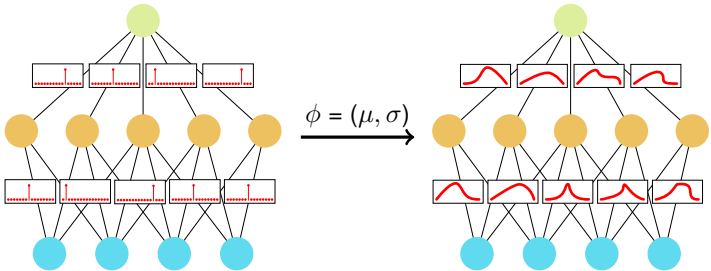


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- NN with 2x #parameters

☞ Careful: many people refer to this architecture as “Bayes Neural Network”

- BNN: any stochastic NN trained using Bayesian inference

Source: Jospin et al. 2022 [8]

# Monte Carlo Dropout

# Monte Carlo Dropout for VI

## Dropout as Bernoulli Sampling [14]

- Recap: Dropout:

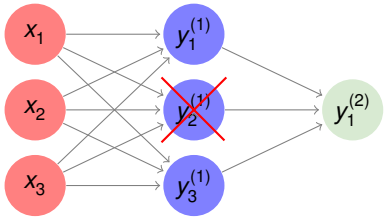
$$z_i \sim \text{Bernoulli}(1-p)$$
$$\hat{\mathbf{W}}_i = \boldsymbol{W}_i \,\text{diag}(\mathbf{z}_i)$$

with:

$p$ : dropout propability
$\mathbf{W}_i$ : weight matrix of layer $i$

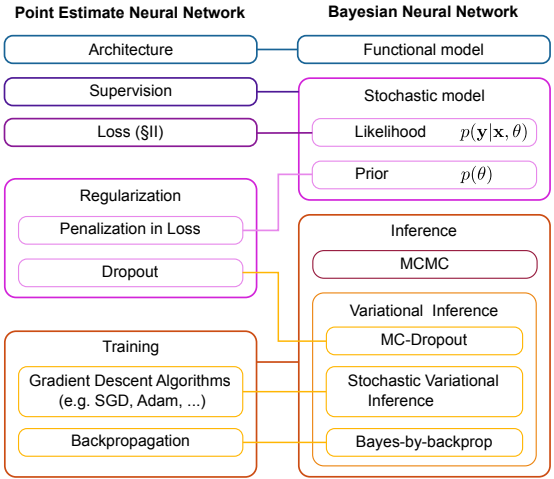
- Apply dropout during Bayesian inference
- Should not be seen as regularization

→ Add other regularization, e.g., $\ell^2$



# Bayesian Neural Networks

## Summary

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# A word of caution...

> For the good of science, please stop calling deep ensembles a “non-Bayesian” competitor to standard approximate Bayesian inference procedures.
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> Wilson and Izmailov, https://cims.nyu.edu/~andrewgw/deepensembles/

[1] is a closer approximation to the Bayesian posterior predictive distribution

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- The posterior for NNs is typically intractable ➔ all methods in Bayesian deep learning provide approximate inference ➔ are “non-Bayesian” in various ways

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- The posterior for NNs is typically intractable ➔ all methods in Bayesian deep learning provide approximate inference ➔ are “non-Bayesian” in various ways
- Bear with me:
  If **method A** is called **“non-Bayesian”**, and **method B “Bayesian”**, but method A behaves more Bayesian[1] than method B, the success of method A cannot serve as evidence that Bayesian methods don’t work very well

[1] is a closer approximation to the Bayesian posterior predictive distribution

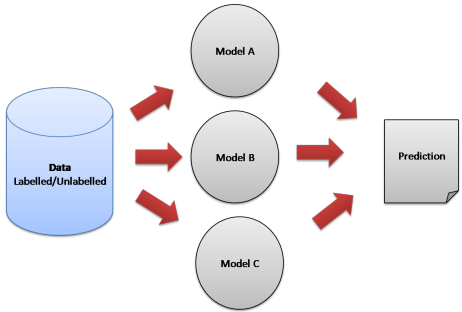
# Approaches for Ensemble-based Bayesian Learning

