

BAYESIAN NEURAL NETWORKS: A TUTORIAL

WESLEY MADDOX



NYU

THANKS TO + MY COLLABORATORS

- ▶ Andrew Wilson
- ▶ Pavel Izmailov & Polina Kirichenko
 - ▶ For the slides :)
- ▶ Greg Benton
- ▶ Slides available at: [https://wjmaddox.github.io/assets/
BNN_tutorial_CILVR.pdf](https://wjmaddox.github.io/assets/BNN_tutorial_CILVR.pdf)

STRUCTURE

- ▶ Motivation
- ▶ Intro to Bayesian Inference
- ▶ Approximate Inference
 - ▶ Variational Inference
 - ▶ Laplace Approximations
 - ▶ MCMC
- ▶ Loss-Geometry Inspired Methods (our work)

MOTIVATION

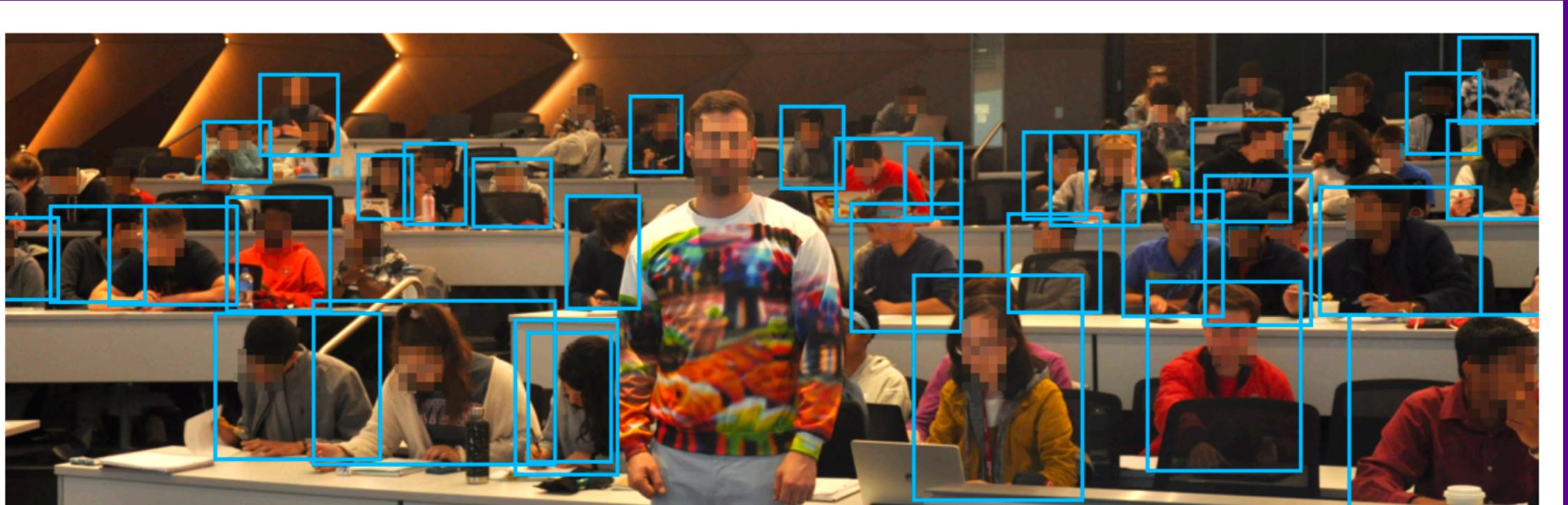


Figure 1: This stylish pullover is a great way to stay warm this winter, whether in the office or on-the-go. It features a stay-dry microfleece lining, a modern fit, and adversarial patterns the evade most common object detectors. In this demonstration, the YOLOv2 detector is evaded using a pattern trained on the COCO dataset with a carefully constructed objective.

From: "Making an Invisibility Cloak: Real World Adversarial Attacks on Object Detectors,"
Wu, Lim, Davis, Goldstein, <https://arxiv.org/pdf/1910.14667.pdf>

DEEP LEARNING SUCCESS

Google Search Results for "deep learning":

- Featured Snippet:** Deep learning is a subset of machine learning in artificial intelligence (AI) that has networks capable of learning unsupervised from data that is unstructured or unlabeled. Also known as **deep neural learning** or **deep neural network**. (Apr 30, 2019)
- Image:** A brain with a circuit board overlay labeled "DEEP LEARNING".
- Search Results:** Deep learning definition from Investopedia, a list of "Deep learning books" (e.g., Deep Learning with Python, Deep Learning), and a "People also search for" section.
- People also ask:** Why is it called deep learning?, What is deep learning examples?, What is deep learning vs Machine Learning?, What is deep learning and how it works?

Smartphone Display: An iPhone screen showing a KLM flight status message: "Dear traveller, your flight has been delayed. We are sorry for the extra wait! Keep an eye on the information screens – just in case your gate number changes. Should you have any questions, our staff will be happy to help." Below it, flight details: KL0605, AMS to SFO, Departure 11:00 AM, Arrival 3:55 PM, Flight Status: DELAYED.

Amazon Echo Devices: Three Amazon Echo Dot smart speakers.

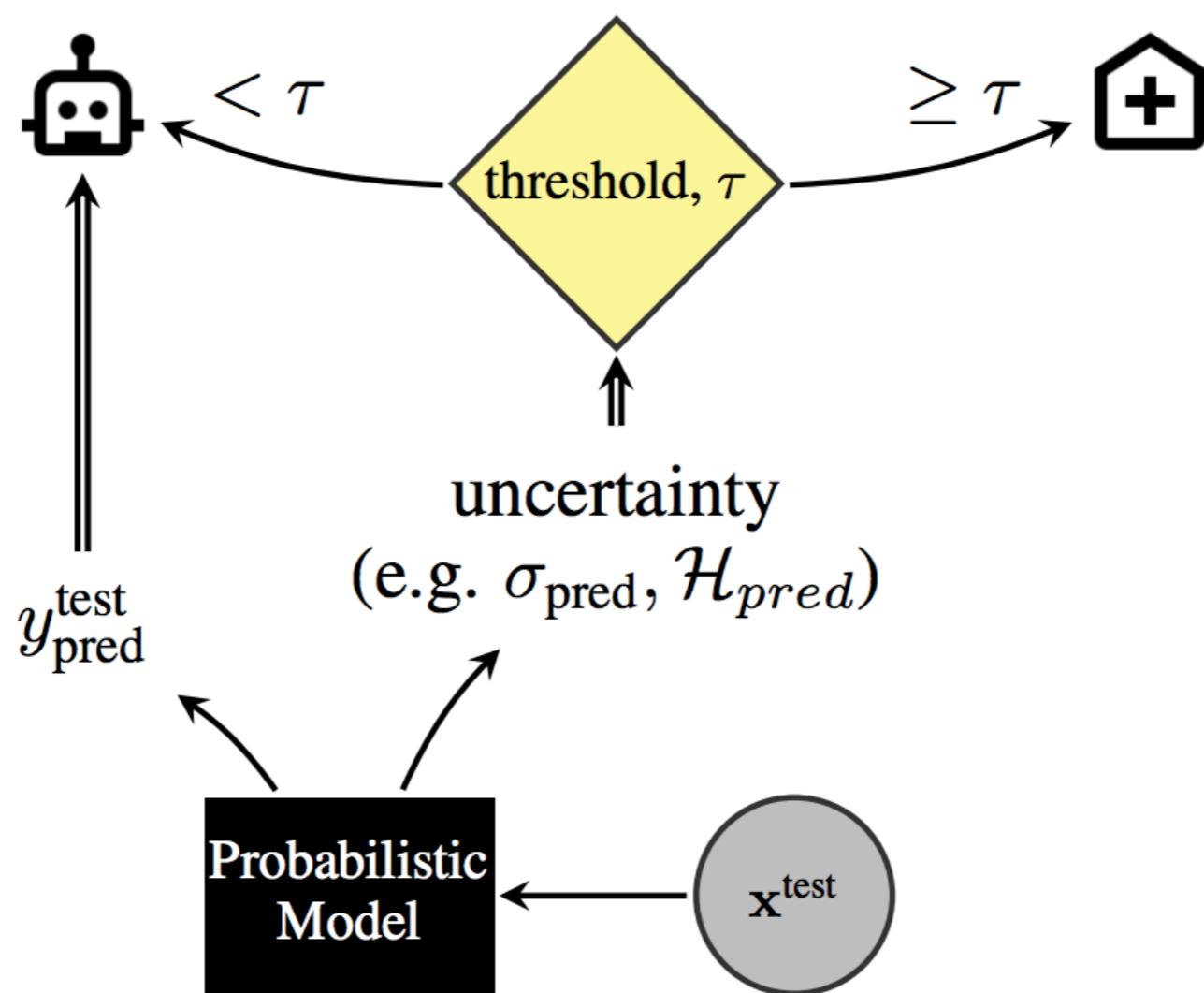
Car with Object Detection: A photograph of a street scene with several vehicles. Green bounding boxes and labels identify them: "traffic light", "car", "truck", "truck", and "truck".

Google Translate Interface: Comparing "city" in English to "ville" in French. It shows definitions, translations, and related terms.

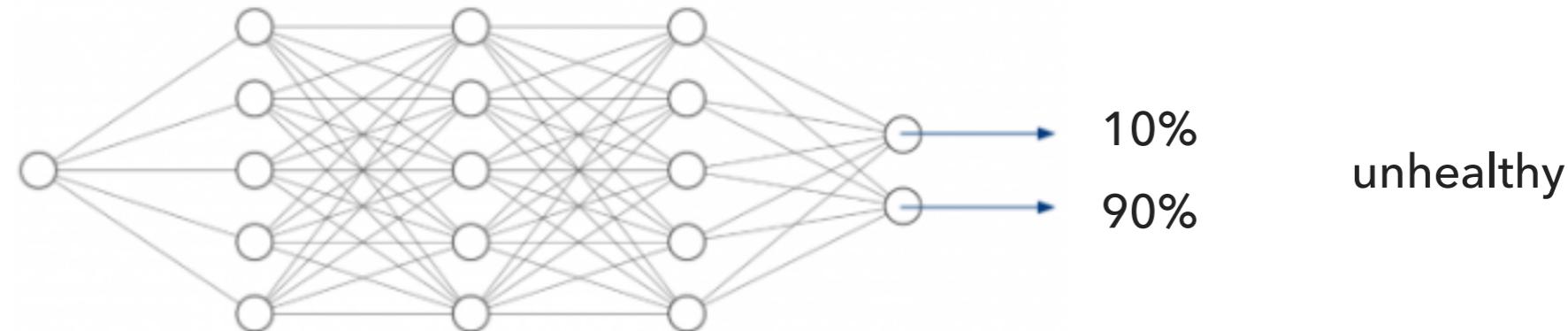
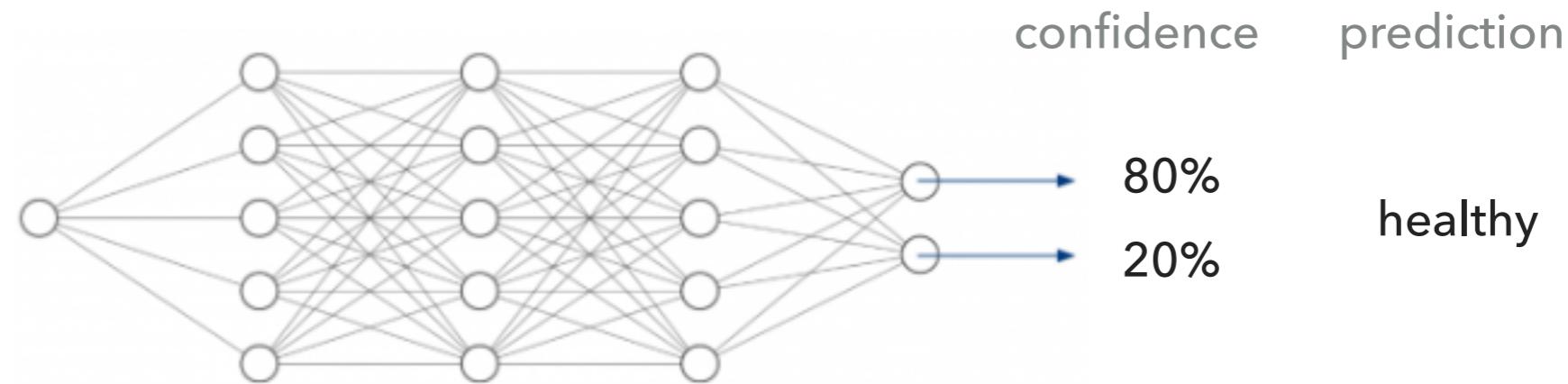
Financial Trading Chart: A candlestick chart on a screen, likely representing stock price movements over time.

UNCERTAINTY IN DEEP LEARNING

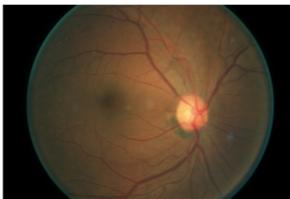
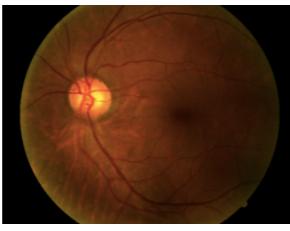
Automated diagnosis: human-in-the-loop



CALIBRATION

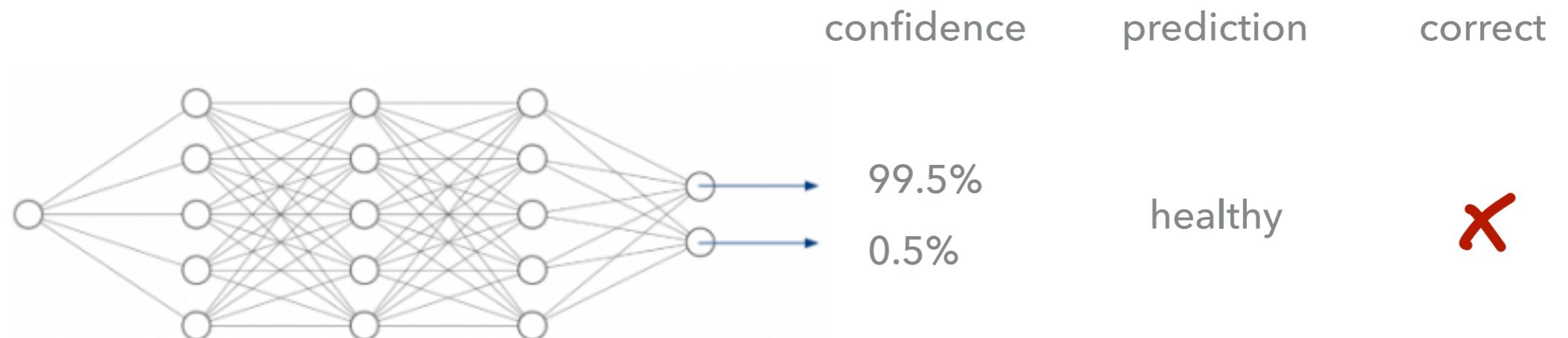


CALIBRATION

	confidence	prediction	correct
	 → 80%  → 20%	healthy	✓
	 → 80%  → 20%	healthy	✓
	 → 80%  → 20%	healthy	✓
	 → 80%  → 20%	healthy	✗
	 → 80%  → 20%	healthy	✓

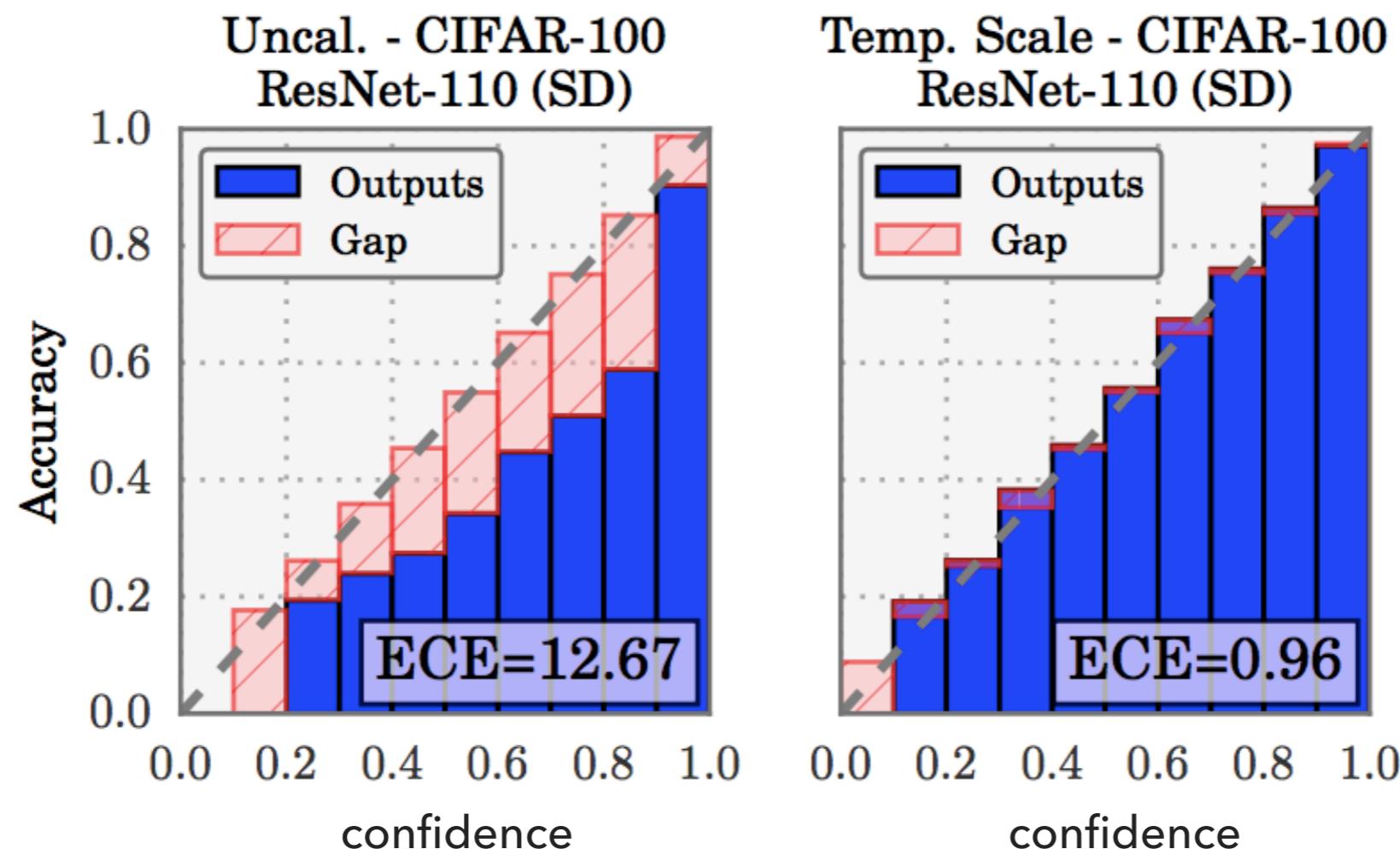
UNCERTAINTY: OVERCONFIDENCE IN NEURAL NETWORKS

- ▶ $p(y|x)$ should represent probabilities of belonging to a class
- ▶ Neural networks are often over-confident in their predictions

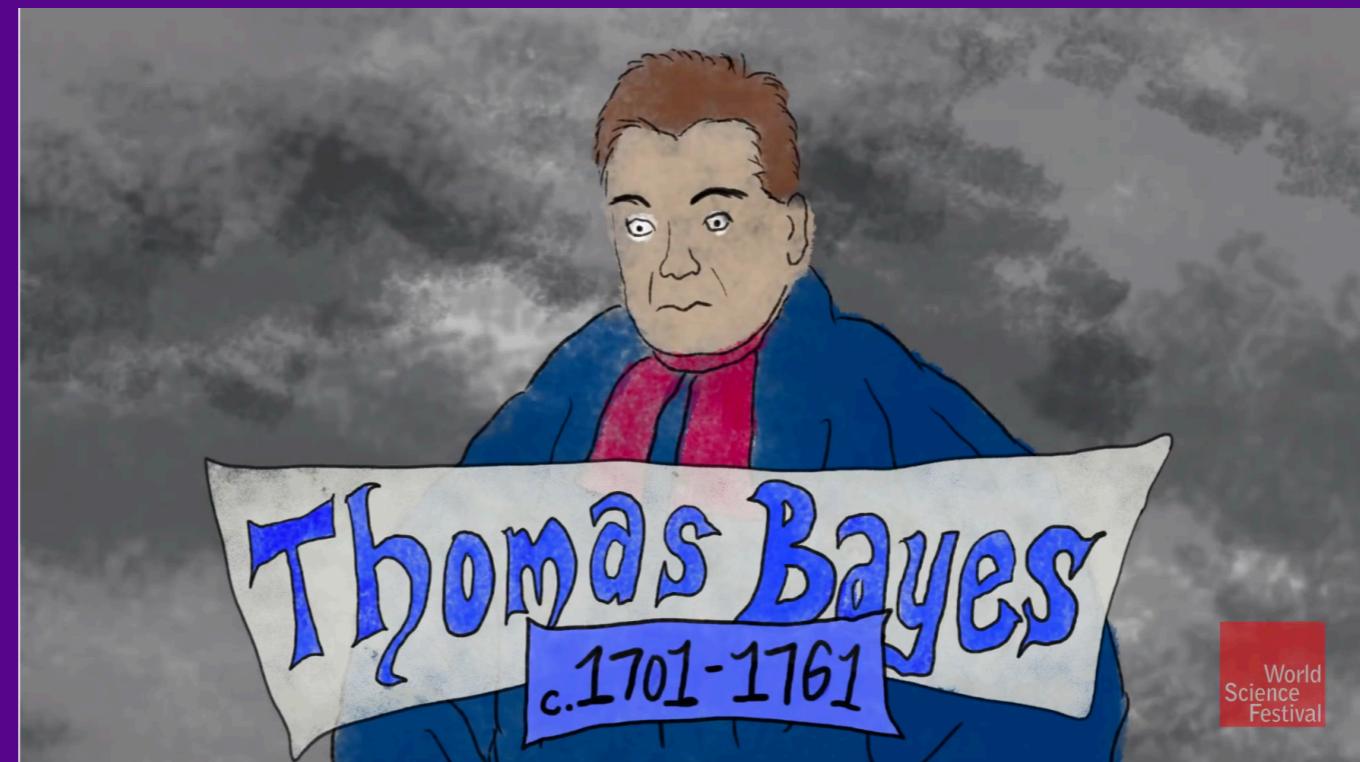


EXPECTED CALIBRATION ERROR (ECE)

ECE is the expected difference between model's confidence and its accuracy



BAYESIAN INFERENCE: A QUICK REVIEW



<https://www.britannica.com/biography/Thomas-Bayes>

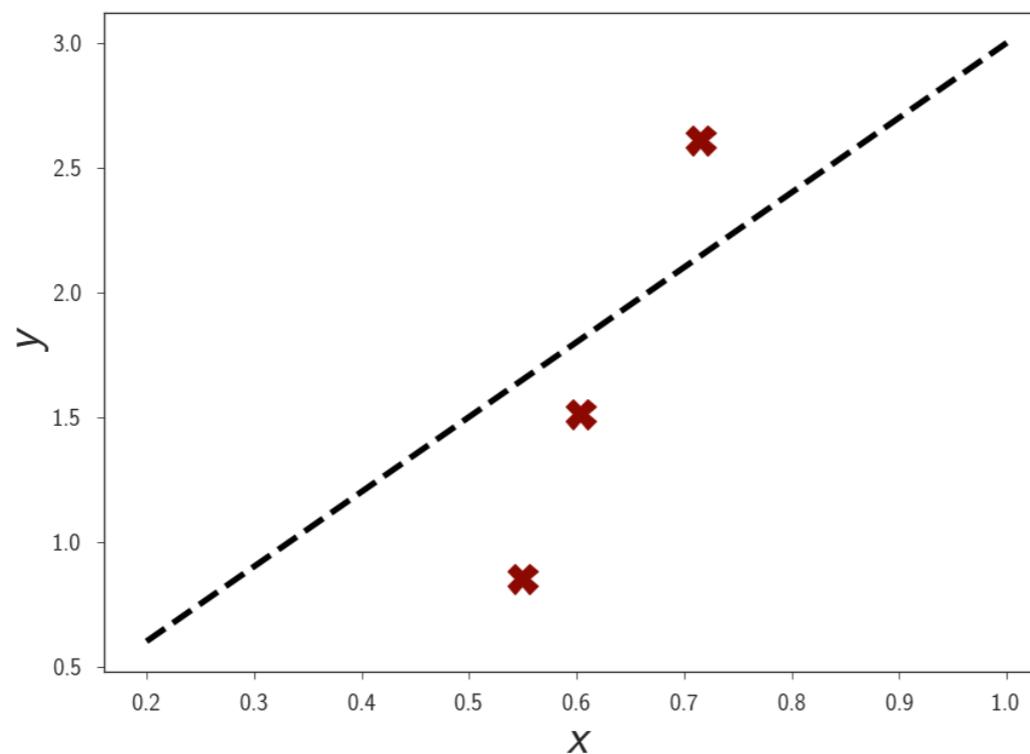
BAYESIAN INFERENCE

- ▶ Likelihood $p(\mathcal{D}|\theta) = p(y|f(x; \theta))$
- ▶ Prior $p(\theta)$
 - ▶ Possibly implicit to the training method
- ▶ Posterior $p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} \approx q(\theta|\mathcal{D})$
- ▶ Inference (Bayesian model averaging)
$$p(y^*|\mathcal{D}) = \mathbb{E}_{p(\theta|\mathcal{D})} p(y^*|\theta) \approx \frac{1}{K} \sum_{k=1}^K p(y^*|\theta_k)$$
$$\theta_k \sim q(\theta|\mathcal{D})$$