- Deep Ensembles [9]
- SWAG [10] & MultiSWAG [11]
- Hyperparameter ensembles [13]
- Batch ensembles [12]

Source: Image by rawpixel.com</a> on Freepik

# Deep Ensembles [9]

- Core idea: Train *M* different models with different initializations (same architecture)

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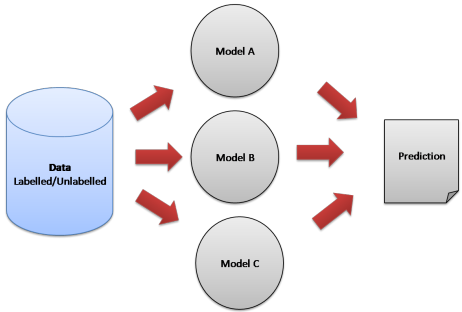
$$p(\mathbf{y}|\mathbf{x}, D) \approx \frac{1}{M} \sum_i p(\mathbf{y}|x, \boldsymbol{\theta}_i) \qquad (1)$$

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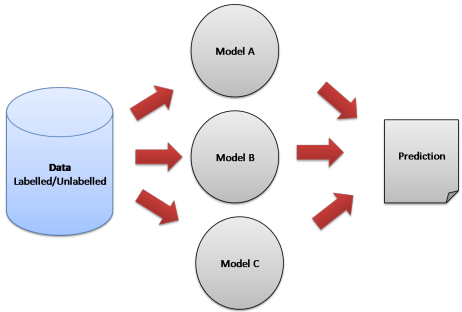
- Loss function should be proper *scoring rule* (e.g., softmax-cross entropy, squared error)

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# Deep Ensembles [9](cont.)

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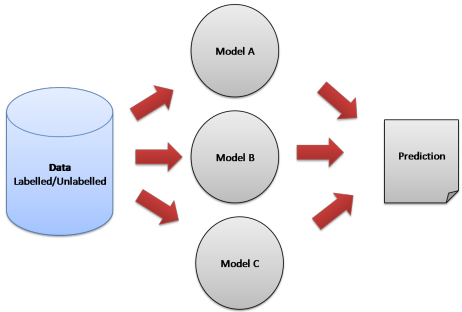
  - Training with adversarial examples [16] to smooth distributions
  - Let network estimate mean and variance, then sample from a Gaussian distribution

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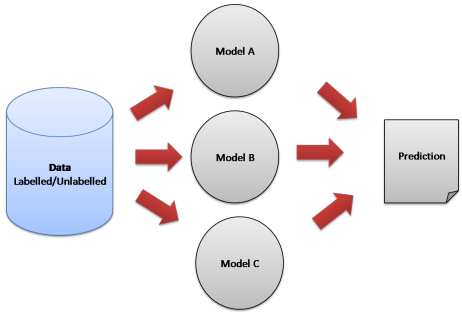


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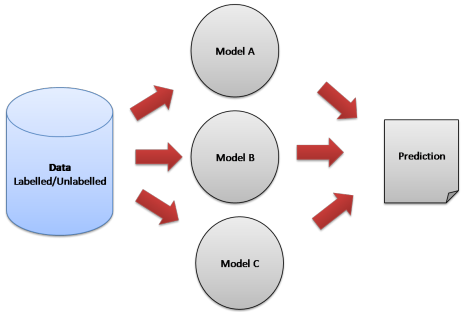
☺ Performance boost compared to MC-dropout
☹ Need to train *M* models

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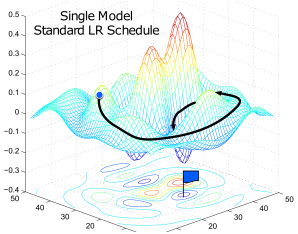
# Better Self-ensembling

- Previously: Separate models trained
- “Self-ensembling”: Re-use same network
  - MC Dropout
  - Reuse different learning stages: Snapshop, Fast Geometric & Averaged

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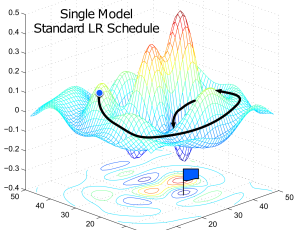