BAYESIAN MACHINE LEARNING

Consider a simple linear regression problem:

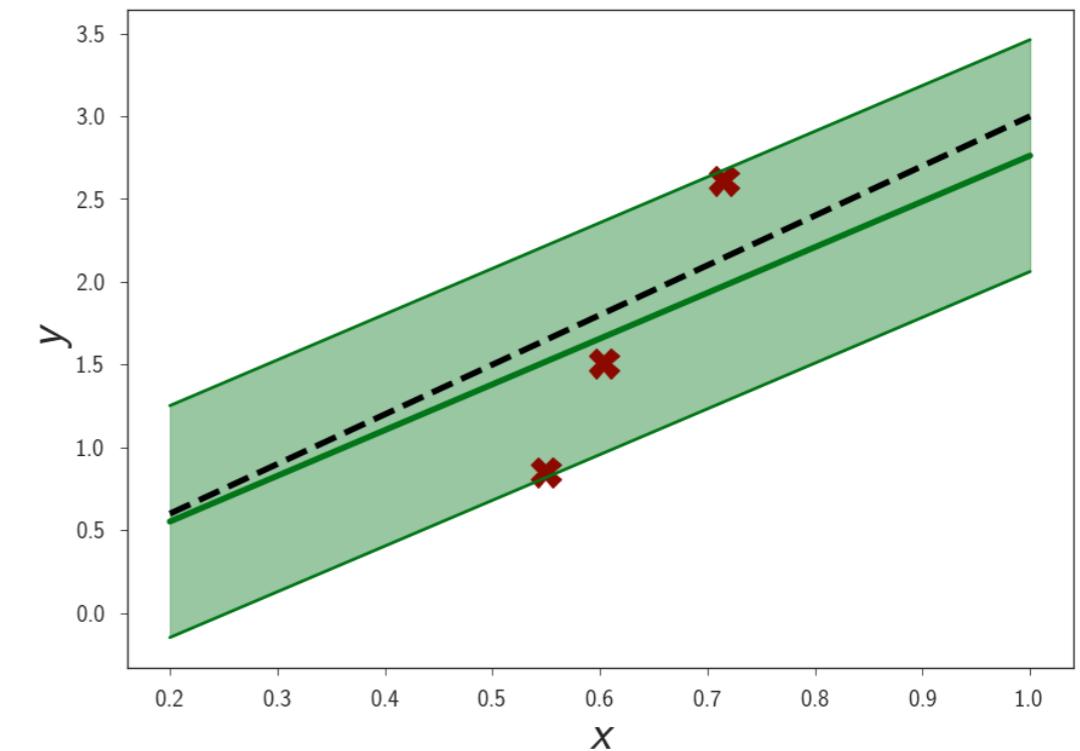
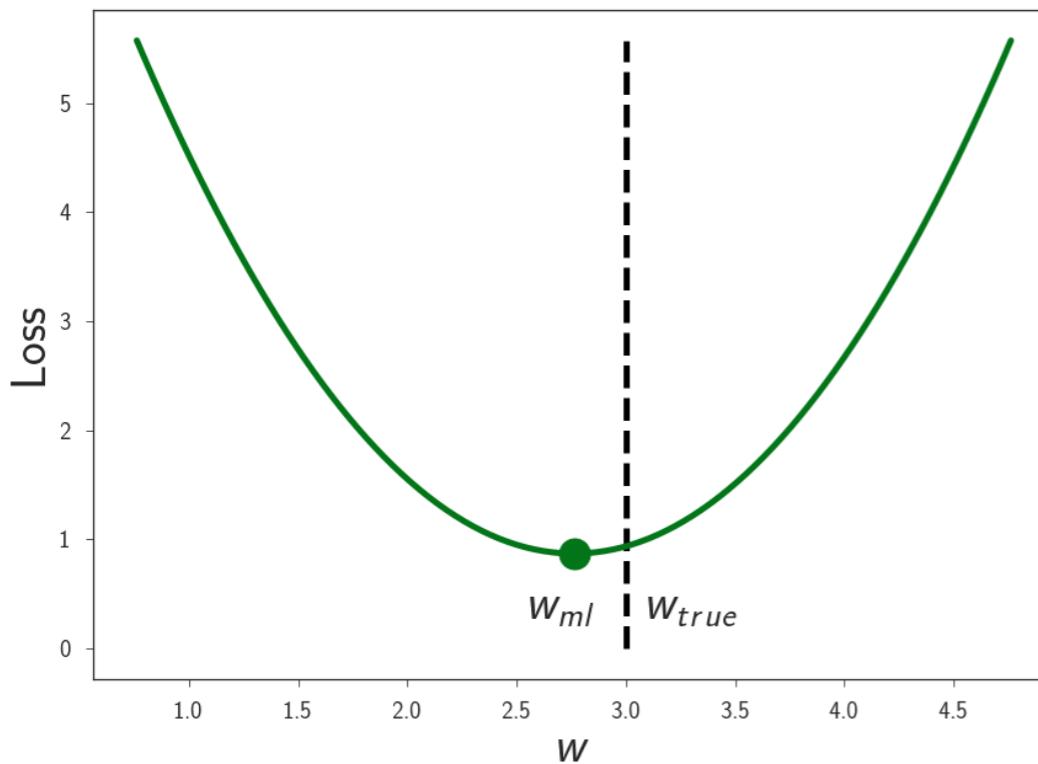
$$y = wx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$



BAYESIAN MACHINE LEARNING

Standard linear regression:

$$\max_w \sum_{i=1}^N \log \mathcal{N}(y_i | wx_i, \sigma^2) \iff \min_w \frac{1}{N} \sum_{i=1}^N (y_i - wx_i)^2$$

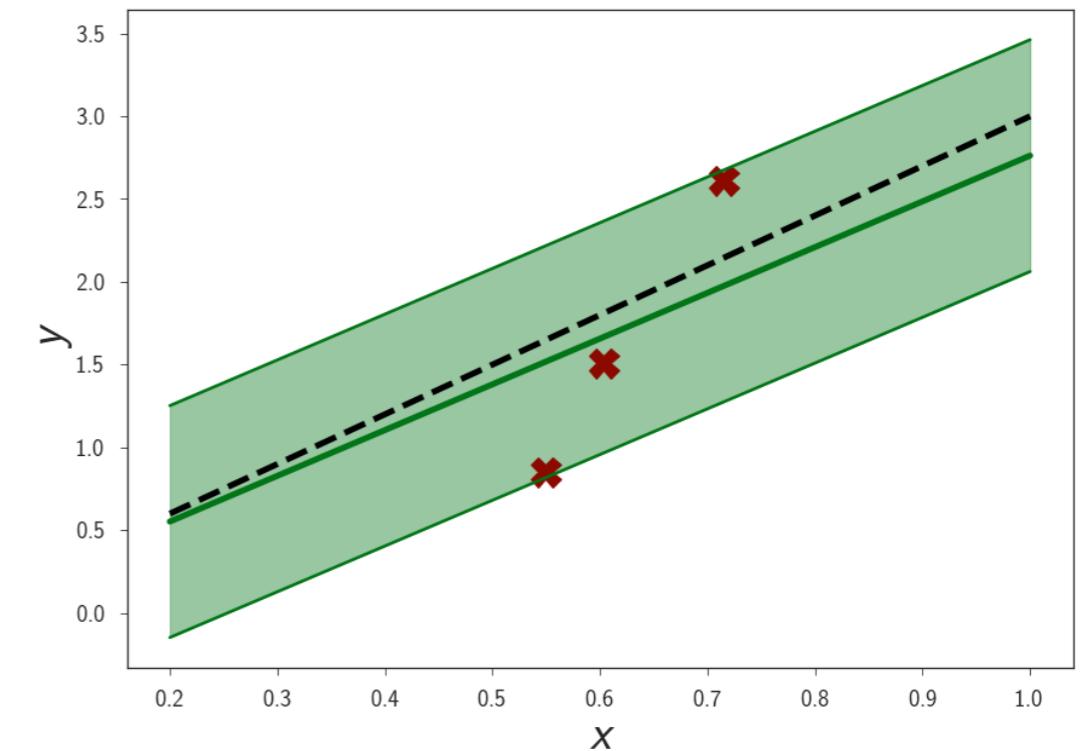
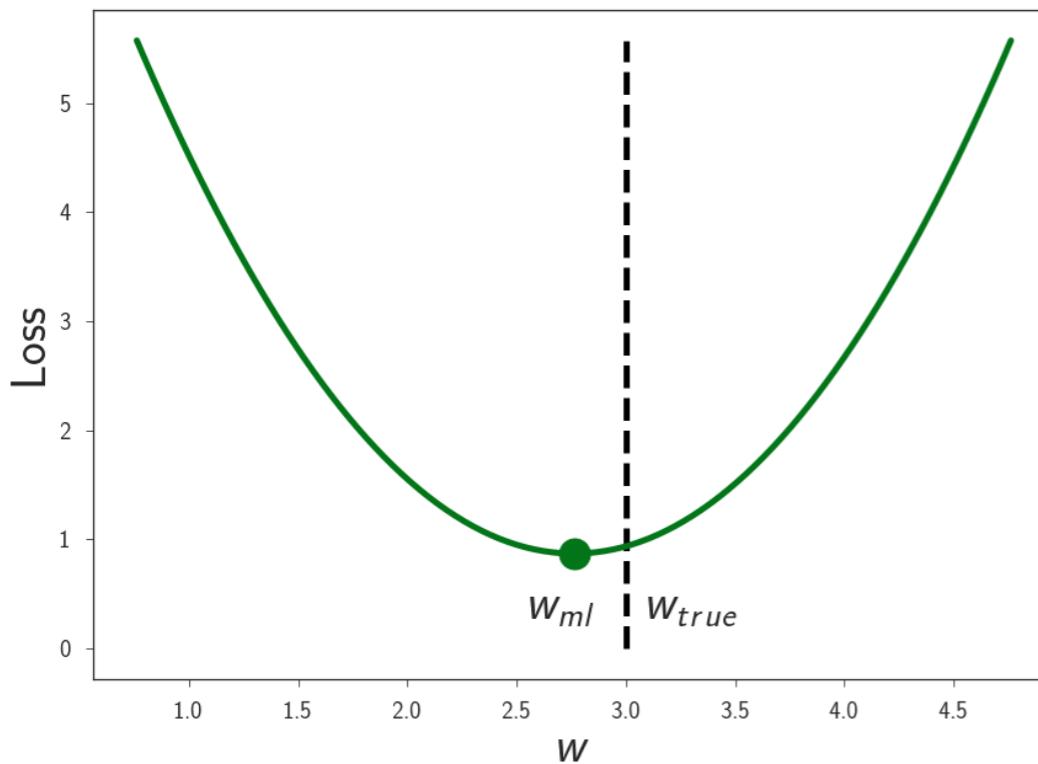


BAYESIAN MACHINE LEARNING

Standard linear regression:

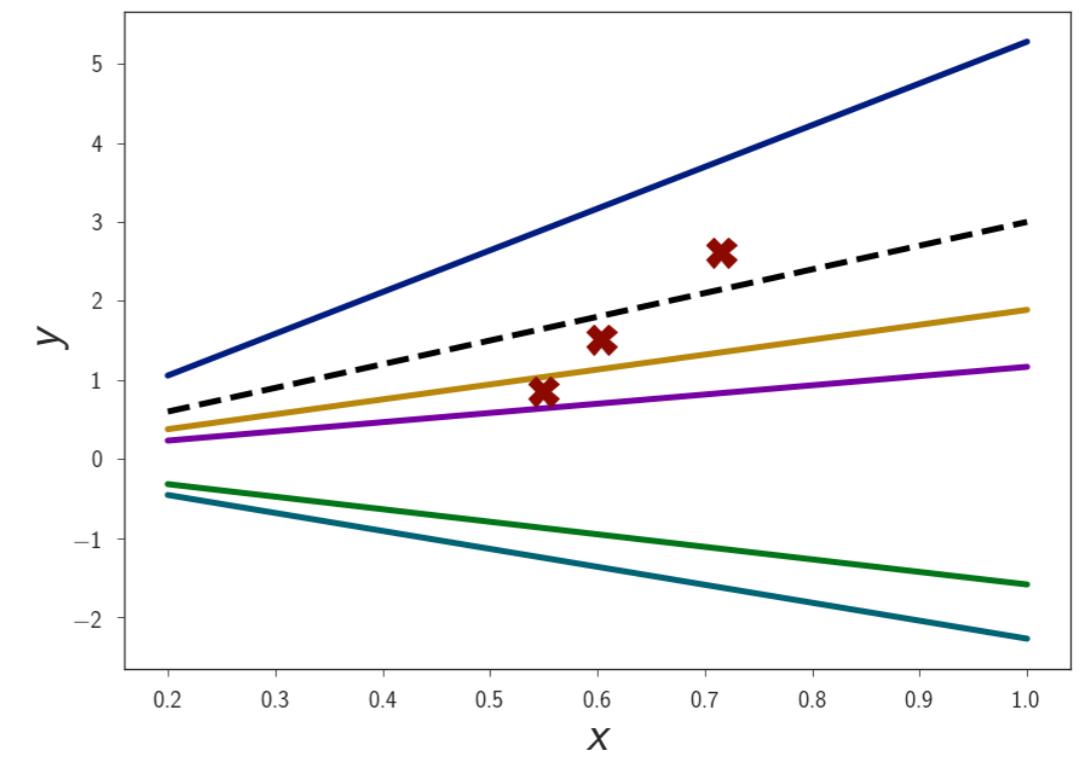
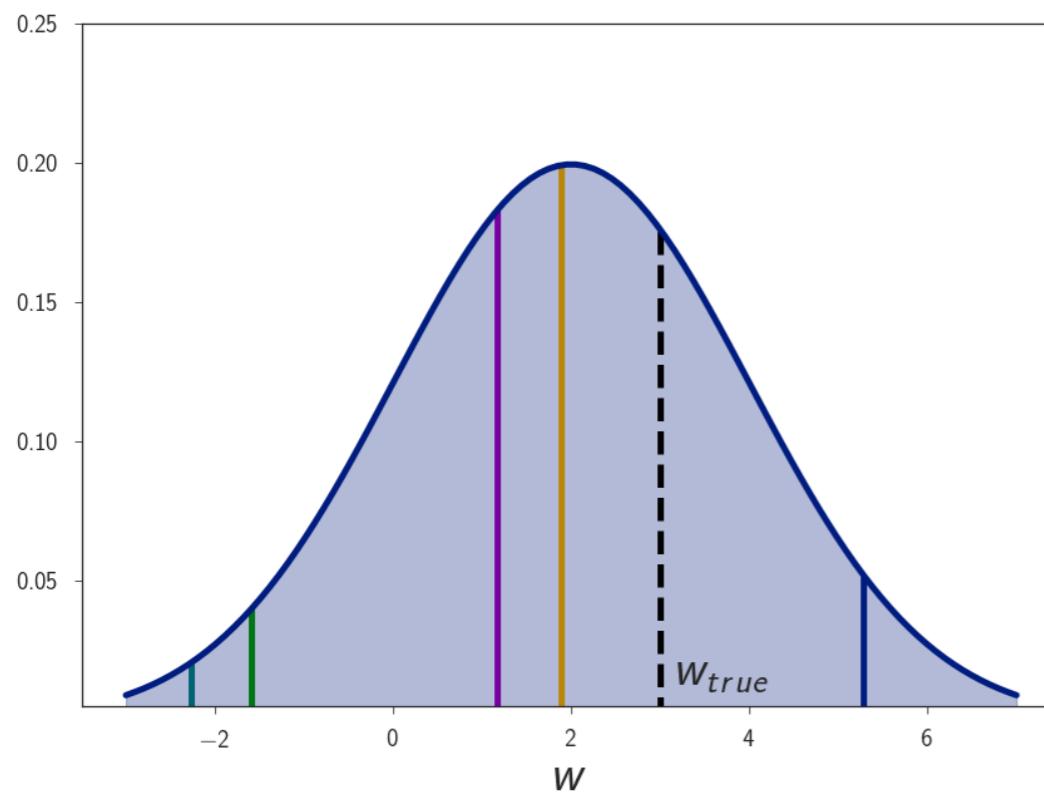
$$\max_w \sum_{i=1}^N \log \mathcal{N}(y_i | wx_i, \sigma^2) \iff \min_w \frac{1}{N} \sum_{i=1}^N (y_i - wx_i)^2$$

We want to model uncertainty over parameters of the model



BAYESIAN LEARNING

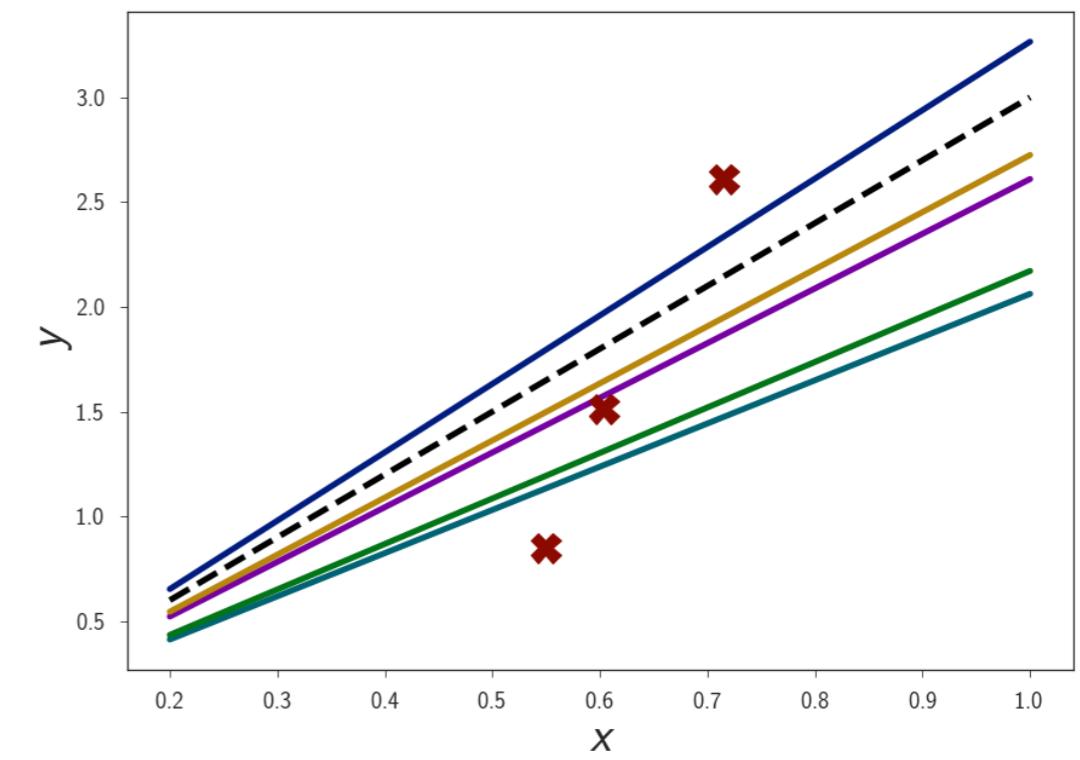
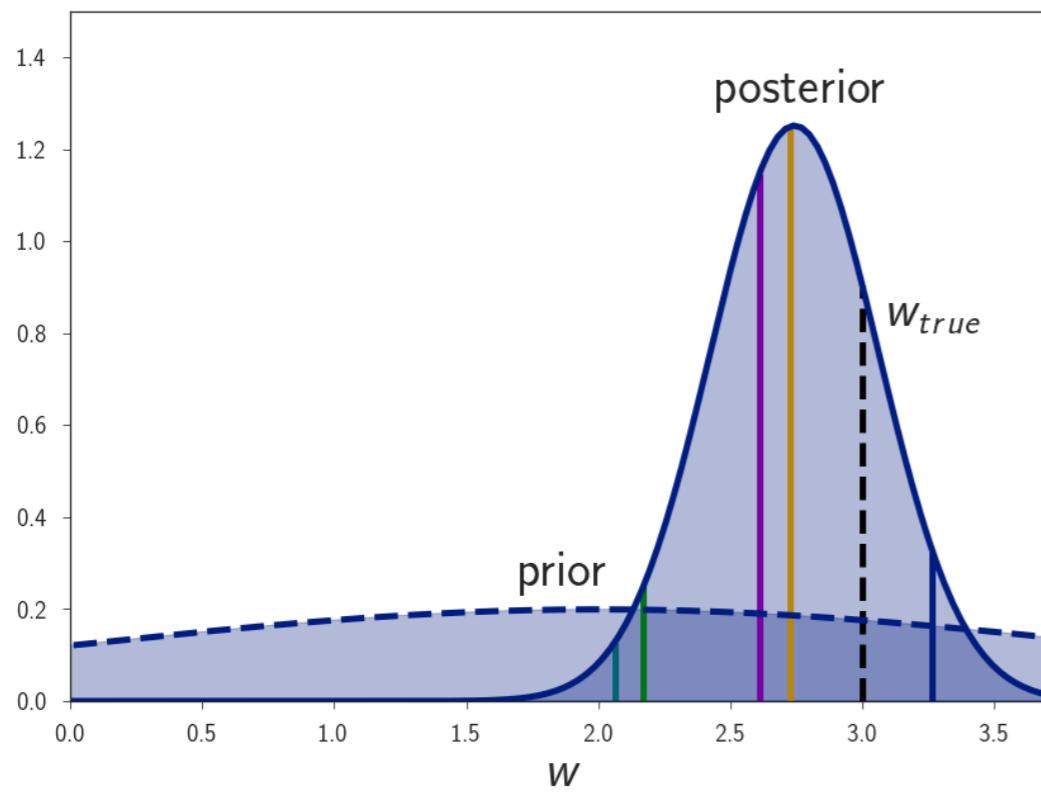
Step 1: introduce a prior distribution $p(w)$ over parameters



BAYESIAN LEARNING

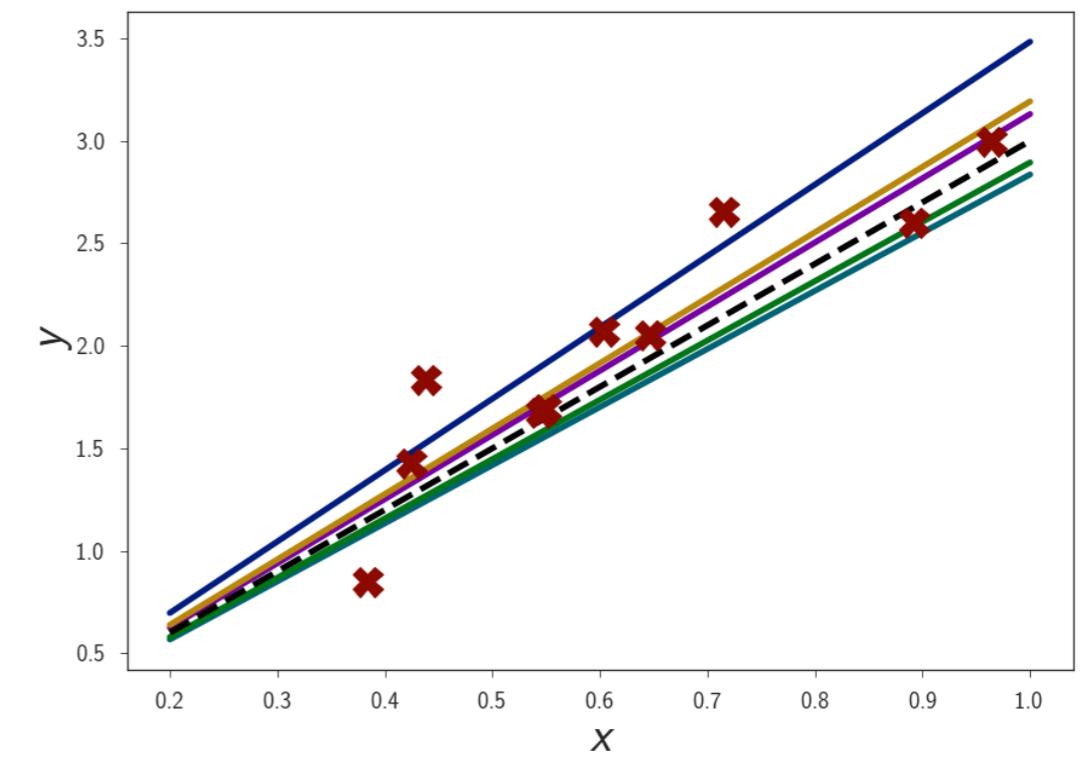
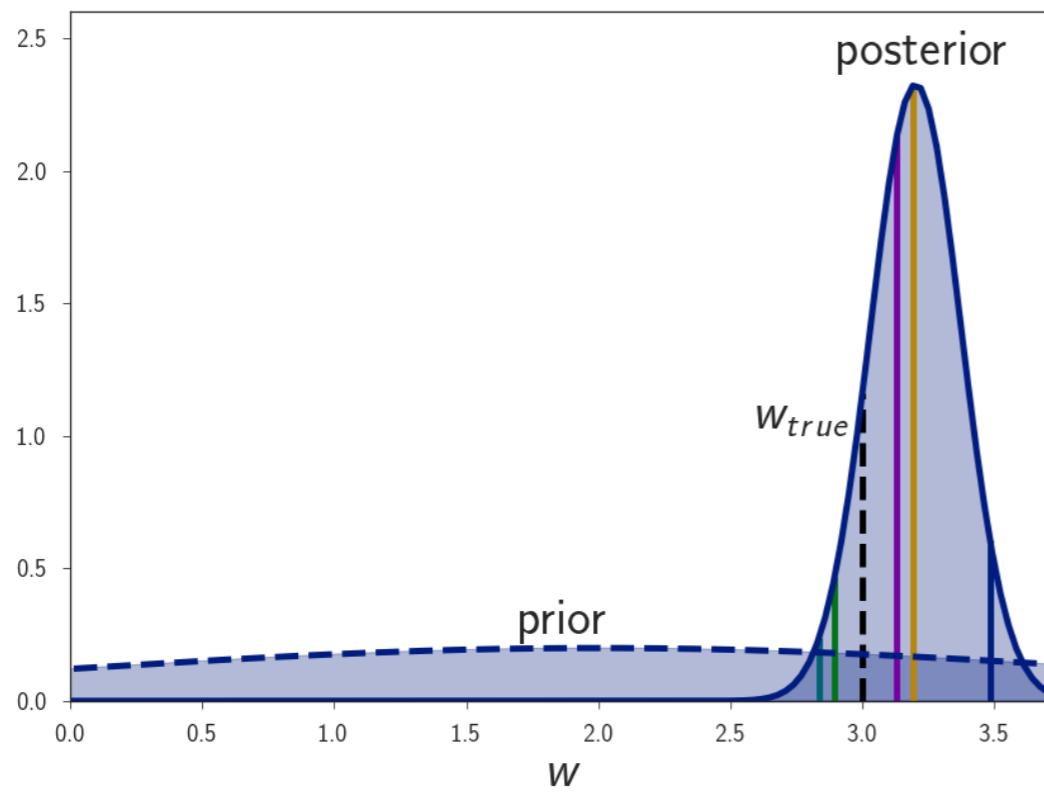
Step 2: Compute posterior $p(w|D)$ using Bayes rule

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)}$$



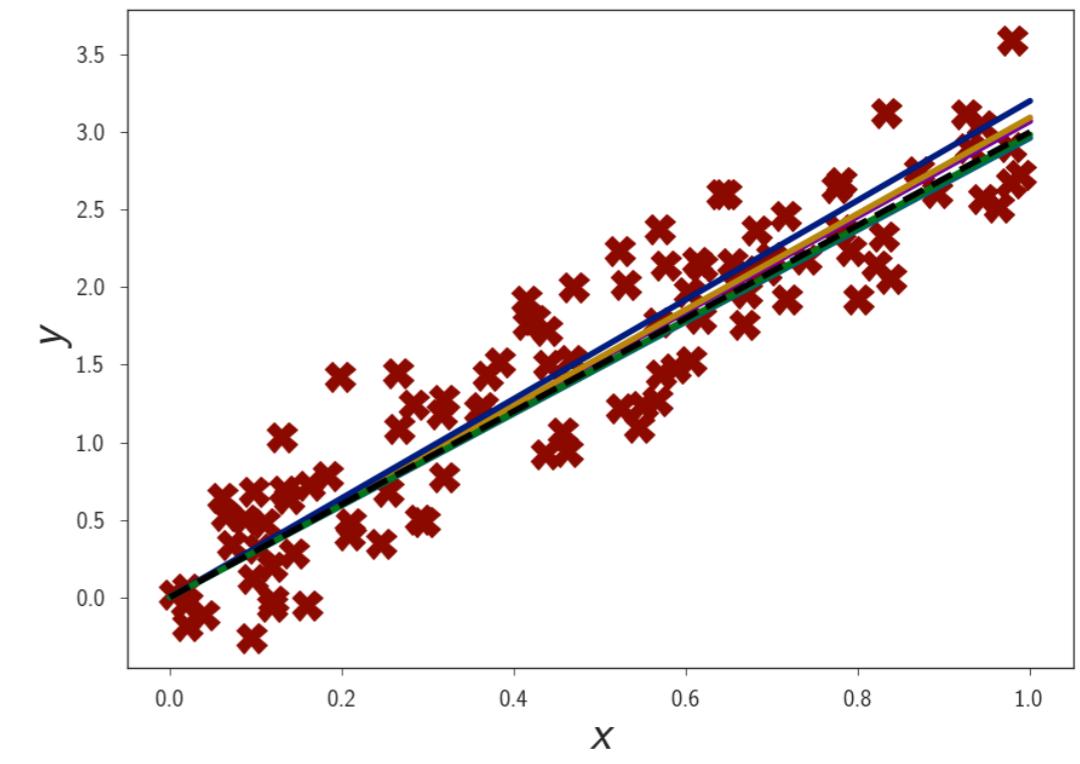
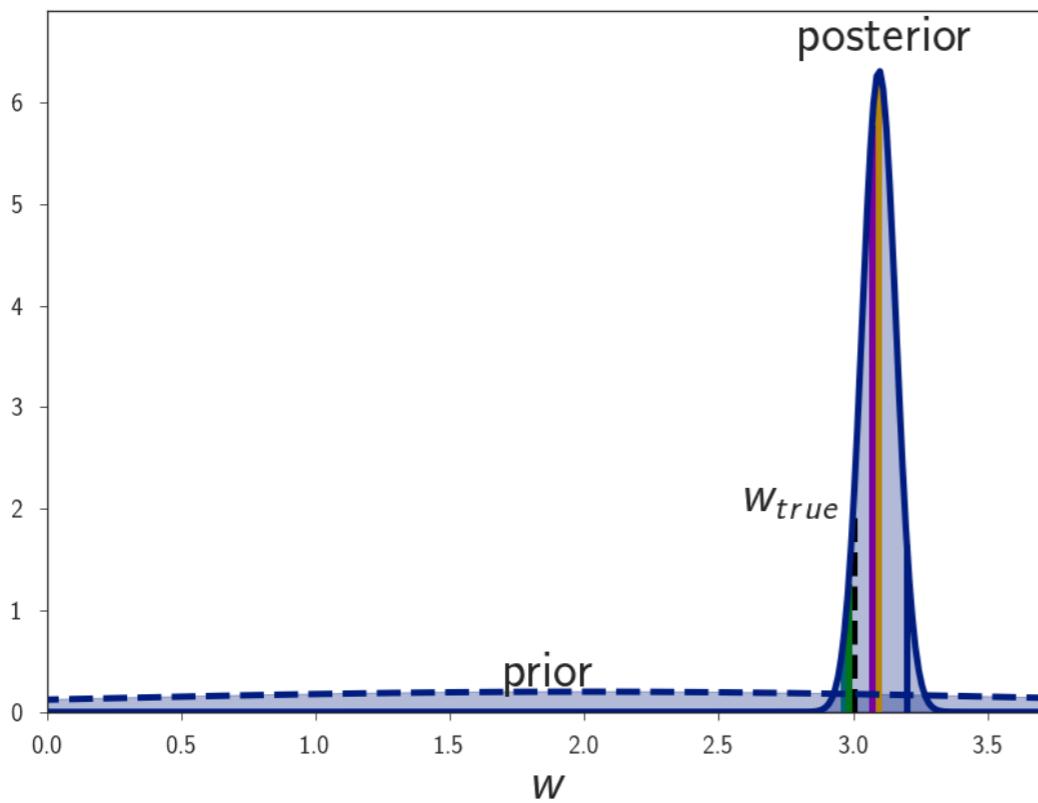
BAYESIAN LEARNING: POSTERIOR CONTRACTION (1)

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)}$$



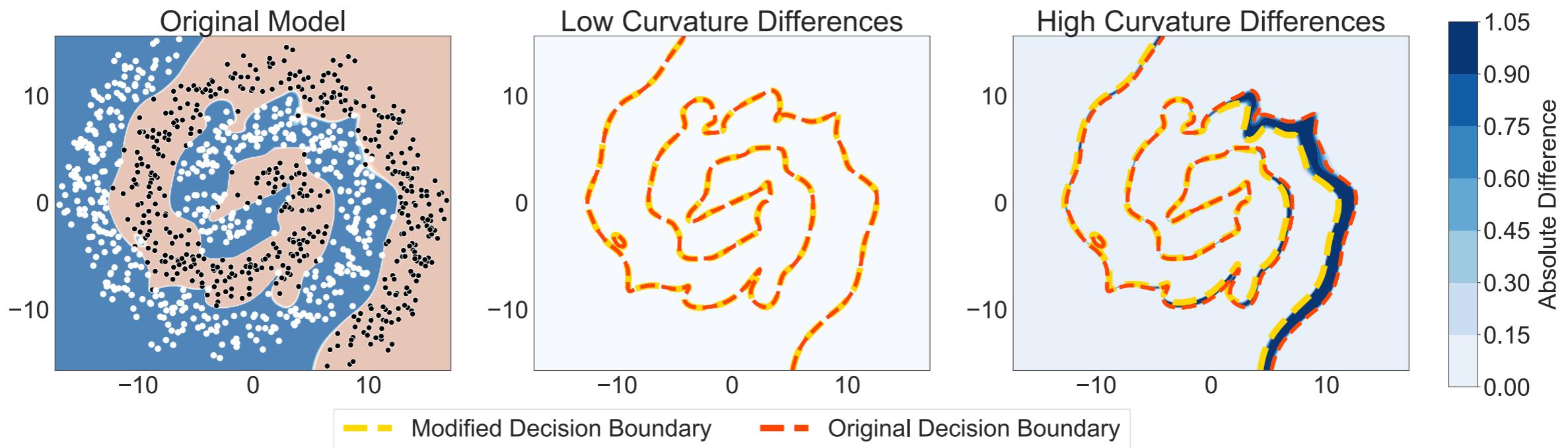
BAYESIAN LEARNING: POSTERIOR CONTRACTION (2)

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)}$$



BAYESIAN LEARNING: POSTERIOR CONTRACTION (3)

What happens if we have more parameters than data points???



Theorem (Function-Space Homogeneity in Linear Models). *Let $\Phi = \Phi(x) \in \mathbb{R}^{n \times k}$ be a feature map of n data observations, x , with $n < k$ and assign isotropic prior $\beta \sim \mathcal{N}(0_k, S_0 = \alpha^2 I_k)$ for parameters $\beta \in \mathbb{R}^k$. The minimal eigenvectors of the Hessian define a $k - n$ dimensional subspace in which parameters can be perturbed without changing the training predictions in function-space.*

Will revisit these results later....

BAYESIAN MODEL AVERAGING

- ▶ We combine aleatoric and epistemic uncertainties via BMA:

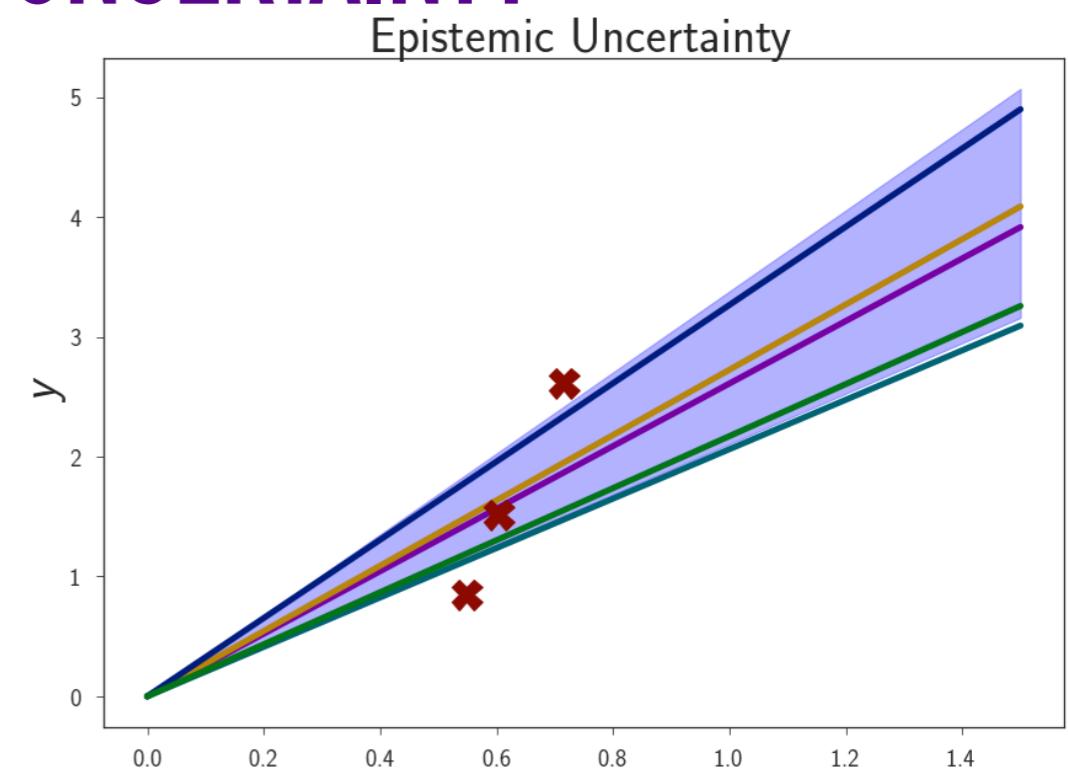
$$p(y^*|x^*, D) = \int_w p(y^*|x^*, w)p(w|D)dw$$

- ▶ Ignoring the uncertainty in the posterior over w leads to overconfident predictions

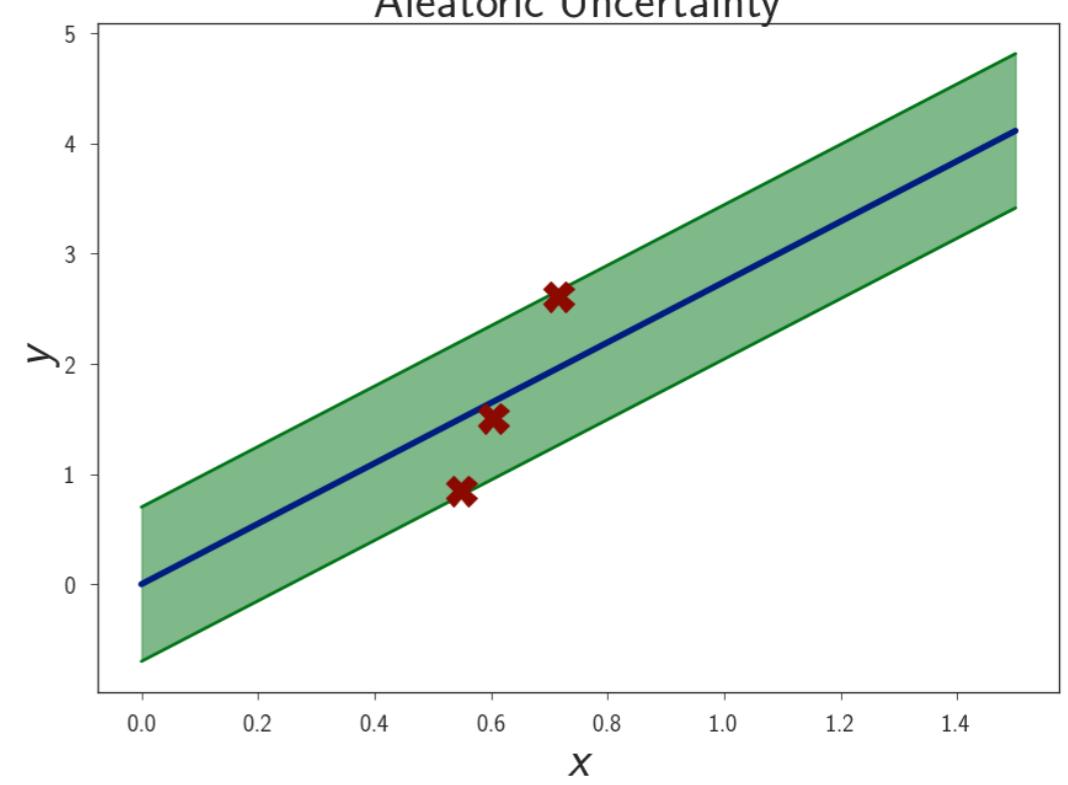
BAYESIAN LEARNING: TWO TYPES OF UNCERTAINTY

Epistemic uncertainty is our uncertainty over the model

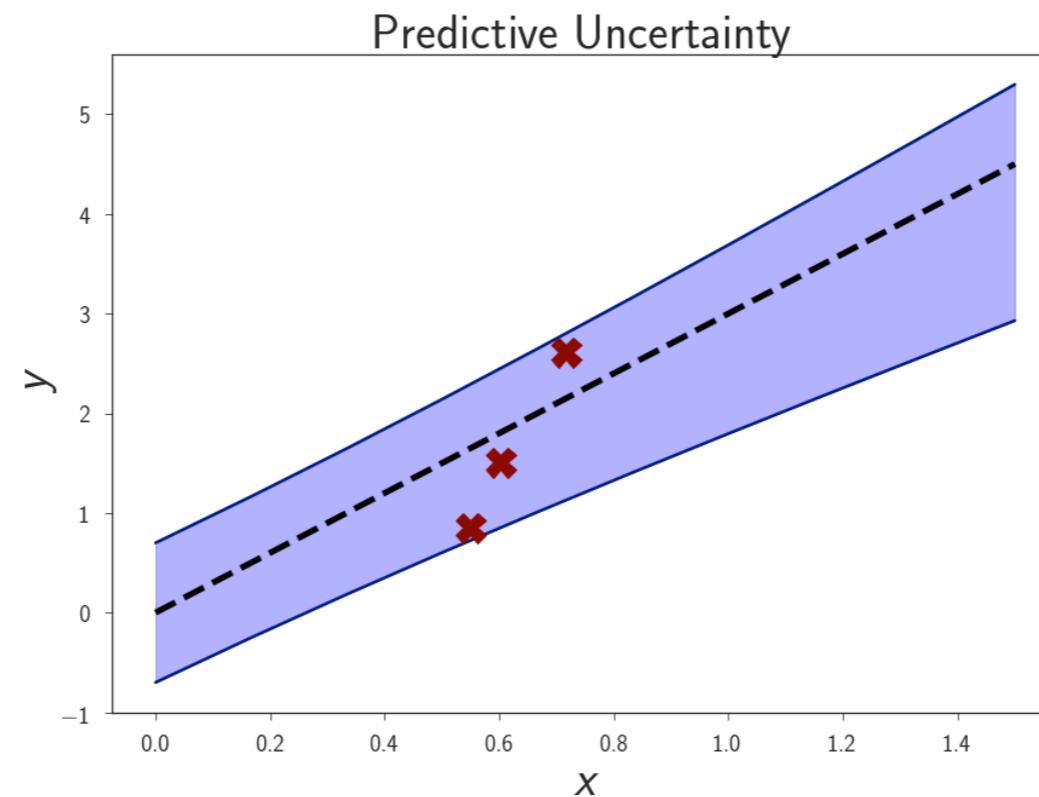
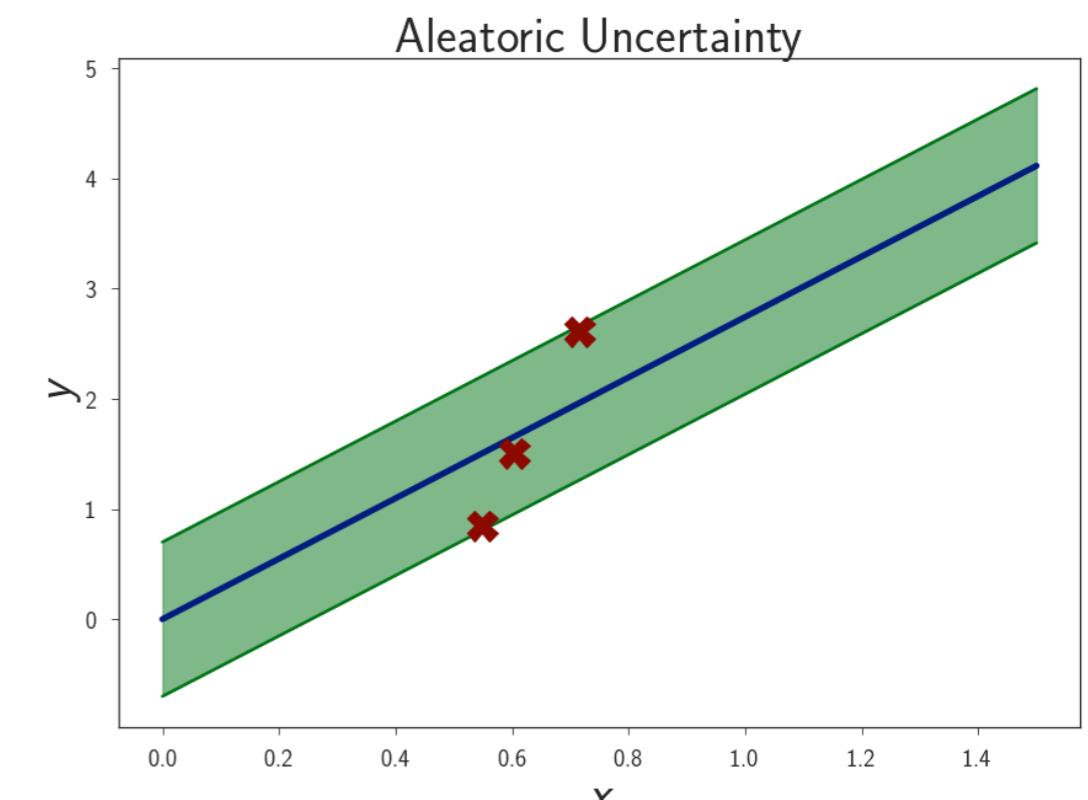
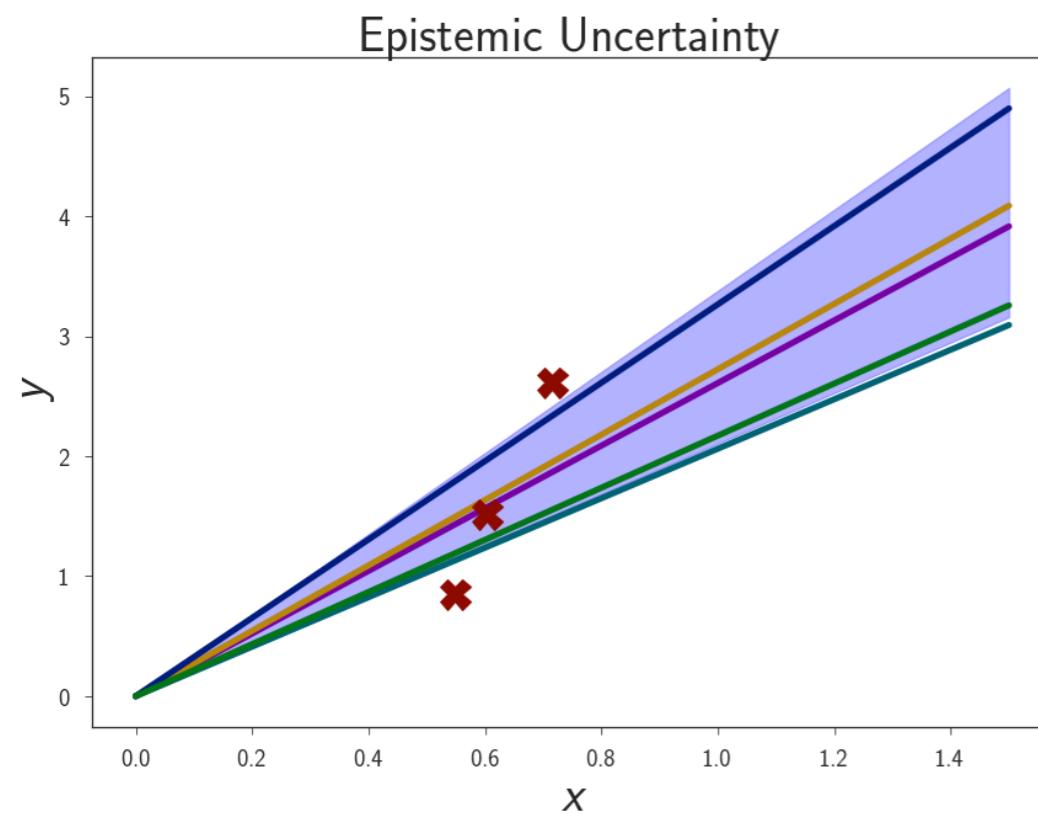
- ▶ Grows with x because uncertainty in w is multiplied by x



Aleatoric uncertainty is our uncertainty over the data for a fixed model, e.g. noise.