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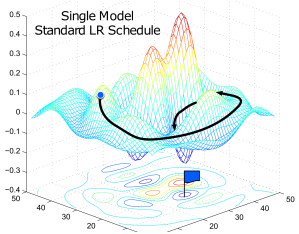


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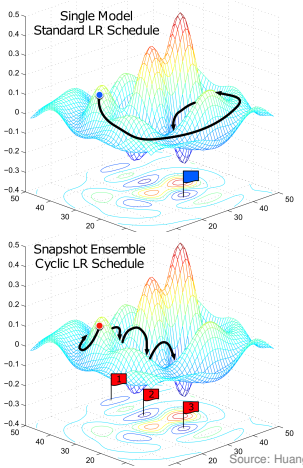
  - Uses a cyclic learning rate
  - Two models:
    **running average** ($\theta_{\text{SWA}}$ and **“normal”** $\theta$)

$$\theta_{SWA} \leftarrow \frac{\theta_{\text{SWA}} \cdot m + \theta}{m + 1} \qquad (2)$$

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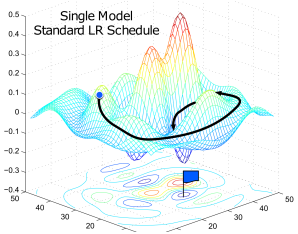
  - ➔ **Single model as ensemble**

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# SWAG [10] & MultiSWAG [11]

Let's leverage this for uncertainty:

- Stochastic Weight Averaging with Gaussian distributions (SWAG)

➔ MultiSwag: Combine "true" and SWAG-Ensembling

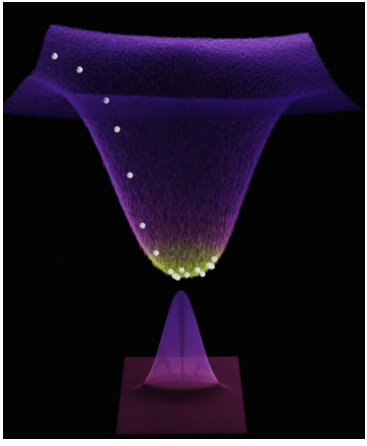
Source: https://www.youtube.com/watch?v=5WOj_ZZJ2wM

# SWAG [10] & MultiSWAG [11]

Let's leverage this for uncertainty:

- Stochastic Weight Averaging with Gaussian distributions (SWAG)
- Idea similar to before:
  Fit Gaussian using SWA solution as mean and low rank (+ diagonal) as covariance

→ MultiSwag: Combine "true" and SWAG-Ensembling



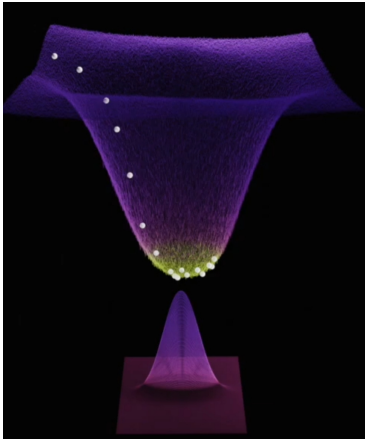
Source: https://www.youtube.com/watch?v=5WOj_ZZJ2wM

# SWAG [10] & MultiSWAG [11]

Let's leverage this for uncertainty:

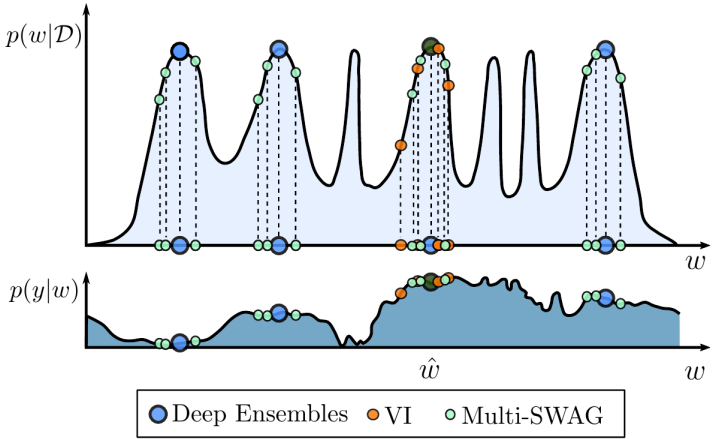
- Stochastic Weight Averaging with Gaussian distributions (SWAG)
- Idea similar to before:
  Fit Gaussian using SWA solution as mean and low rank (+ diagonal) as covariance
- Sample from Gaussian to perform Bayesian Model Averaging