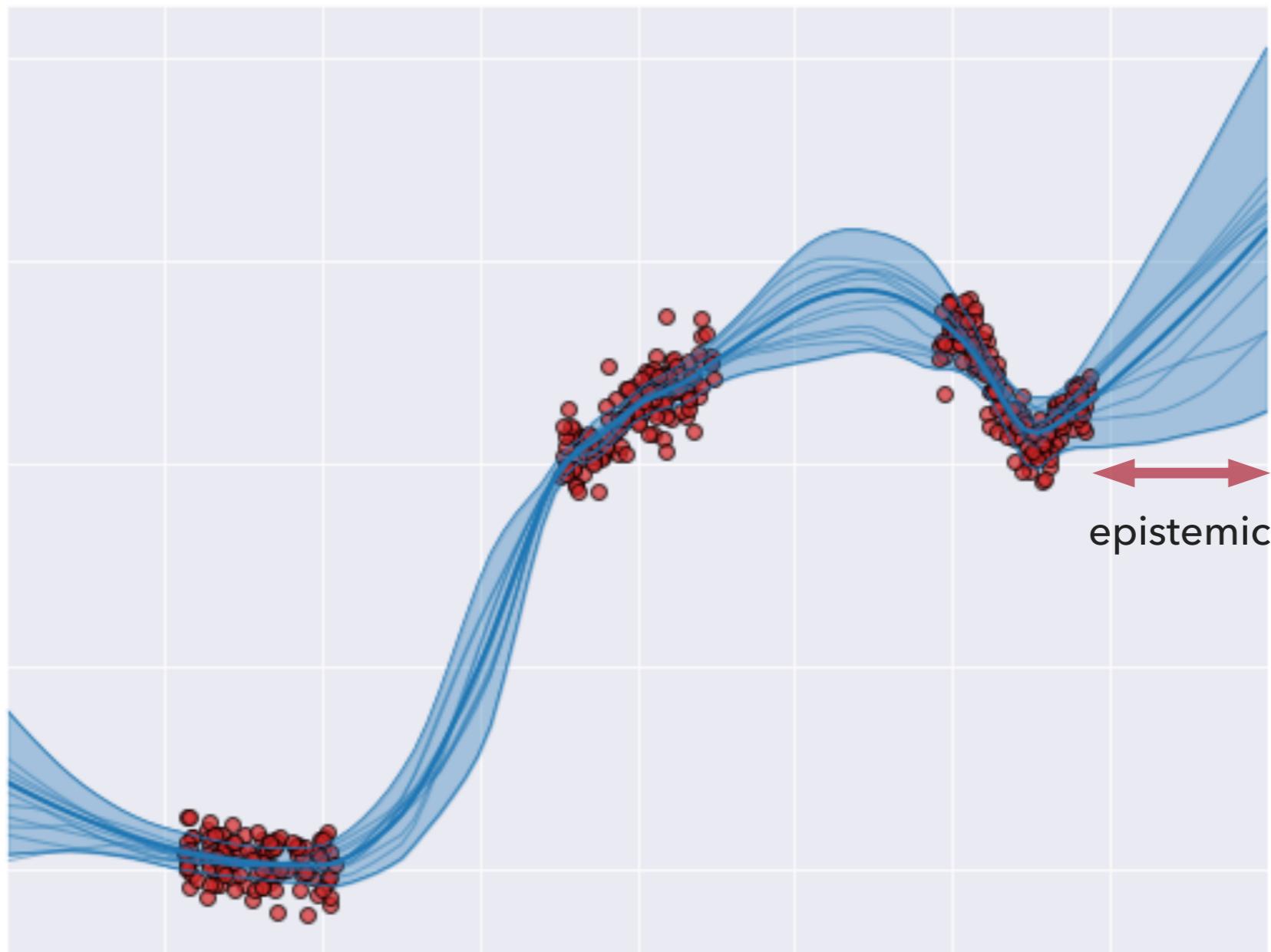


BAYESIAN LEARNING: BAYESIAN MODEL AVERAGING



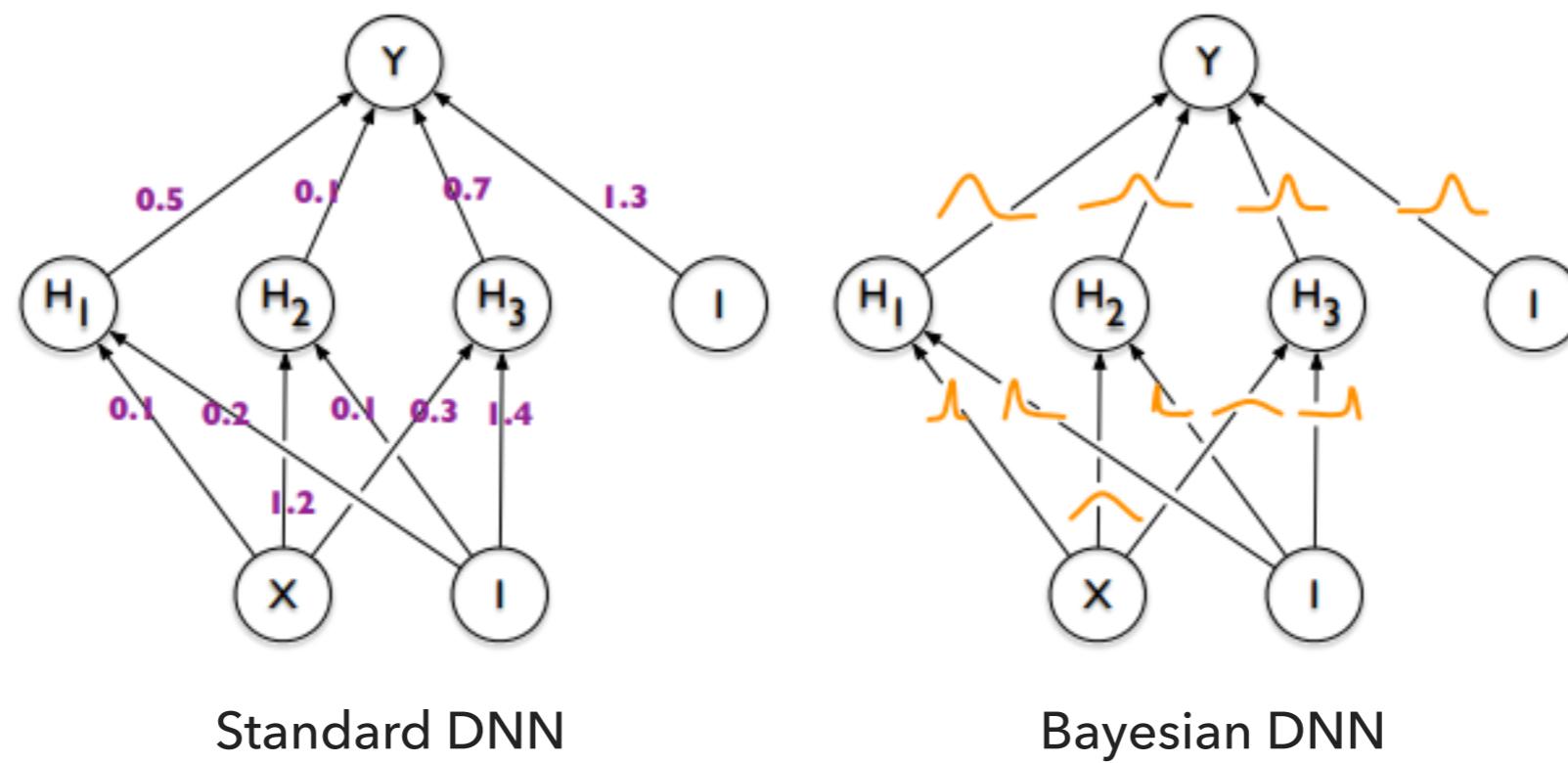
BAYESIAN LEARNING: TWO TYPES OF UNCERTAINTY

Epistemic uncertainty: non-linear model



BAYESIAN DEEP LEARNING

- ▶ In Bayesian deep learning we model posterior distribution over the weights of neural networks
- ▶ In theory, leads to better predictions and well-calibrated uncertainty



BAYESIAN DEEP LEARNING: CHALLENGES

Bayesian inference for deep neural networks is extremely challenging

- ▶ Posterior is intractable
- ▶ Millions of parameters
- ▶ Large datasets
- ▶ Unclear which priors to use

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int_{w'} p(D|w')p(w')dw'}$$

BAYESIAN DEEP LEARNING: CHALLENGES

Bayesian inference for deep neural networks is extremely challenging

- ▶ Posterior is intractable Is the likelihood correct?
 - ▶ Millions of parameters What do these parameters mean?
 - ▶ Large datasets Can we run MCMC for 1 million steps on ImageNet??
 - ▶ Unclear which priors to use Is the prior correct?

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int_{w'} p(D|w')p(w')dw'}$$

BAYESIAN DEEP LEARNING: CHALLENGES

Bayesian inference for deep neural networks is extremely challenging

- ▶ Posterior is intractable Is the likelihood correct? Probably
- ▶ Millions of parameters What do these parameters mean? Care about functions instead
- ▶ Large datasets Can we run MCMC for 1 million steps on ImageNet?? We don't need to
- ▶ Unclear which priors to use Is the prior correct? Probably

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int_{w'} p(D|w')p(w')dw'}$$

BAYESIAN DEEP LEARNING: CHALLENGES

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$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int_{w'} p(D|w')p(w')dw'}$$

A photograph of a man in a dark suit and red tie standing on a large, light-colored, textured rock formation that slopes down from the left. He is looking down at the rock. The background is a dramatic, cloudy sky.

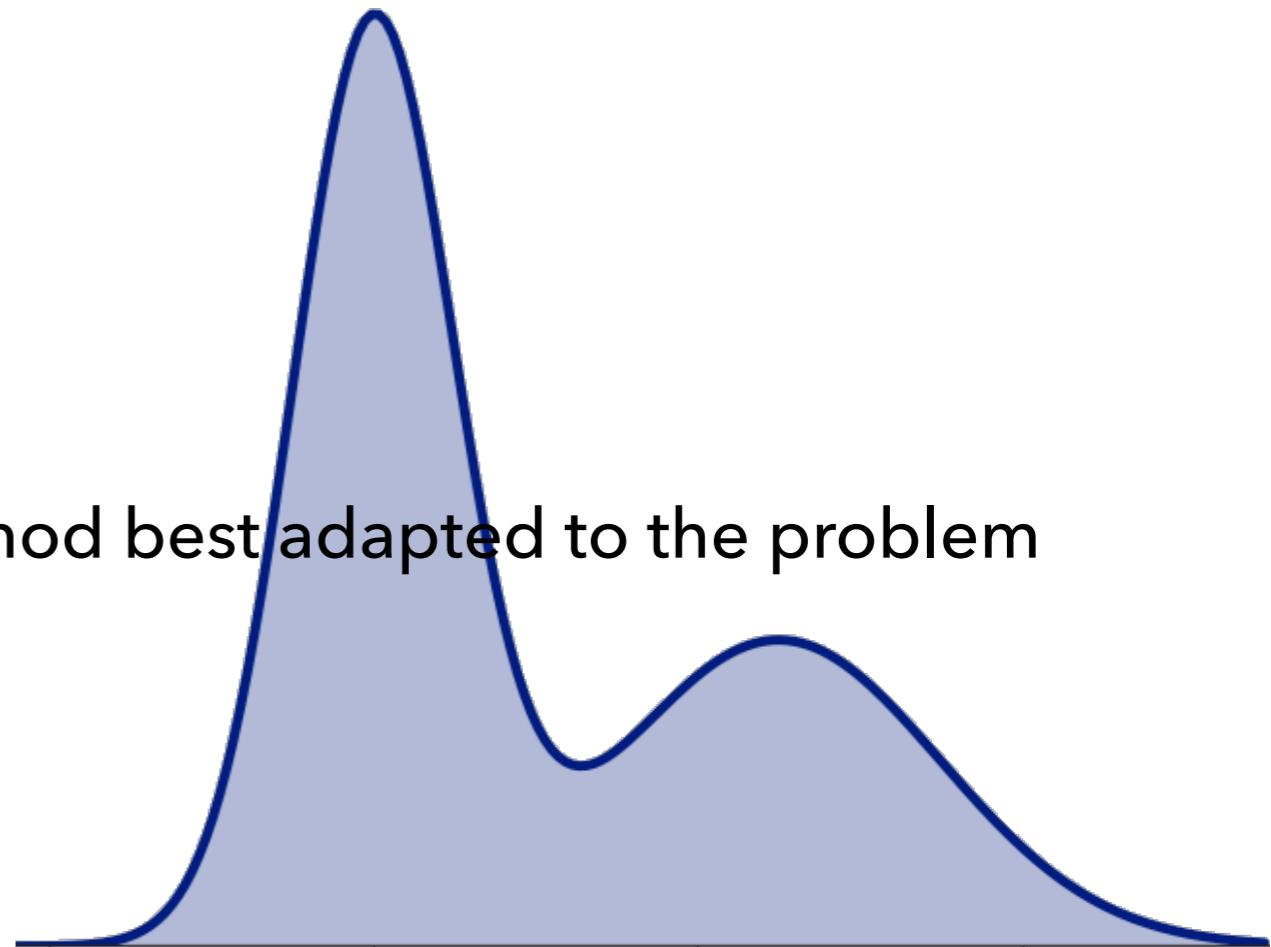
APPROXIMATE INFERENCE

HOW CAN WE DO APPROXIMATE BAYESIAN INFERENCE?

Posterior Approximation:

- ▶ Laplace Approximation
- ▶ Variational Inference
- ▶ Markov Chain Monte Carlo
- ▶ Geometrically Inspired Methods

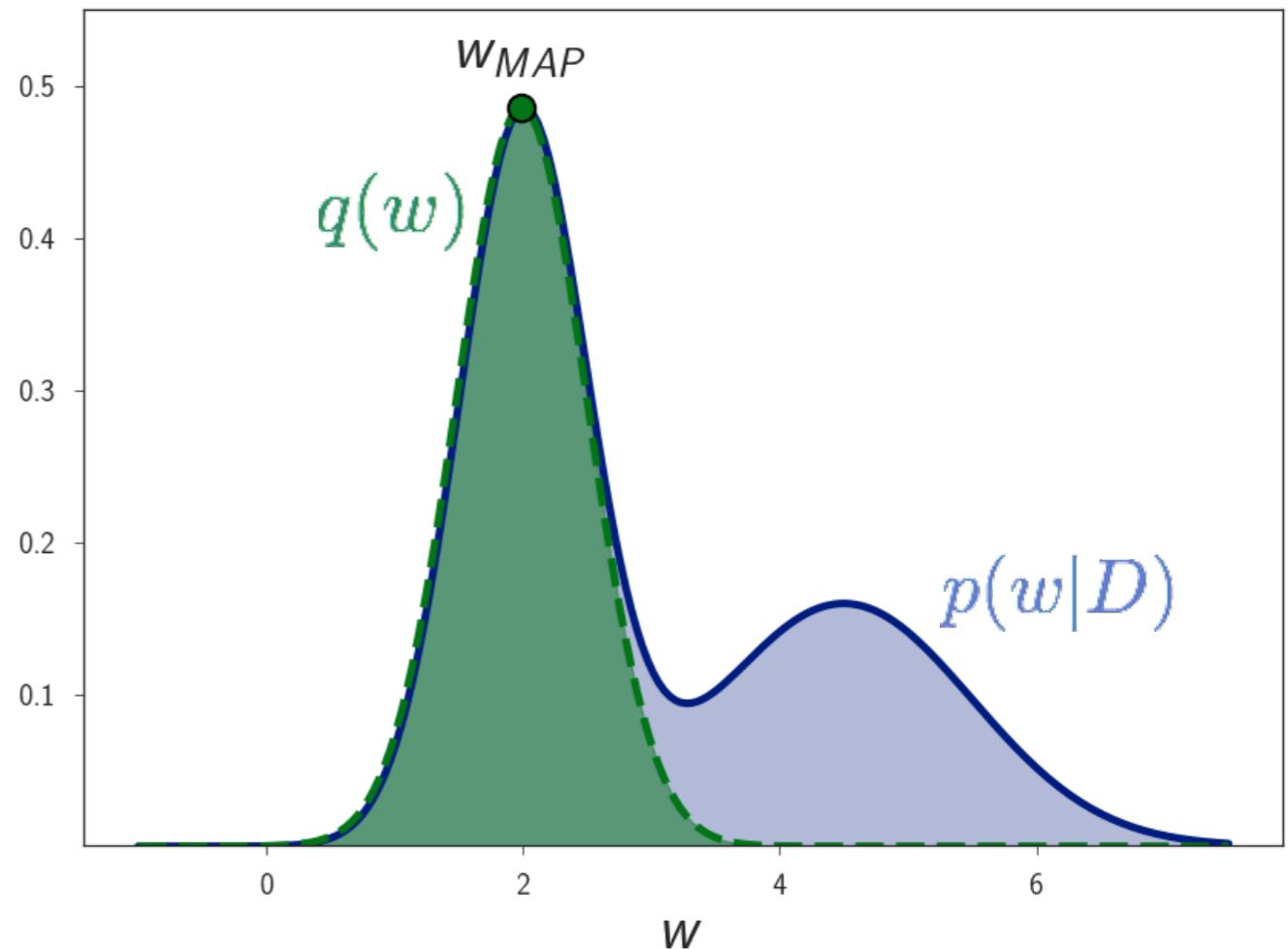
There's no one best method - use the method best adapted to the problem



LAPLACE APPROXIMATION

Approximate posterior with a Gaussian $\mathcal{N}(w|\mu, A^{-1})$

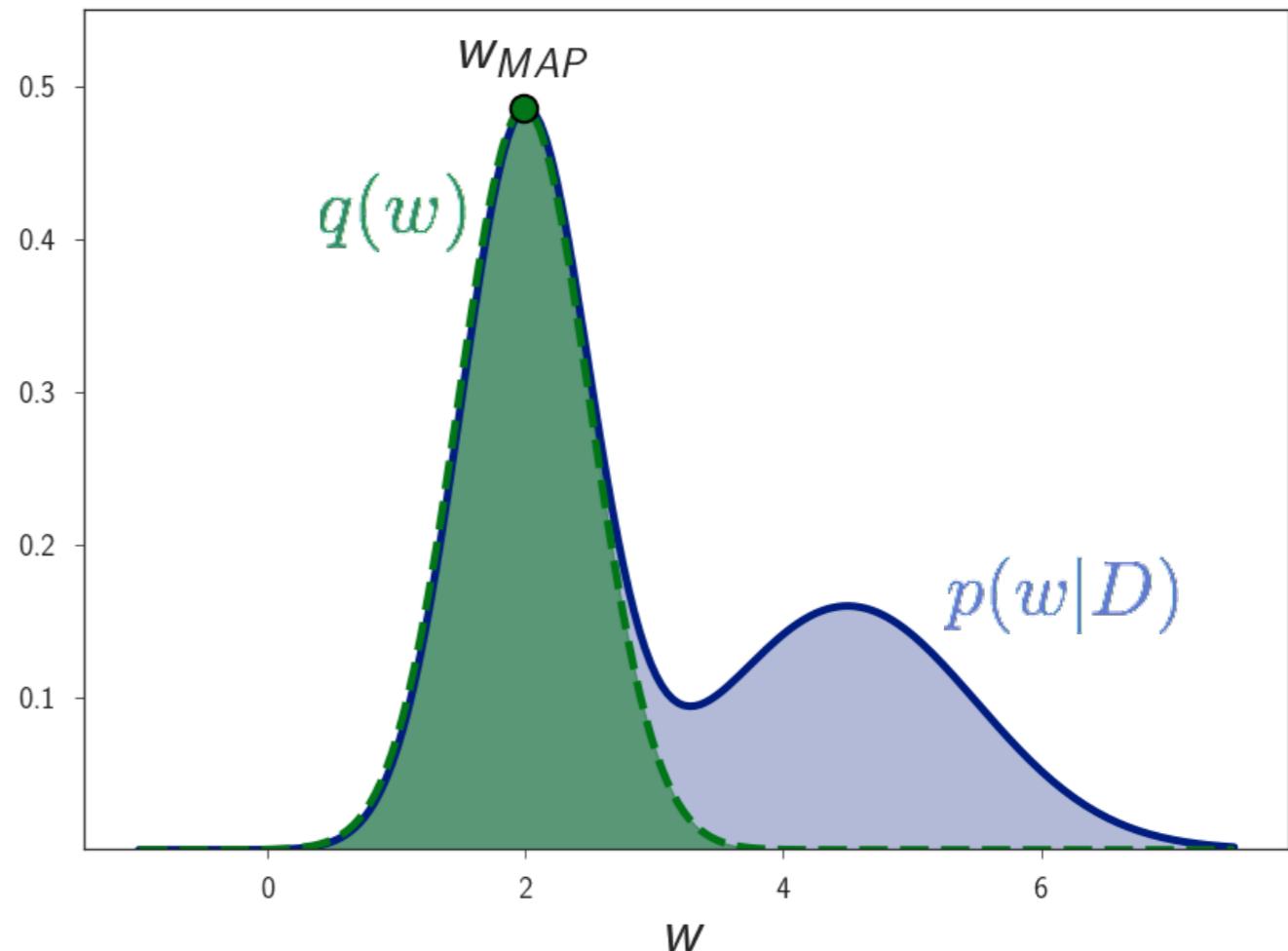
- ▶ $w = w_{MAP}$ mode (local maximum) of $p(w|D)$
- ▶ $A = -\nabla\nabla \log[p(D|w)p(w)]$
- ▶ Only captures a single mode



LAPLACE APPROXIMATION

Approximate posterior with a Gaussian $\mathcal{N}(w|\mu, A^{-1})$

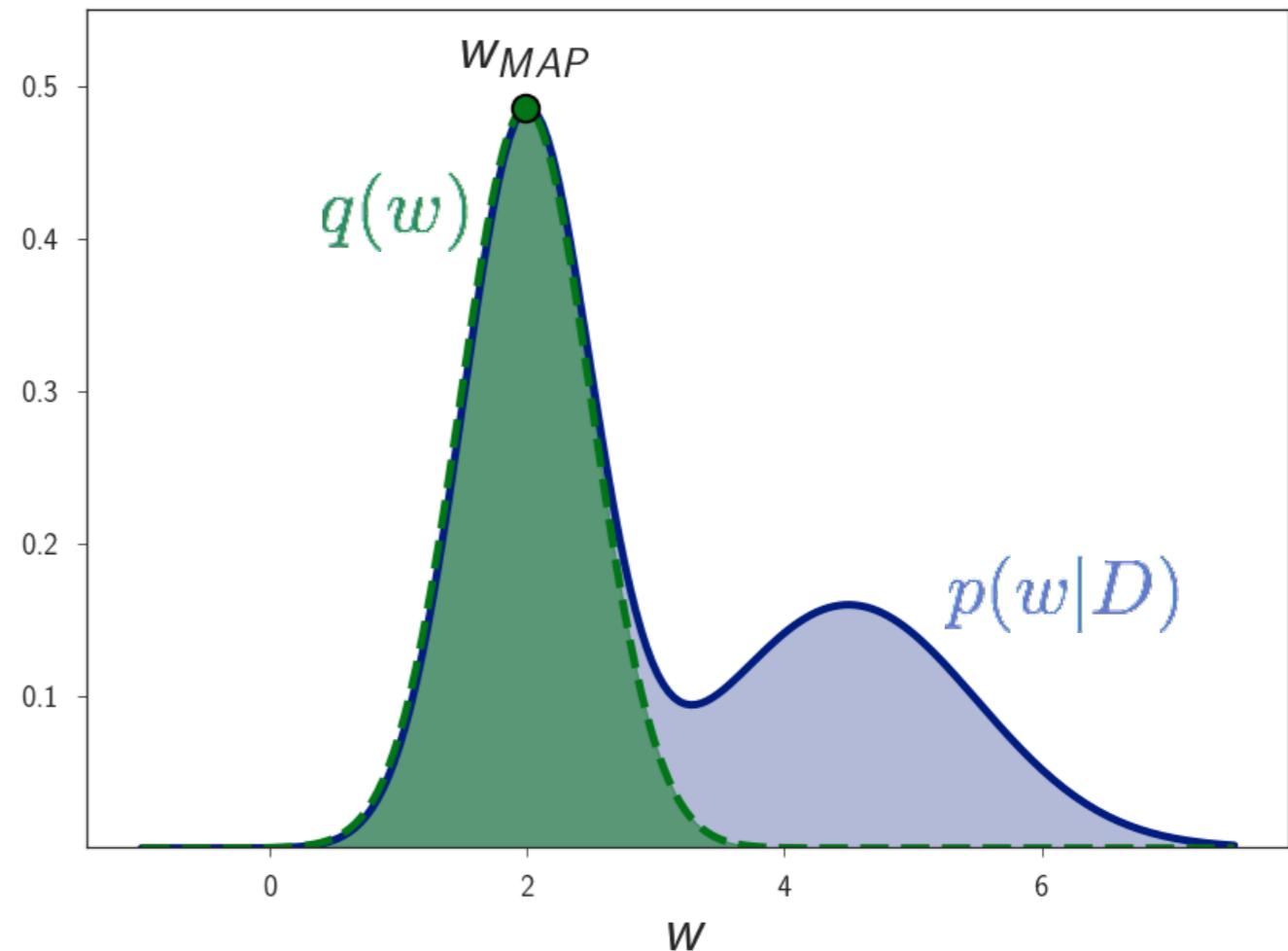
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- ▶ **Is a single mode a bad thing?**



LAPLACE APPROXIMATION

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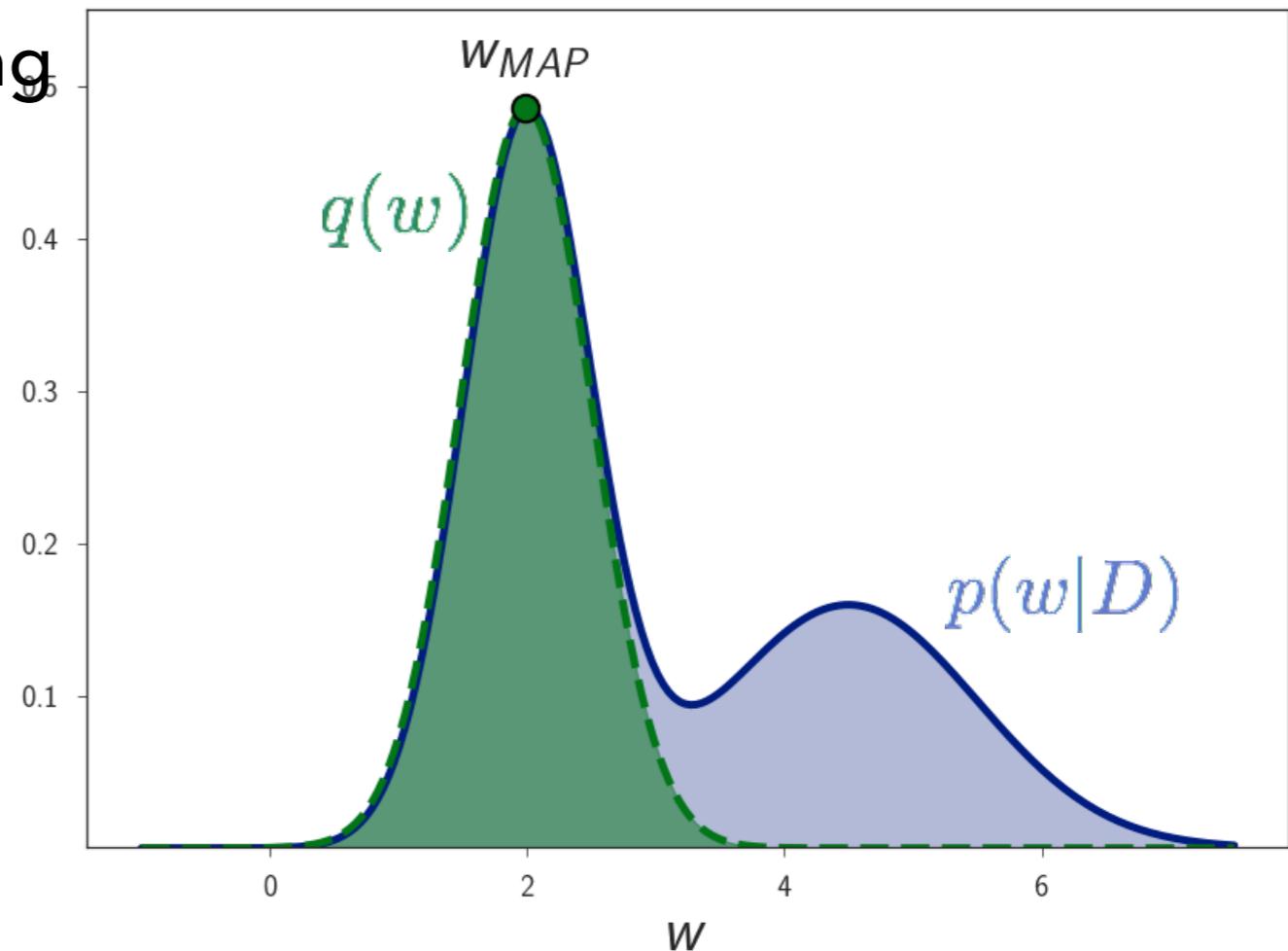
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- ▶ $A = -\nabla\nabla \log[p(D|w)p(w)]$
- ▶ Only captures a single mode
- ▶ **Is a single mode a bad thing?**



LAPLACE APPROXIMATION: DEEP LEARNING

Approximate posterior with a Gaussian $\mathcal{N}(w|\mu, A^{-1})$

- ▶ $w = w_{MAP}$ mode (local maximum) of $p(w|D)$
- ▶ Approximate A with a KFAC (tri-diagonal) – Ritter et al., 2018a
- ▶ Application: Catastrophic forgetting
(Ritter et al, 2018b)
- ▶ Originally from Mackay, '92

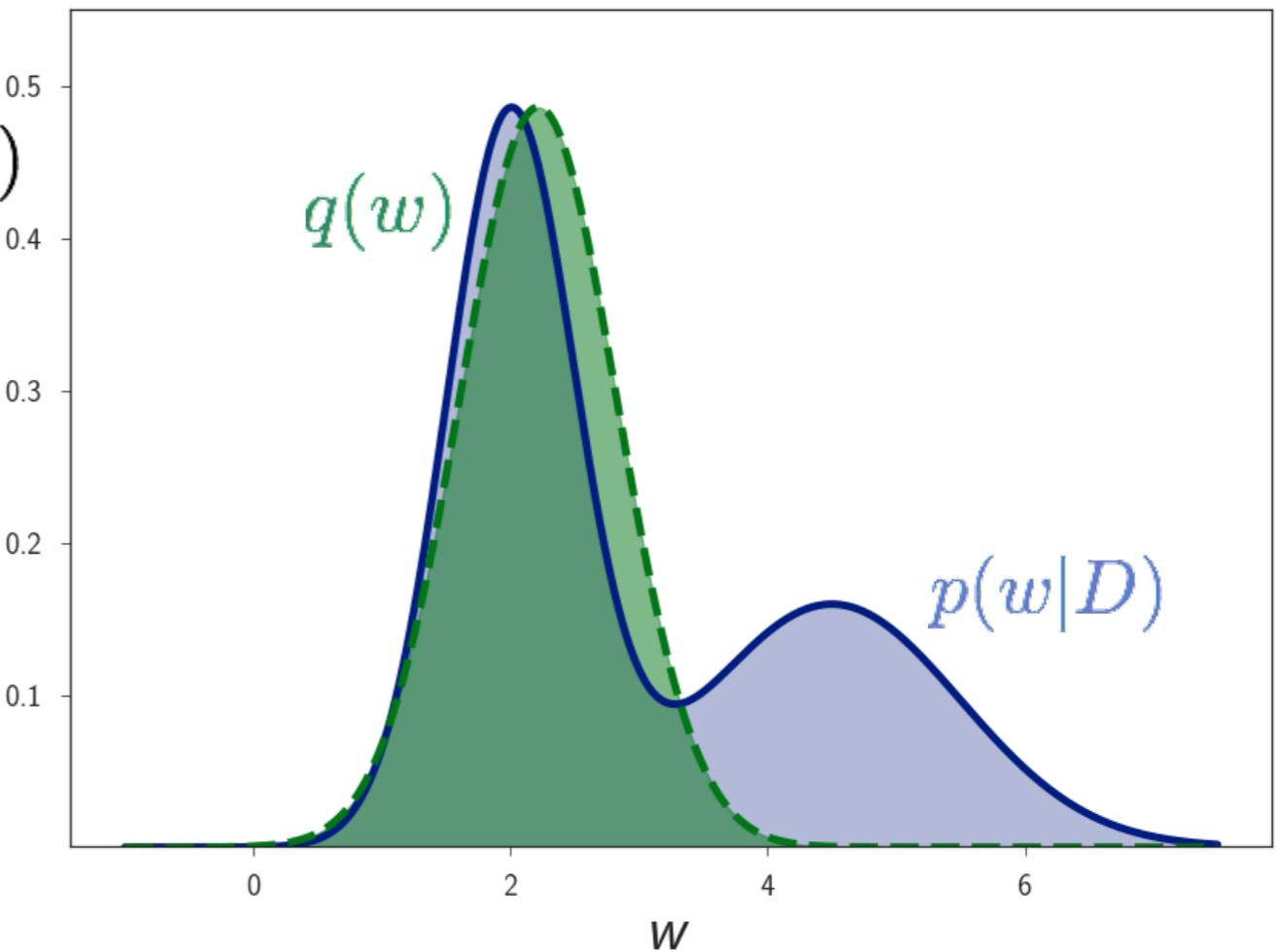


VARIATIONAL INFERENCE

We can find the best approximating distribution within a given family with respect to KL-divergence

$$\triangleright KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$

$$\triangleright \text{ If } q = \mathcal{N}(\mu, \Sigma), \text{ then } \min_{\mu, \Sigma} KL(q||p)$$



VARIATIONAL INFERENCE

We can find the best approximating distribution within a given family with respect to KL-divergence

- ▶
$$KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$
- ▶ Stochastic variational inference (Hoffman et al, '13, Kucelkibir, et al, '17, Graves, 2011)

$$ELBO(w) = E_{q(w)}(\log p(\mathcal{D}|w)) - KL(q(w)||p(w))$$

Traditionally... $q(w) = \mathcal{N}(\mu_i, \sigma_i^2)$

- ▶ Minimizing the KL divergence is “consistent” statistically (Wang & Blei, '19) & optimal in other settings (Knoblauch, et al, '19)
- ▶ Can somewhat evaluate if it works (Yao, et al, '18)

VARIATIONAL INFERENCE: DEEP LEARNING (2)

We can find the best approximating distribution within a given family with respect to KL-divergence

- ▶
$$KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$
- ▶ Other bounds exist...
 - ▶ Chi-Square (Dieng, et al, '17), F-divergences (Wang, et al, '17), Perturbative divergences (Bamler et al, '17), VPNG (Tang & Ranganath, '19)
 - ▶ Better approximation distributions....
 - ▶ Matrix-variate Gaussians (Louizos, et al, '16), Normalizing flows (Louizos, et al, '17), Bayes by Backprop (Blundell, et al, 16)

VARIATIONAL INFERENCE: DEEP LEARNING (3)

We can find the best approximating distribution within a given family with respect to KL-divergence

- ▶
$$KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$
- ▶ Other bounds exist...
 - ▶ Renyi-divergences (Li & Turner, '16), robust divergences (Futami, et al, '17), operator divergences (Ranganath, et al, 16), etc...
 - ▶ Better approximation distributions....
 - ▶ Implicit distributions (Tran, Ranganath, Blei, '17), GANs (Huszar, '17), boosting (Miller et al, '17), smoothed dropout (Gal, et al, '17), etc...

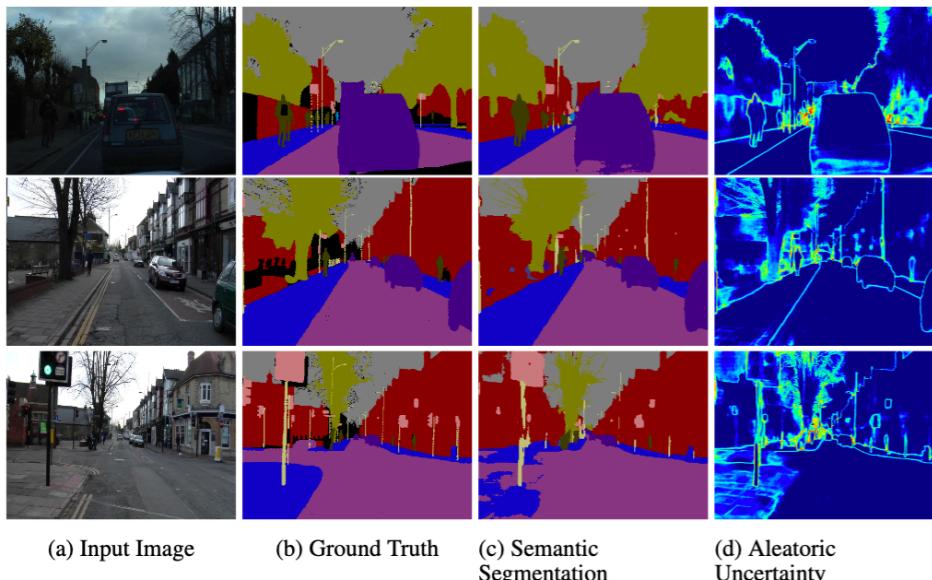
VARIATIONAL INFERENCE: DEEP LEARNING

We can find the best approximating distribution within a given family with respect to KL-divergence

- ▶
$$KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$
- ▶ Dropout at test time ([Gal & Ghahramani, '15](#), Gal & Ghahramani, '16, Gal, '16, Gal & Li, '17)
- ▶ $q(w) = Bernoulli(p)\mathcal{N}(\mu_i, \sigma)$
- ▶ KL un-defined so it's actually minimizing a quasi-KL divergence...
(Hron et al, '18)

VARIATIONAL INFERENCE: DROPOUT

- ▶ Applications of dropout
 - ▶ Segmentation for autonomous driving(Kendall & Gal '17)



From Kendall & Gal

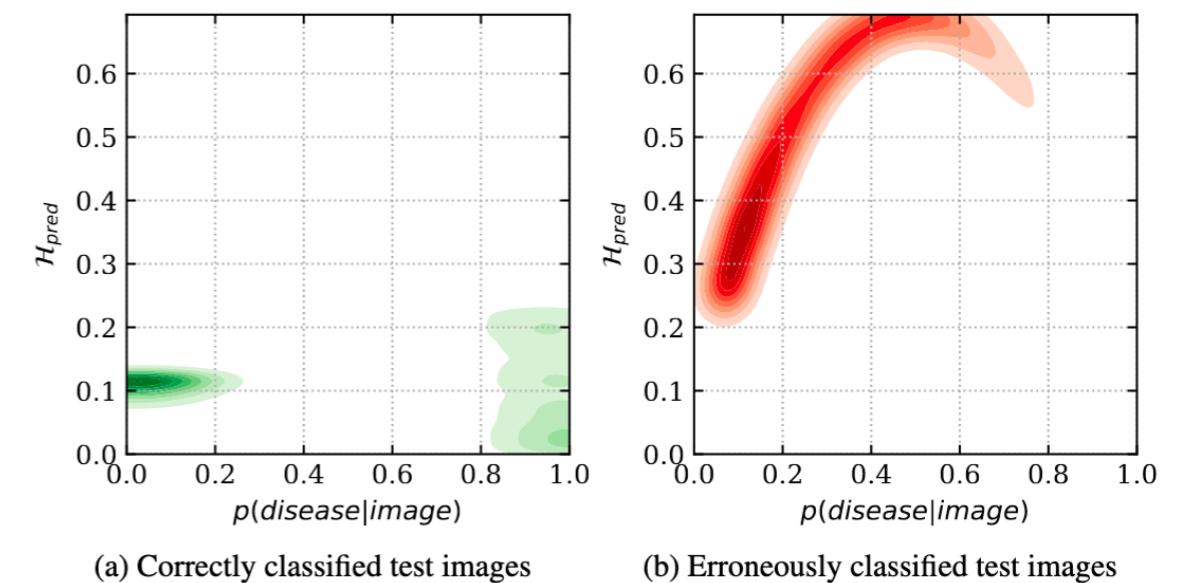


Figure 4: Relation between predictive uncertainty (i.e. entropy), $\mathcal{H}_{\text{pred}}$, of MC Dropout model, and maximum-likelihood, i.e. sigmoid probabilities $p(\text{disease}|\text{image})$. The model has higher uncertainty for the miss-classified images, hence it can be used as an indicator to drive referral.

From Filiots et al, 2019

- ▶ Segmentation for clinical applications

VARIATIONAL INFERENCE: DEEP LEARNING (6)

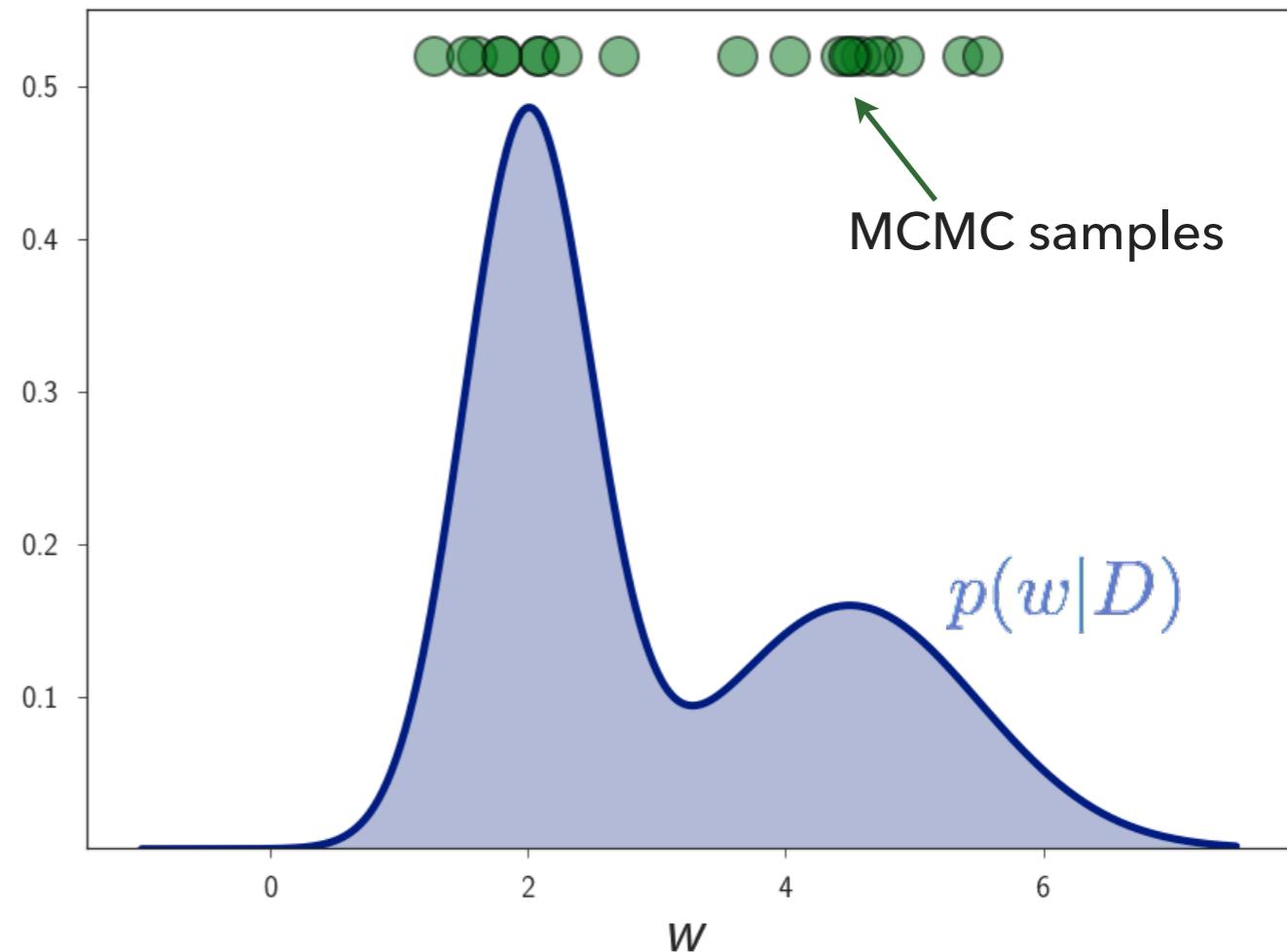
We can find the best approximating distribution within a given family with respect to KL-divergence

- ▶
$$KL(q||p) = \int_w q(w) \log \frac{q(w)}{p(w|D)} dw$$
- ▶ Variational interpretations of stochastic optimization....
 - ▶ Early stopping (Duvenaud, et al, '16)
 - ▶ Constant SGD (Mandt, Hoffman, Blei, '17) **[more later]**
 - ▶ Adam (Khan et al, '18, [Osawa et al, '19](#))
 - ▶ Natural Gradient descent (Zhang et al, '18, Bae et al, 19)
 - ▶ MCMC (Hoffman & Ma, '19)

MARKOV CHAIN MONTE CARLO

We can produce samples from the exact posterior by defining specific Markov Chains

- ▶ Software packages:
 - ▶ Stan, PyMC4, Pyro
 - ▶ Langevin dynamics (SGLD) (Neal '93, Welling & Teh, '11)
 - ▶ Hamiltonian dynamics
 - ▶ Neal, '95, '96
 - ▶ Stochastic version - Chen et al, '14



CYCLIC SGMC (ZHANG ET AL, ICLR 2020)

<https://github.com/ruqizhang/csgmcmc>

- ▶ Run stochastic Hamiltonian Monte Carlo with a cyclic learning rate

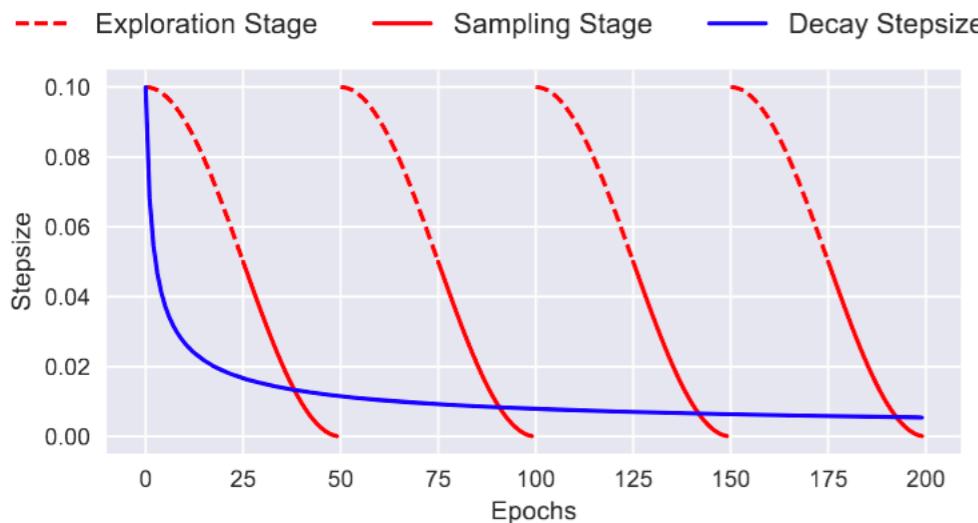


Figure 1. Illustration of the proposed cyclical stepsize schedule (red) and the traditional decreasing stepsize schedule (blue) for SG-MCMC algorithms.