➔ MultiSwag: Combine "true" and SWAG-Ensembling



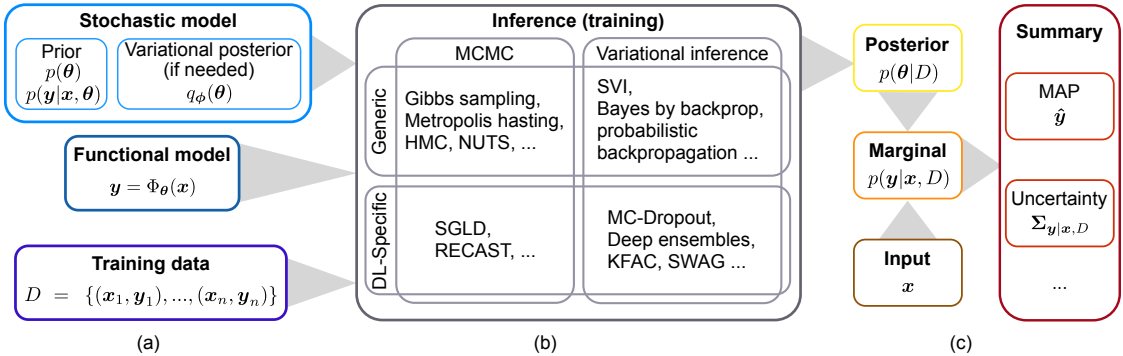
Source: https://www.youtube.com/watch?v=5WOj_ZZJ2wM

# Sampling the Posteriors




Source: Adapted from https://cims.nyu.edu/~andrewgw/deepensembles/

# Summary



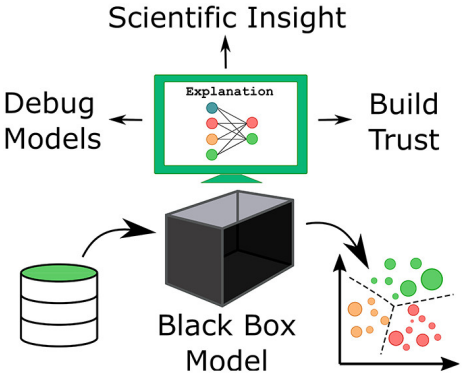

Source: Jospin et al. 2022 [8]

# NEXT TIME

ADVANCED

ON DEEP LEARNING

# Interpretable DL & Causal DL




Source: Oviedo et al. 22 [15]

# Comprehensive Questions

- Which types/sources of uncertainties exist?
- Why can we not use a normal NN for uncertainty classification?
- What is the main problem of Bayesian learning?
- What is the predictive distribution?
- Which approximation methods for the posterior exist?
- How does Bayes by backprop work?
- How does Dropout work?
- How does ensembling work?
- How does SWAG work?

# Further Reading

- Blog about Bayesian inference
  https://www.cs.toronto.edu/~duvenaud/distill_bayes_net/public/
- Another blog
  https://jorisbaan.nl/2021/03/02/introduction-to-bayesian-deep-learning.html
- Argument for Ensembles as Bayesian Approaches:
  https://cims.nyu.edu/~andrewgw/deepensembles/
- Yarin Gal's lecture on Bayesian DLL: https://www.youtube.com/watch?v=G6tUZRHnJYc
- Nice blog post on Stochastic Weight Averaging:
  https://pechyonkin.me/stochastic-weight-averaging/
- Jospin et al. "Hands-on Bayesian Neural Networks – A Tutorial for Deep Learning Users" [8]

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