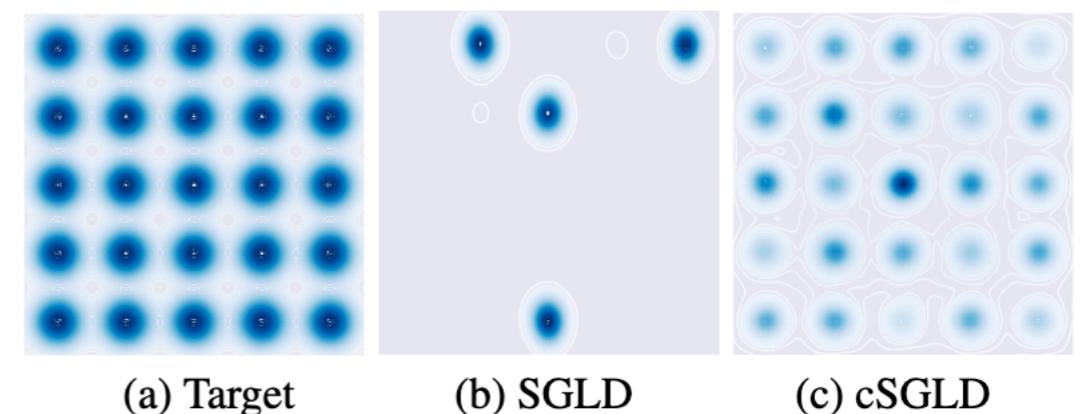
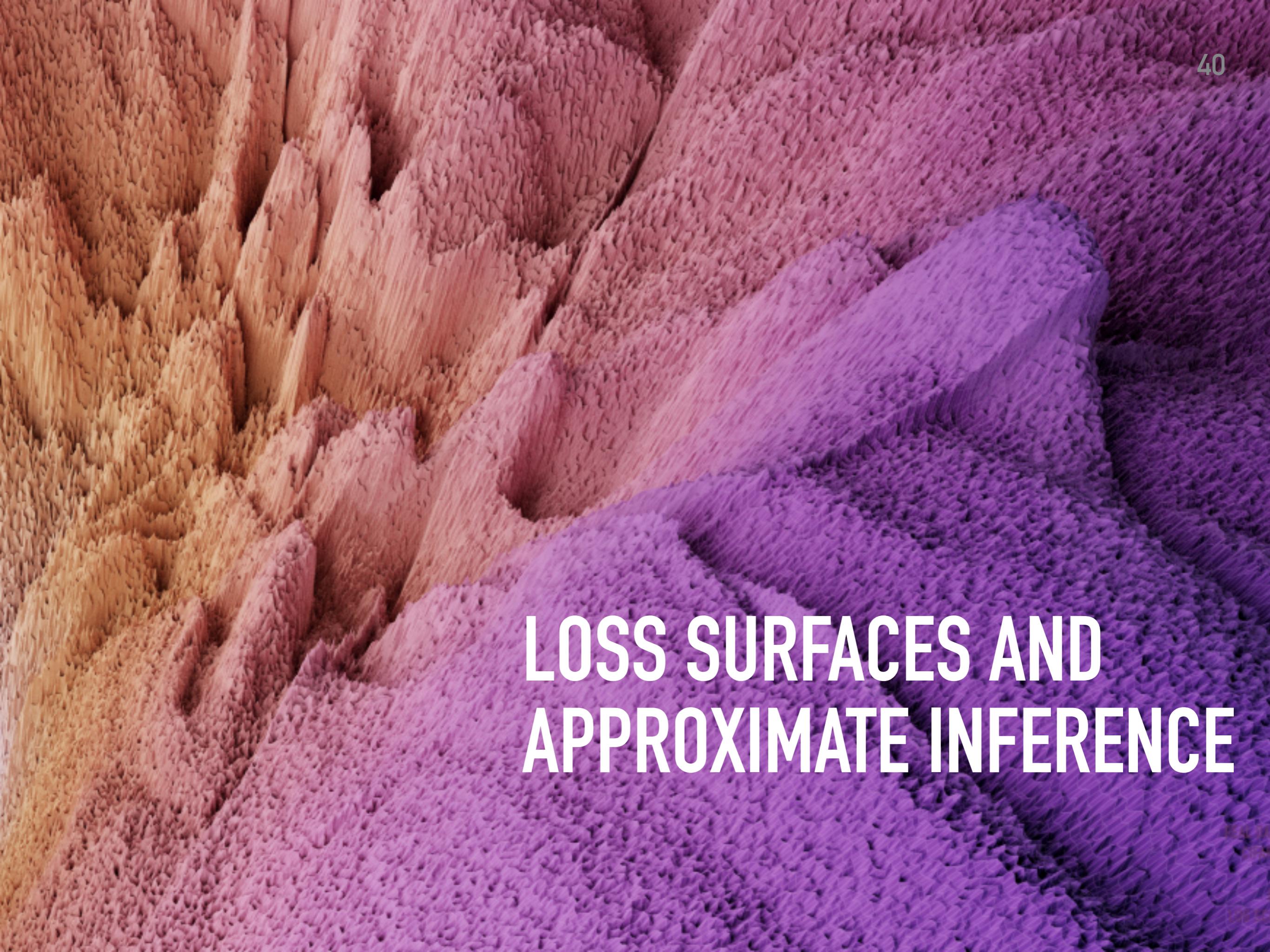


Figure 2. Sampling from a mixture of 25 Gaussians shown in (a) for the parallel setting. With a budget of $50k \times 4 = 200k$ samples, traditional SGLD in (b) has only discovered 4 of the 25 modes, while our cSGLD in (c) has fully explored the distribution.

Converges faster to the posterior than standard SGHMC in terms of Wasserstein distance

A 3D surface plot of a loss function, characterized by numerous sharp peaks and deep valleys, creating a complex landscape of local minima.

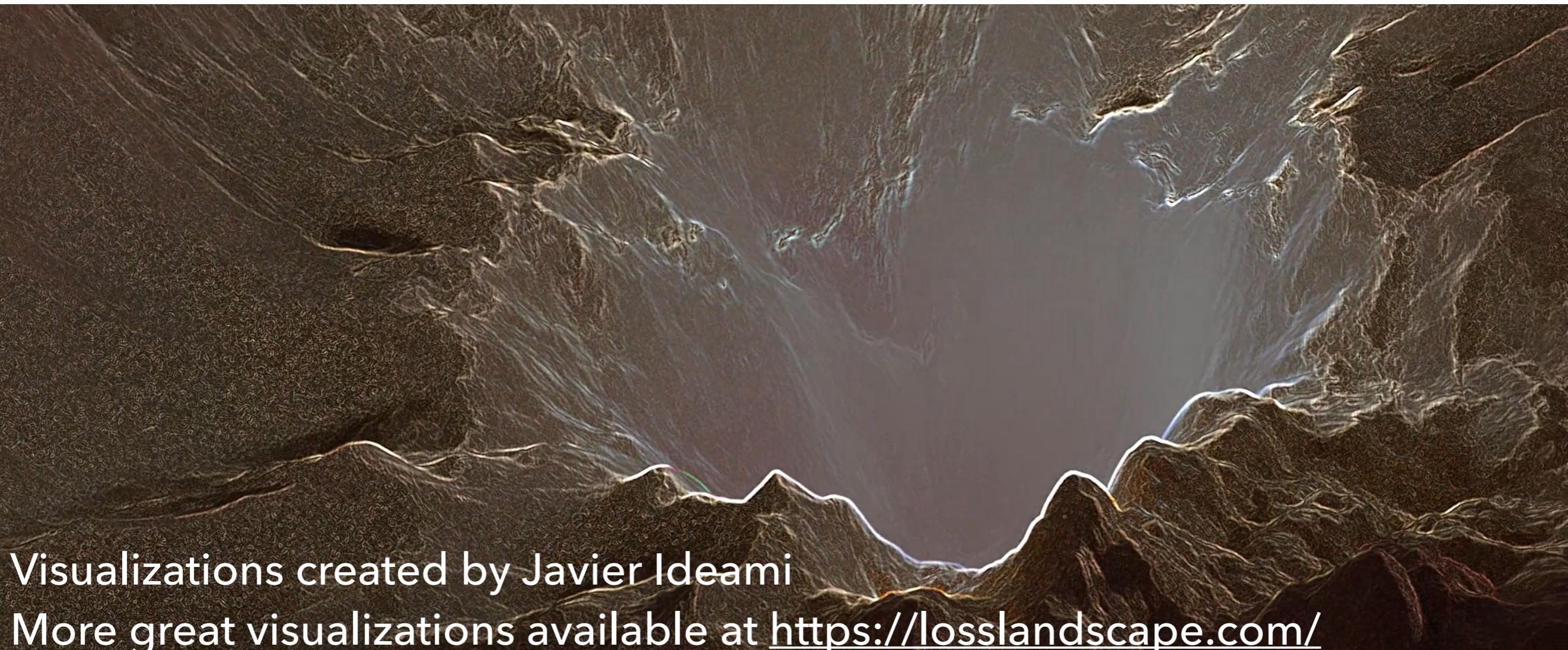
LOSS SURFACES AND APPROXIMATE INFERENCE

BASED OFF OF

- ▶ “A Simple Baseline for Bayesian Uncertainty in Deep Learning,” Maddox, Garipov, Izmailov, Vetrov, Wilson, <https://arxiv.org/abs/1902.02476>, NeurIPS, 2019
 - ▶ Code: https://github.com/wjmaddox/swa_gaussian
- ▶ “Subspace Inference for Bayesian Deep Learning,” Izmailov, Maddox, Kirichenko, Garipov, Vetrov, Wilson, <https://arxiv.org/abs/1907.07504>, UAI, 2019.
 - ▶ Code: <https://github.com/wjmaddox/drbayes>

LOSS SURFACES: WHY DO WE CARE?

- ▶ Better approximate Bayesian Inference
 - $\text{loss} = -\log p(w|D)$, so understanding loss surfaces is crucial for approximate Bayesian inference

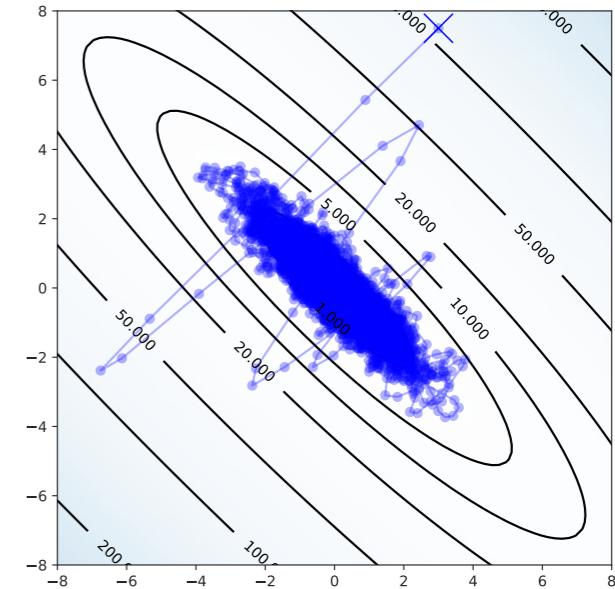


Visualizations created by Javier Ideami

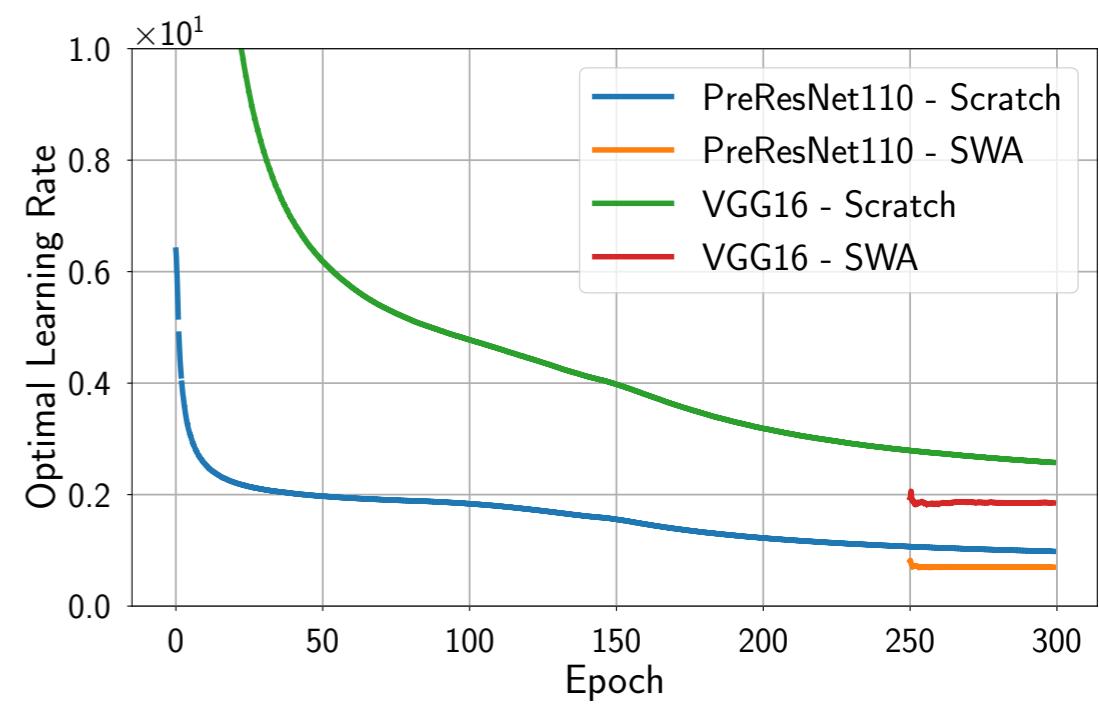
More great visualizations available at <https://losslandscape.com/>

SGD AS APPROXIMATE BAYESIAN INFERENCE - MANDT, ET AL, JMLR, '17

- ▶ SGD with isotropic noise follows the shape of the posterior



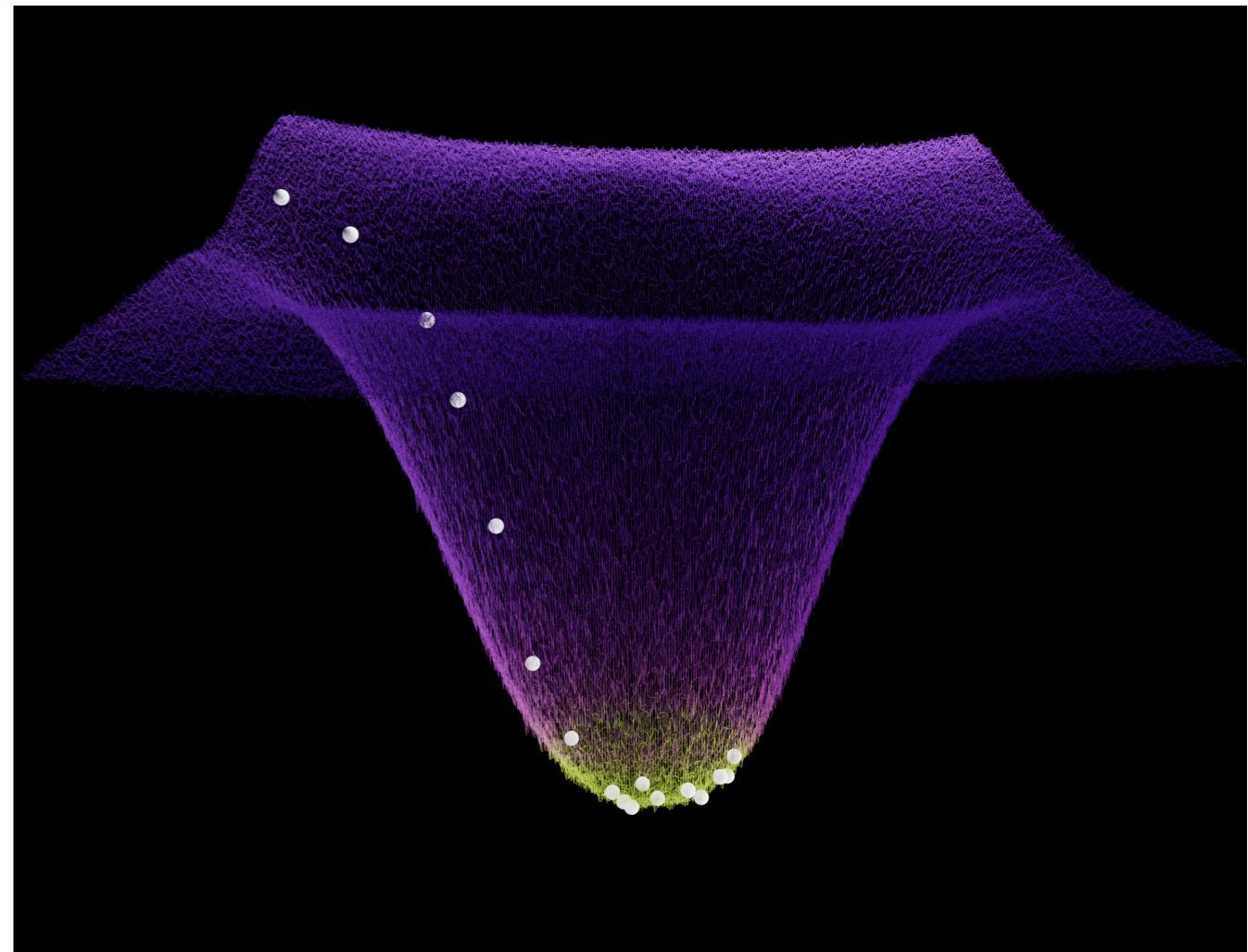
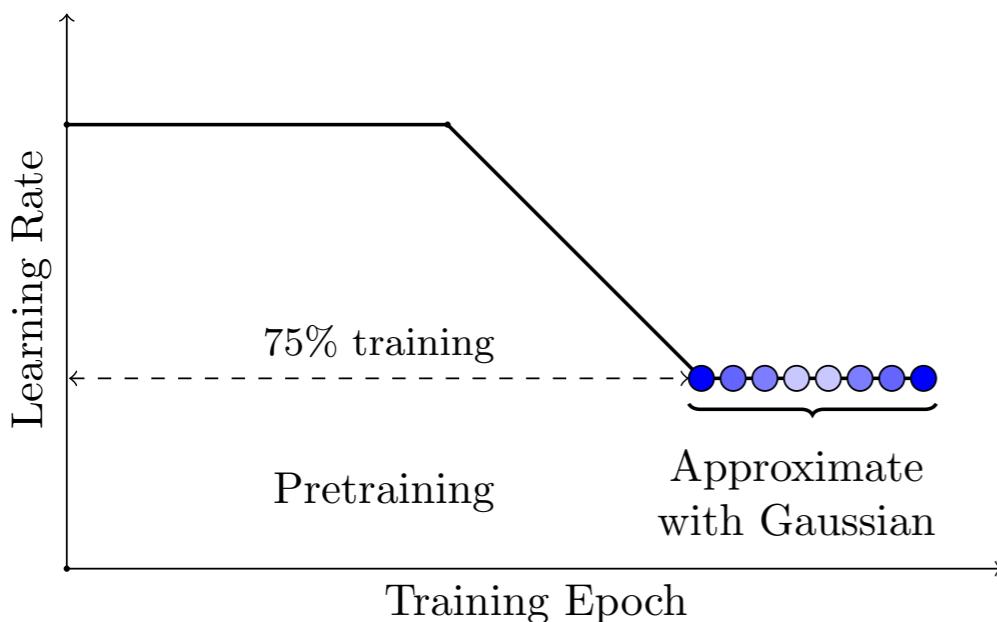
- ▶ Assumptions of analysis don't quite hold for DNNs
- ▶ But... we can use the same idea to approximate the posterior for DNNs



STOCHASTIC WEIGHT AVERAGING GAUSSIAN (SWAG) - MADDOX ET AL, NEURIPS, '19

https://github.com/wjmaddox/swa_gaussian

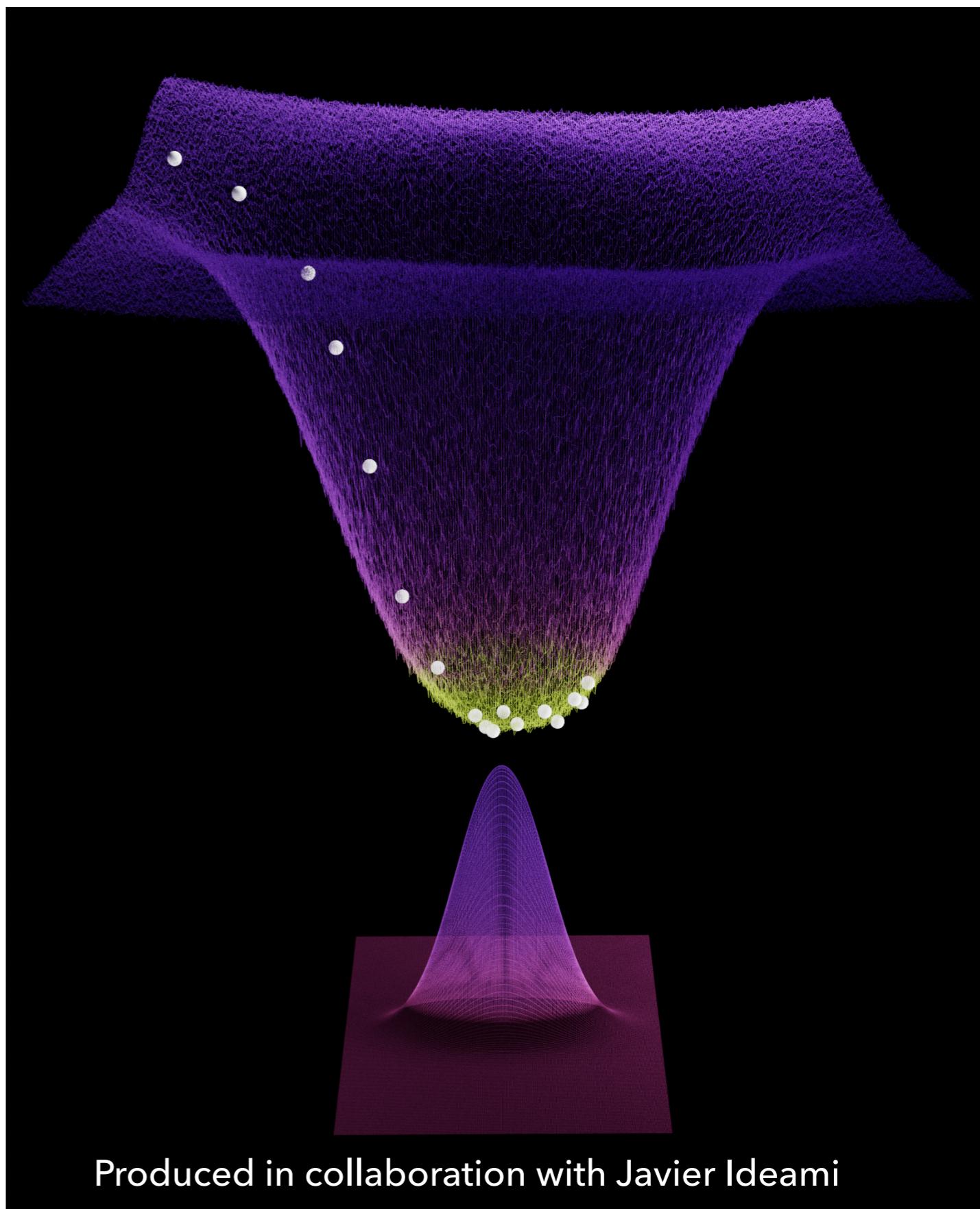
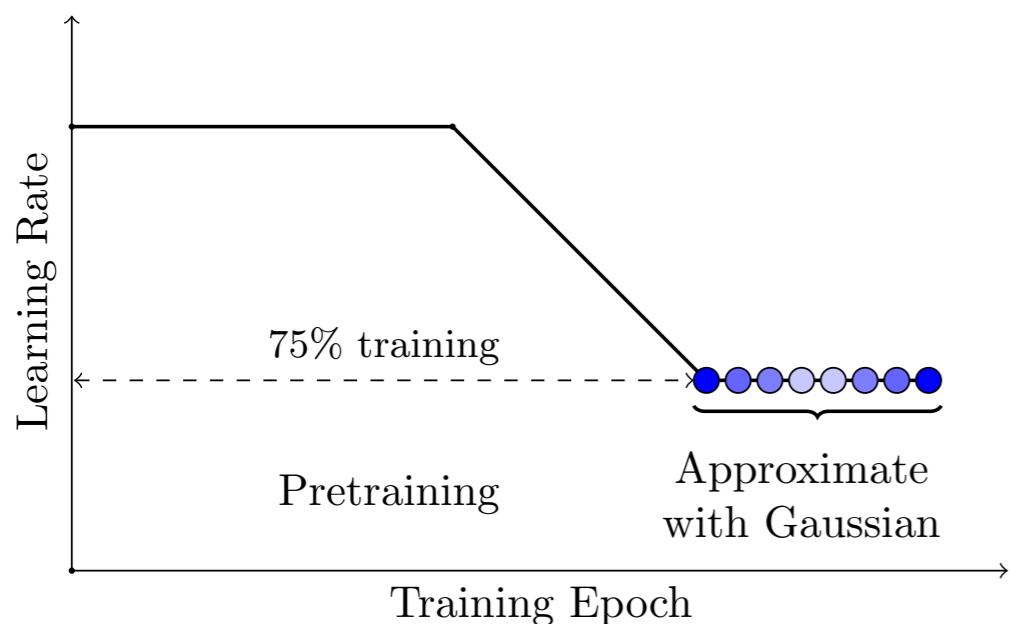
During training



Produced in collaboration with Javier Ideami

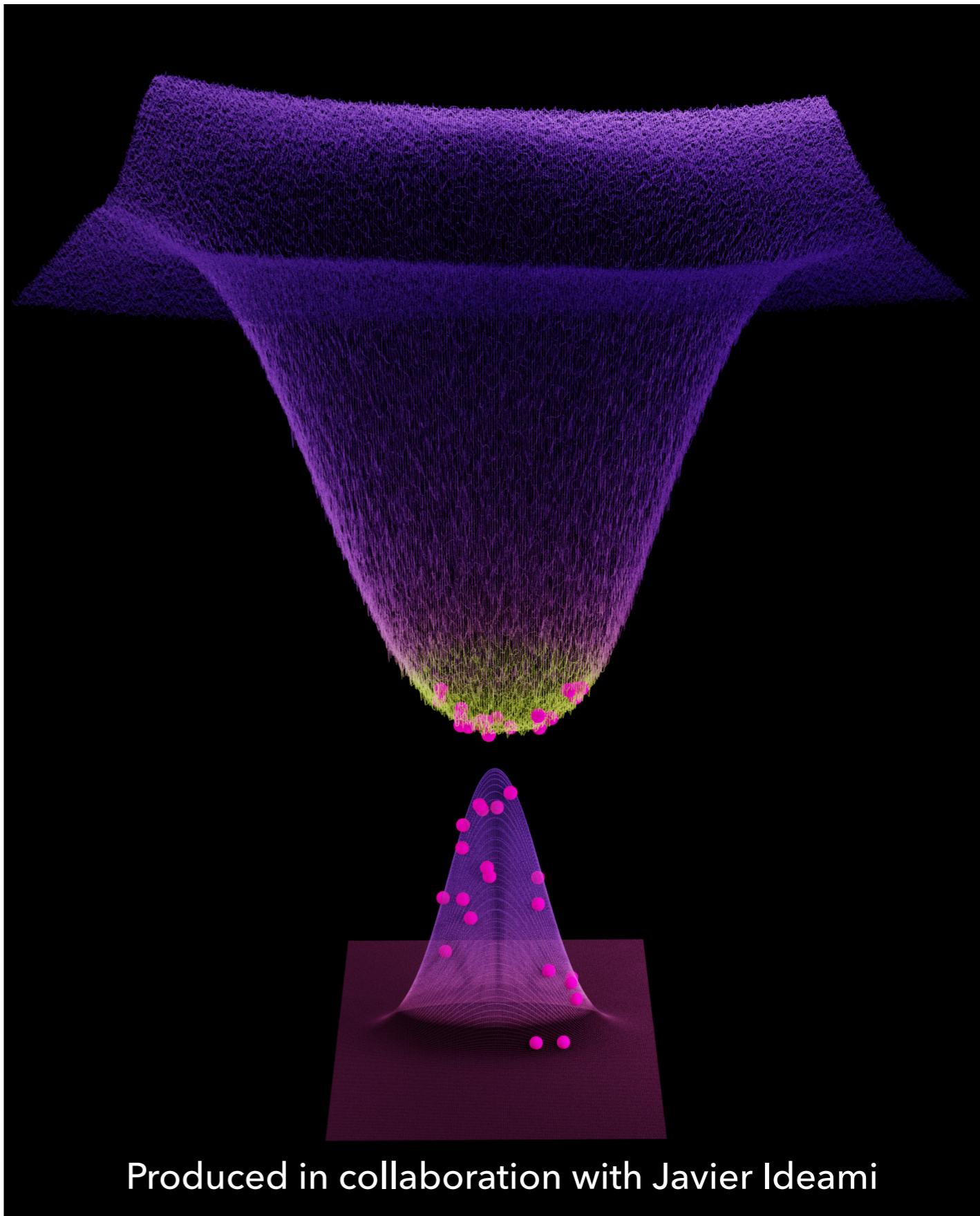
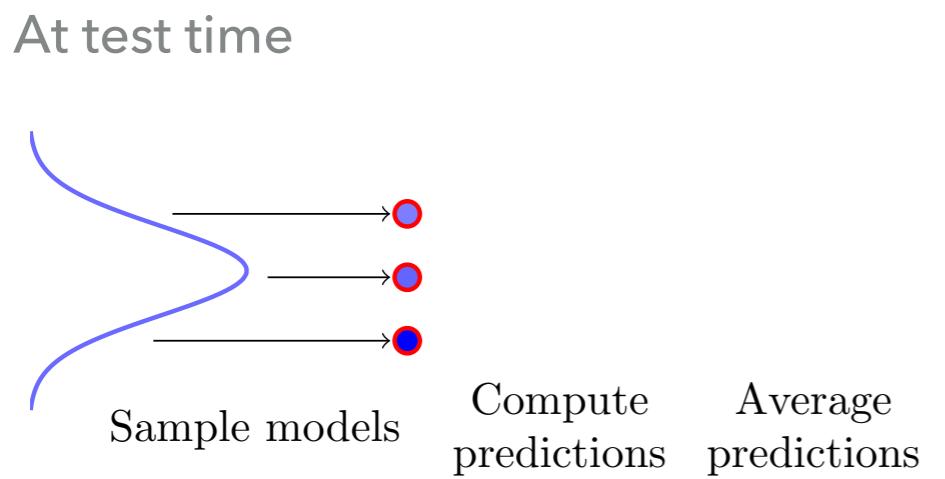
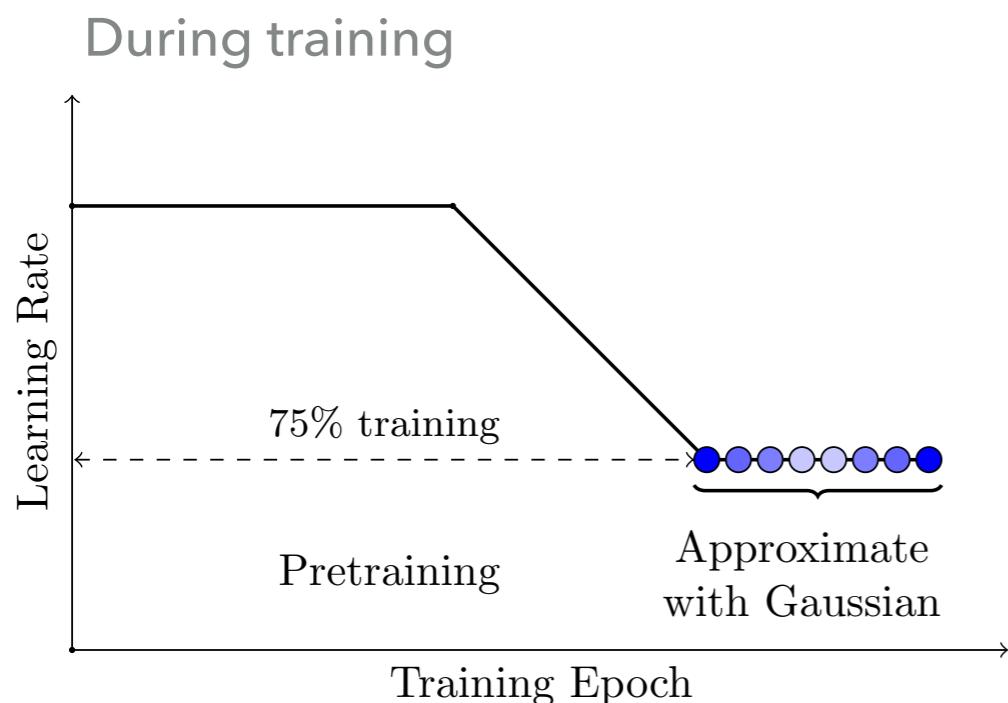
SWAG

During training

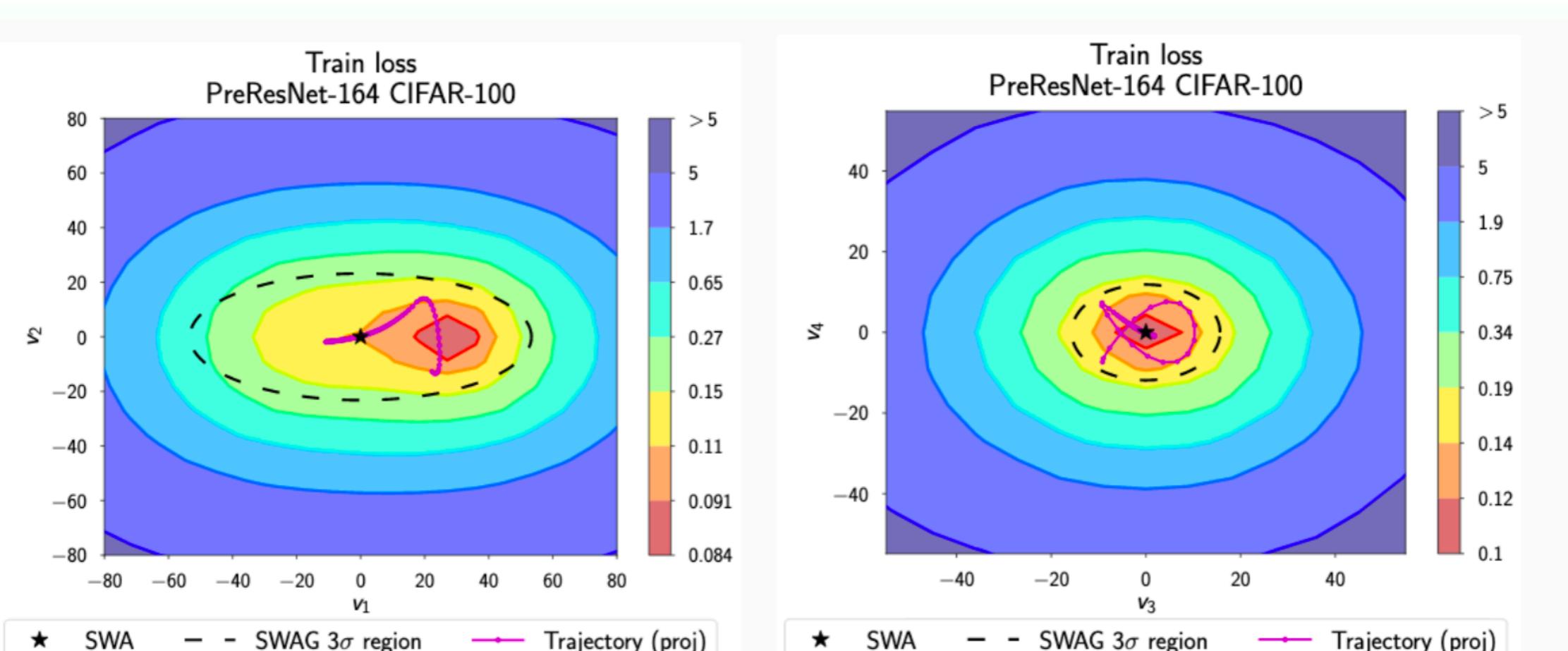


Produced in collaboration with Javier Ideami

SWAG

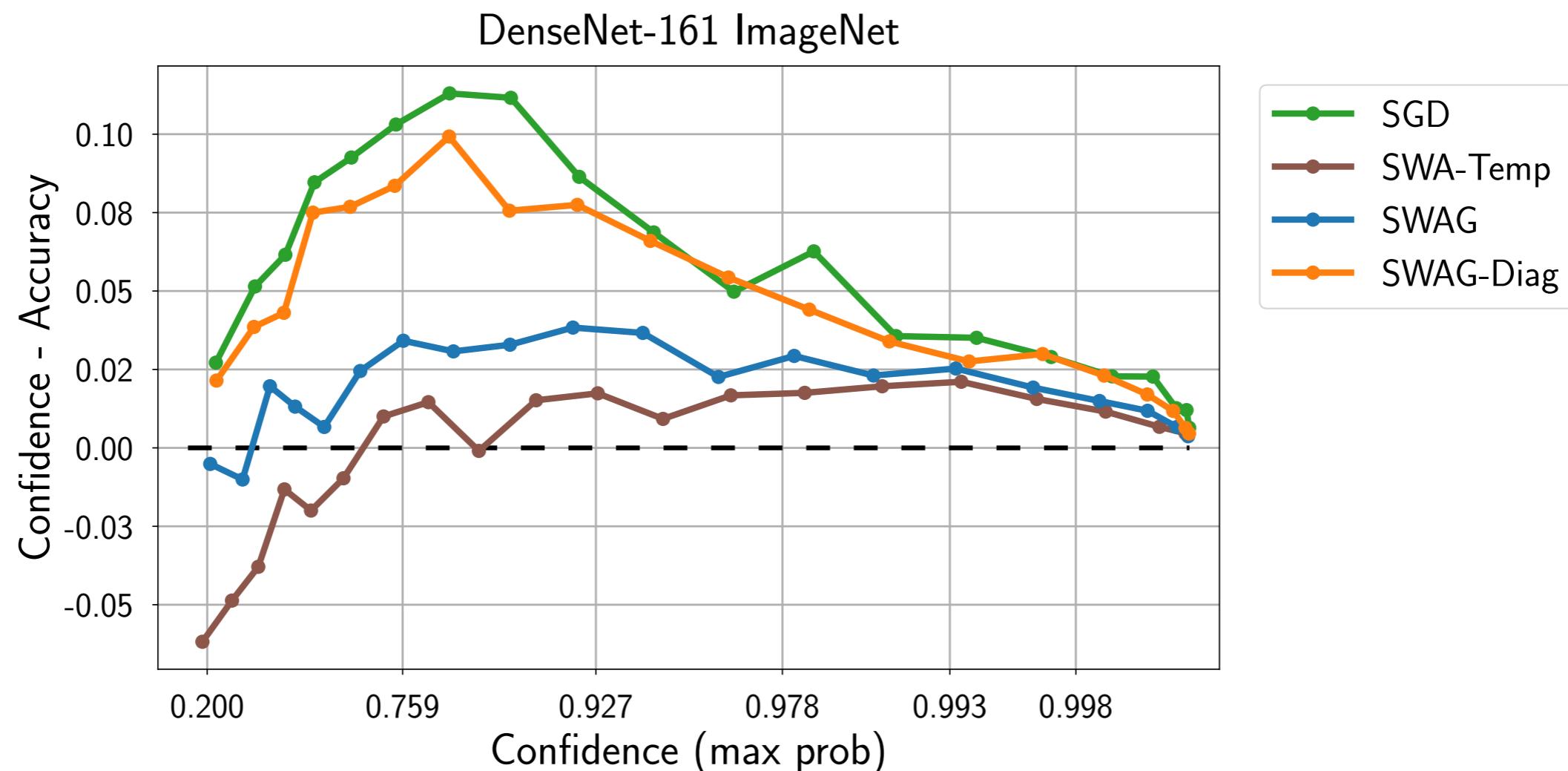


SWAG - EMPIRICAL MOTIVATION



$$\psi(t_1, t_2) = \mathcal{L}(\theta_{\text{SWA}} + t_1 \cdot \frac{v_i}{\|v_i\|} + t_2 \cdot \frac{v_j}{\|v_j\|})$$

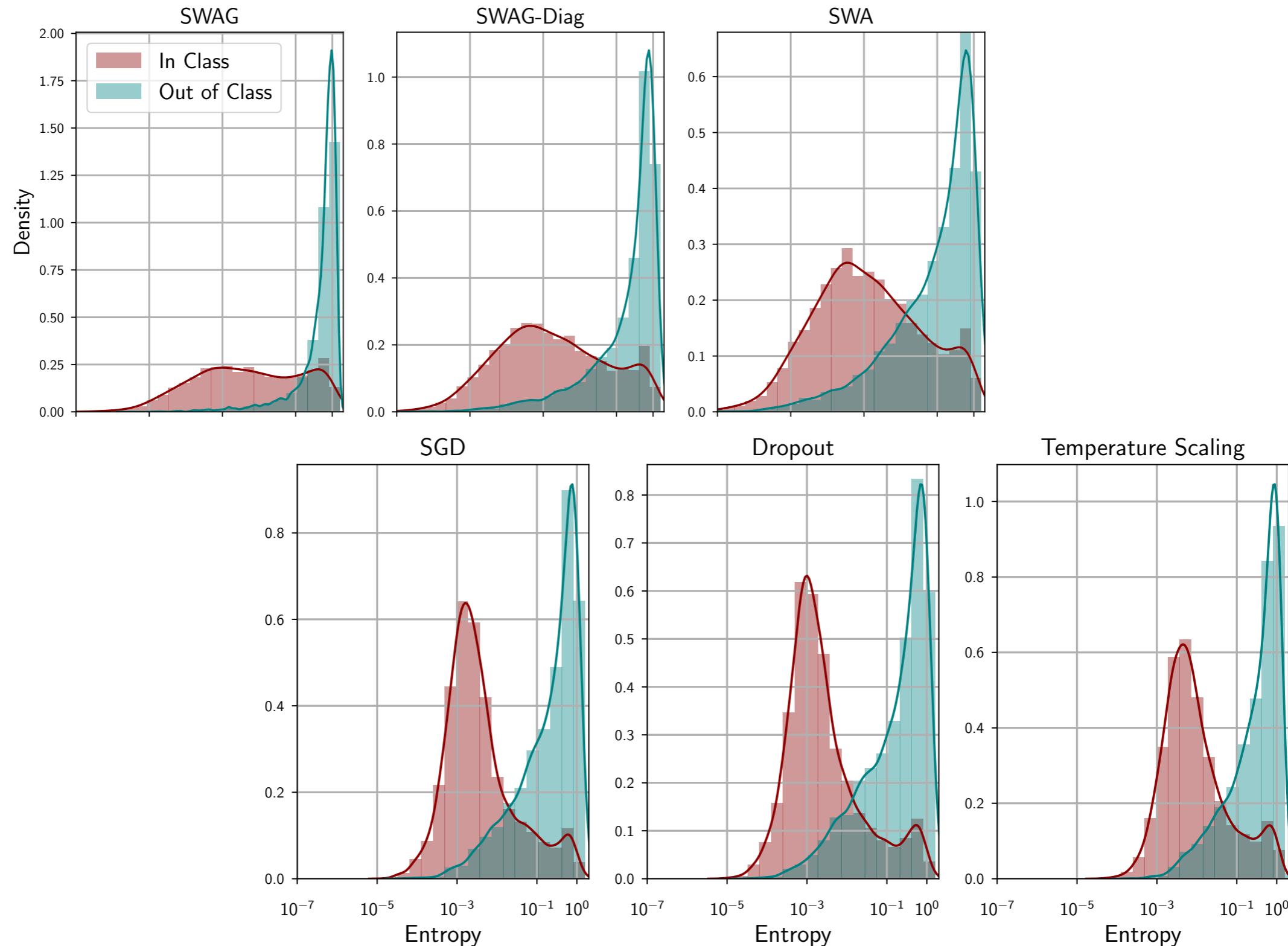
SWAG - CALIBRATION



SWAG - BAYESIAN MODEL AVERAGING

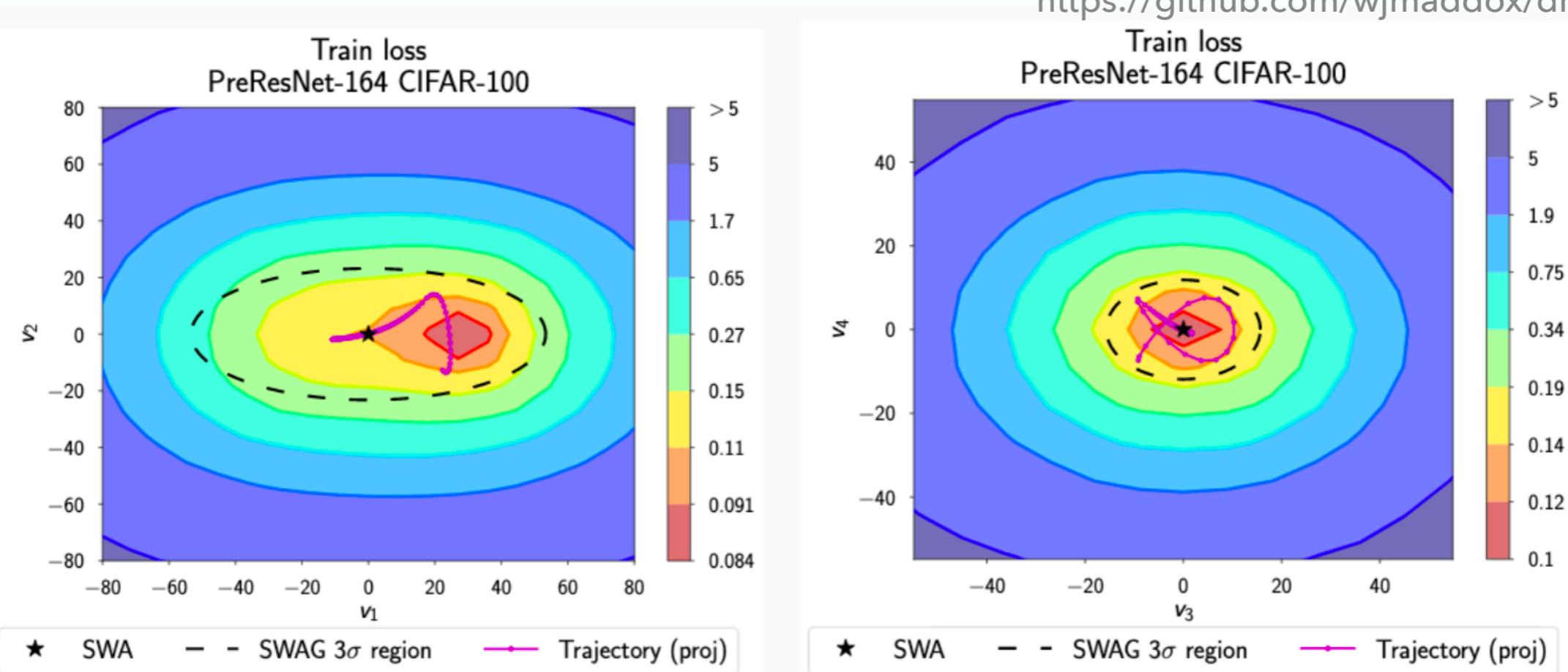
Dataset	Model	SGD	SWA	SWAG-Diag	SWAG	KFAC-Laplace	SWA-Dropout	SWA-Temp
CIFAR-10	VGG-16	93.17	93.61	93.66	93.60	92.65	93.23	93.61
CIFAR-10	PreResNet-164	95.49	96.09	96.03	96.03	95.49	96.18	96.09
CIFAR-10	WideResNet28x10	96.41	96.46	96.41	96.32	96.17	96.39	96.46
CIFAR-100	VGG-16	73.15	74.30	74.68	74.77	72.38	72.50	74.30
CIFAR-100	PreResNet-164	78.50	80.19	80.18	79.90	78.51		80.19
CIFAR-100	WideResNet28x10	80.76	82.40	82.40	82.23	80.94	82.30	82.40
ImageNet	DenseNet-161	77.79	78.60	78.59	78.59			78.60
ImageNet	ResNet-152	78.39	78.92	78.96	79.08			78.92
CIFAR10 → STL10	VGG-16	72.42	71.92	72.09	72.19		71.45	71.92
CIFAR10 → STL10	PreResNet-164	75.56	76.02	75.95	75.88			76.02
CIFAR10 → STL10	WideResNet28x10	76.75	77.50	77.26	77.09		76.91	77.50

SWAG - OUT OF SAMPLE DETECTION



SUBSPACE INFERENCE FOR BAYESIAN DEEP LEARNING - IZMAILOV, ET AL, UAI, '19

<https://github.com/wjmaddox/drbayes>

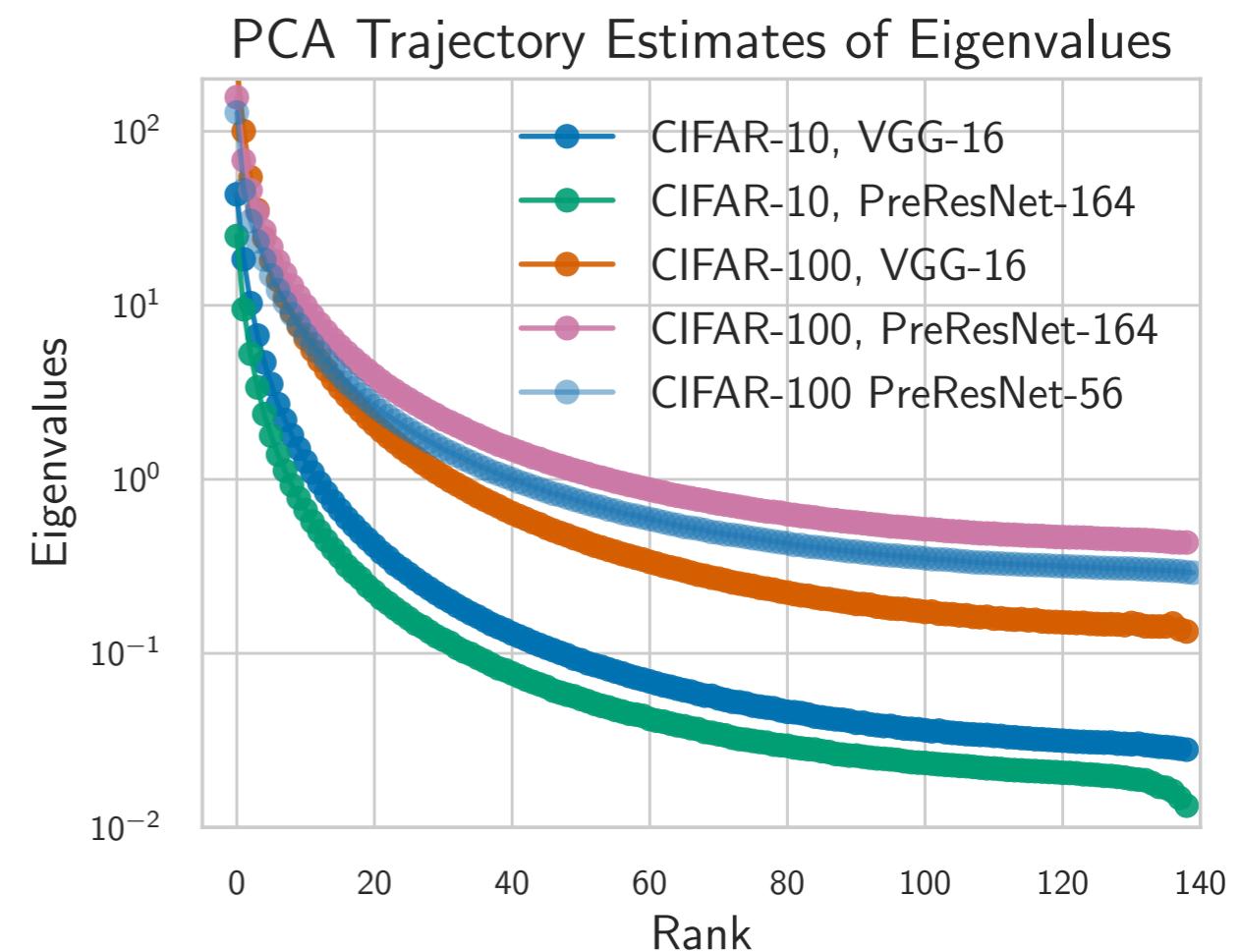


$$\psi(t_1, t_2) = \mathcal{L}(\theta_{\text{SWA}} + t_1 \cdot \frac{v_i}{\|v_i\|} + t_2 \cdot \frac{v_j}{\|v_j\|})$$

- ▶ Remember this plot?

SUBSPACE INFERENCE

- ▶ SGD trajectory happens in a very small subspace
 - ▶ Summarize the information from the trajectory in very low dimensions
 - ▶ Also seen in Gur-Ari, et al, '19



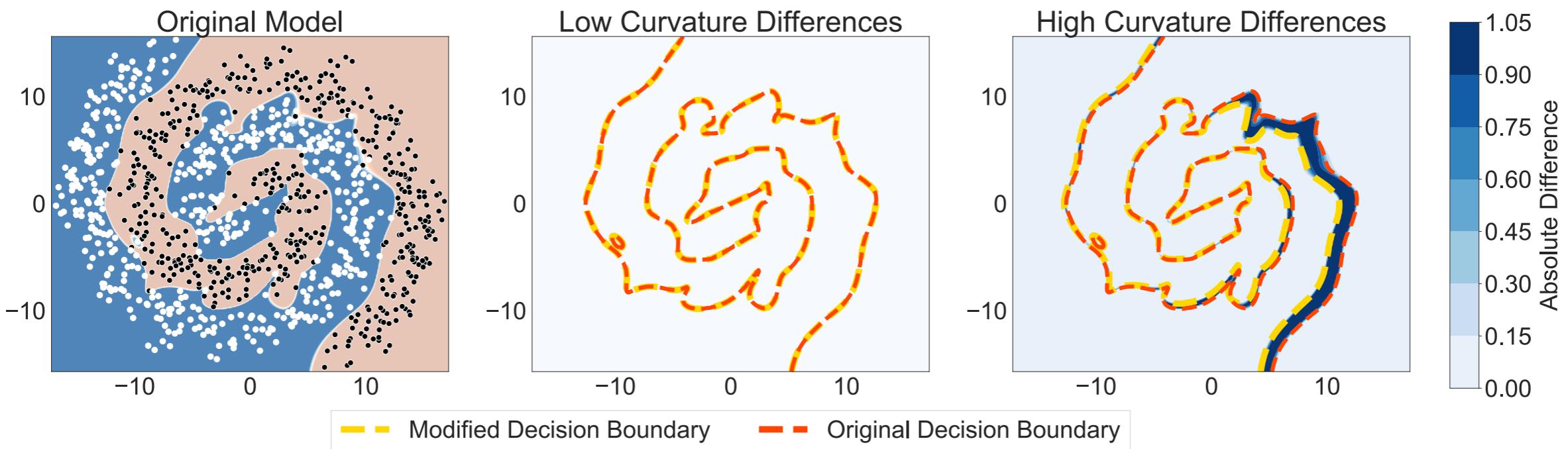
SUBSPACE INFERENCE

- ▶ A modular approach
 - ▶ Design subspace
 - ▶ Approximate posterior over parameters in that subspace
 - ▶ Sample from approximate posterior for bayesian model averaging

We can approximate posterior of 36 million dimensional WideResNet in 5D subspace and get state-of-the-art results!

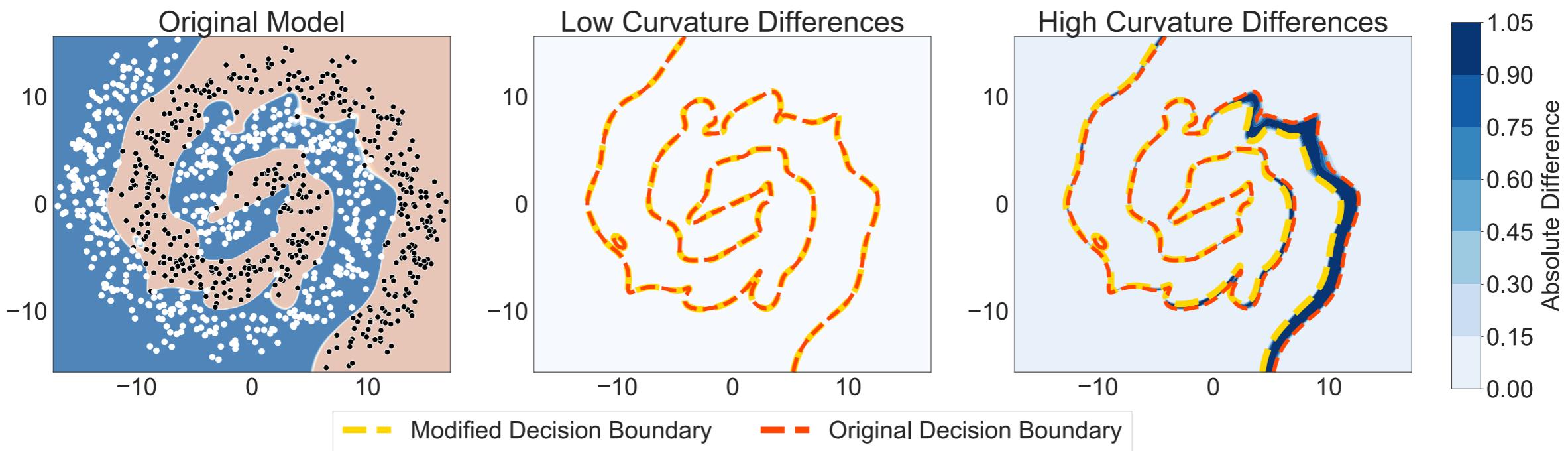
POSTERIOR CONTRACTION (REVISITED)

- ▶ If $N \gg p$, can we even learn interesting distributions in p dimensions?



POSTERIOR CONTRACTION (REVISITED)

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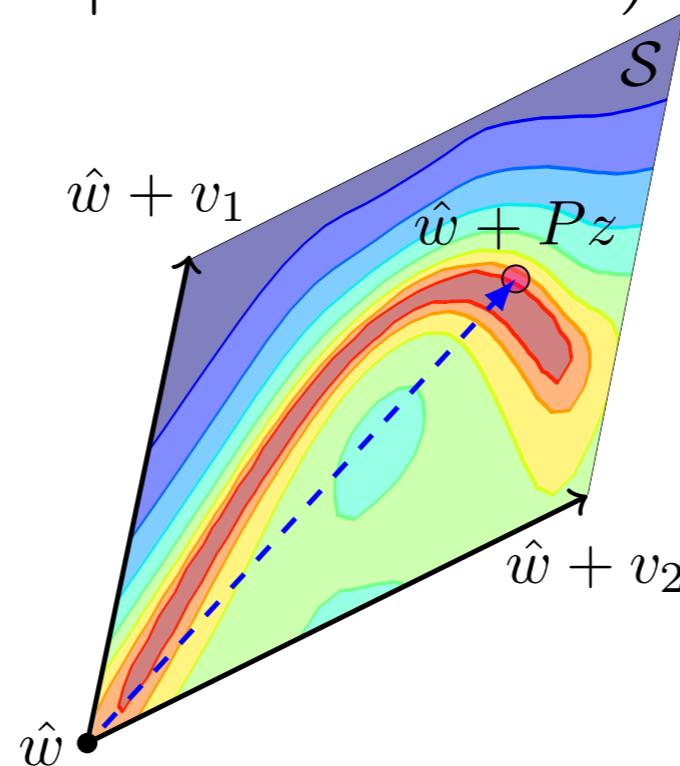


Probably not

CREATING THE SUBSPACE

- ▶ Choose shift \hat{w} and basis vectors $\{d_1, \dots, d_K\}$
- ▶ Define subspace $\mathcal{S} = \{w | w = \hat{w} + \underbrace{d_1 z_1 + \dots + d_K z_K}_{Pz}\}$
- ▶ Likelihood

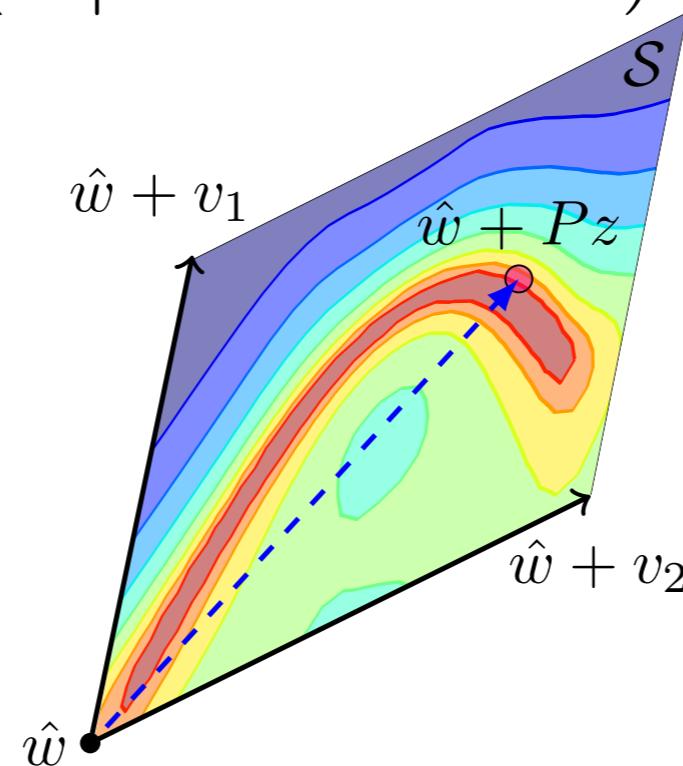
$$p(\mathcal{D}|z) = p_{\mathcal{M}}(\mathcal{D}|w = \hat{w} + Pz)^{1/T}$$



CREATING THE SUBSPACE

- ▶ Choose shift \hat{w} and basis vectors $\{d_1, \dots, d_K\}$
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- ▶ Likelihood

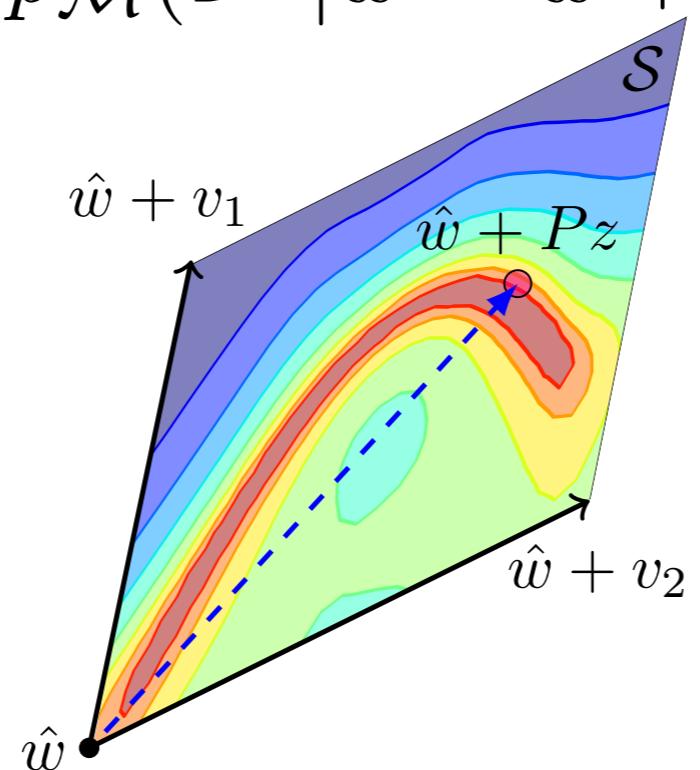
$$p(\mathcal{D}|z) = p_{\mathcal{M}}(\mathcal{D}|w = \hat{w} + Pz)^{1/T}$$



$T \gg 1$: to increase prior dependency & reduce effect of likelihood

INFERENCE IN THE SUBSPACE

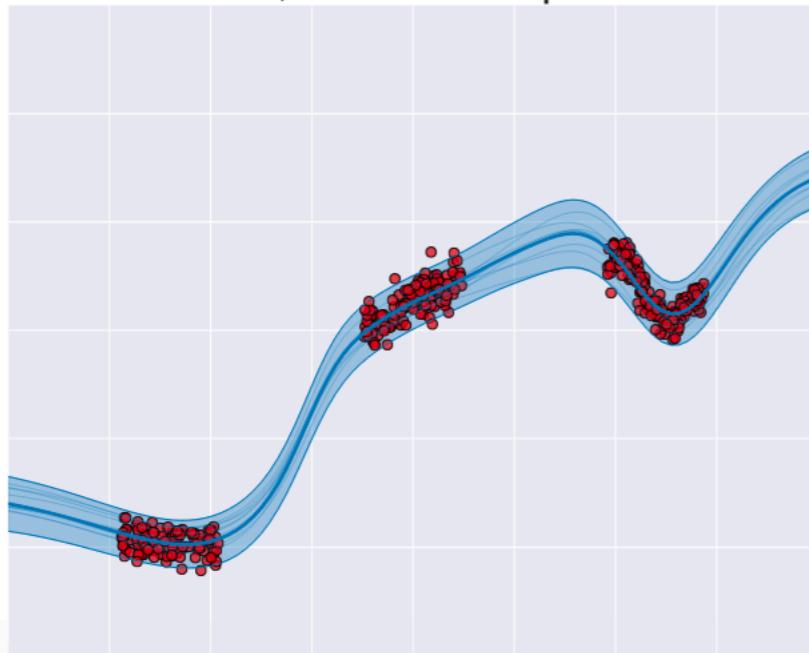
- ▶ Approximate inference over parameters
 - ▶ MCMC, VI, Normalizing Flows, ...
- ▶ Bayesian model averaging at test time
- ▶ $p(\mathcal{D}^* | \mathcal{D}) = \frac{1}{J} \sum_{j=1}^J p_{\mathcal{M}}(\mathcal{D}^* | w = \hat{w} + P\tilde{z}_j), \tilde{z}_j \sim q(\tilde{z} | \mathcal{D})$



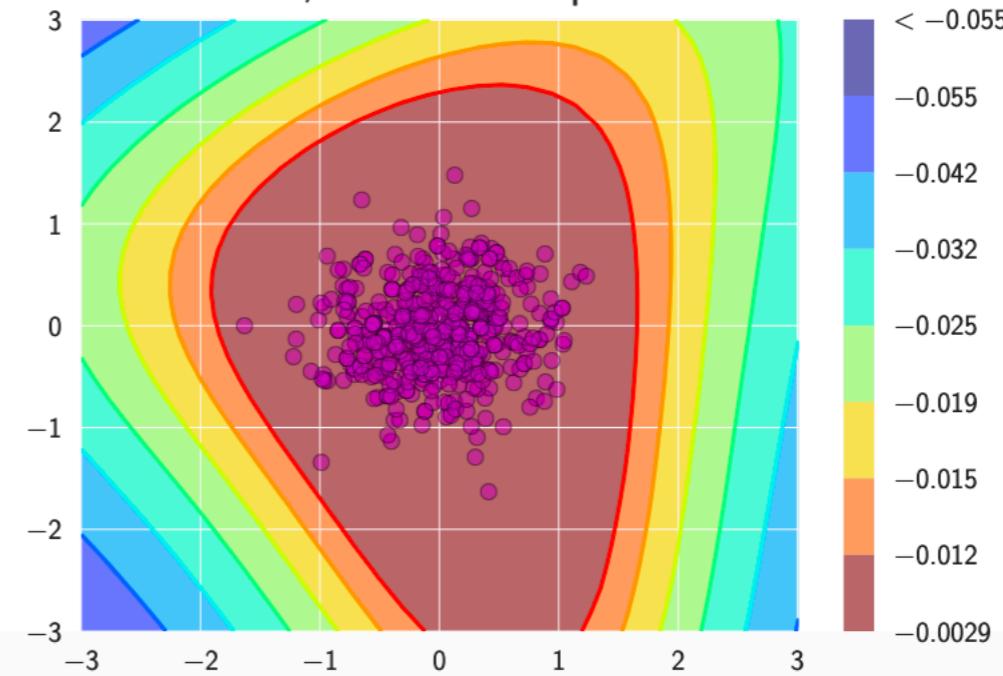
WHICH SUBSPACE? (RANDOM SUBSPACE)

- ▶ Random directions: $d_1, \dots, d_K \sim \mathcal{N}(0, I_K)$
- ▶ Use pre-trained solution as shift \hat{w}
- ▶ Subspace $S = \{w | w = \hat{w} + Pz\}$

Predictive Distribution
ESS, Random Subspace



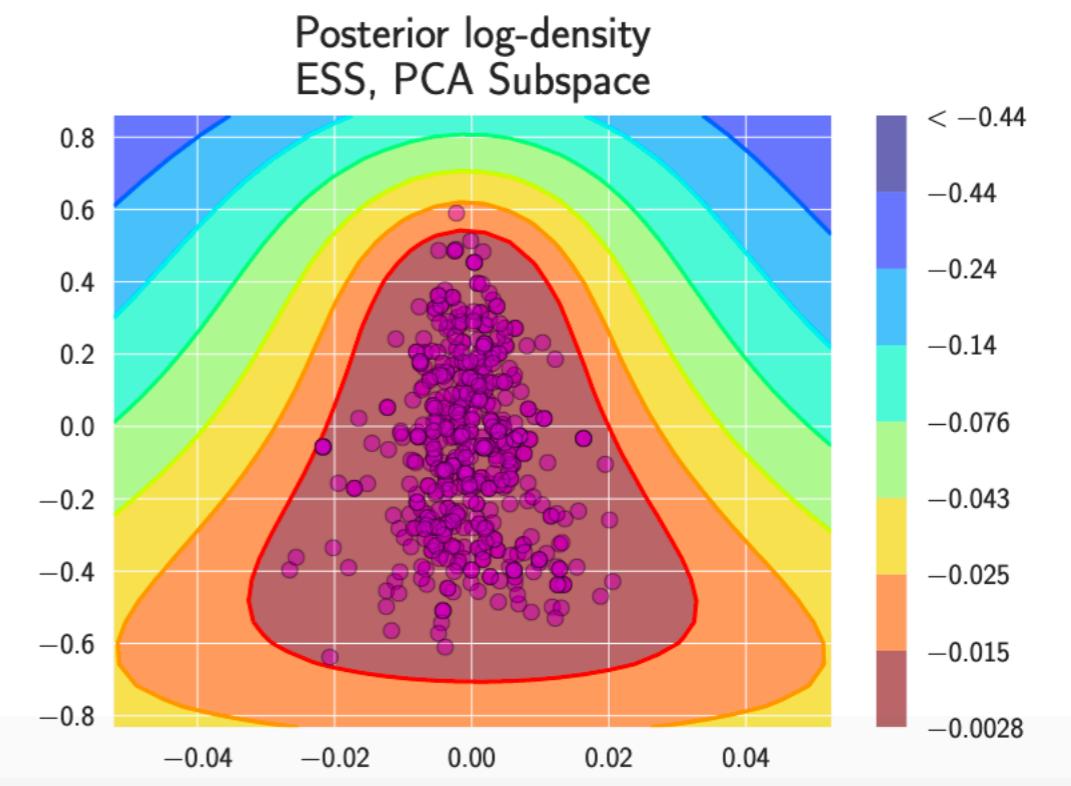
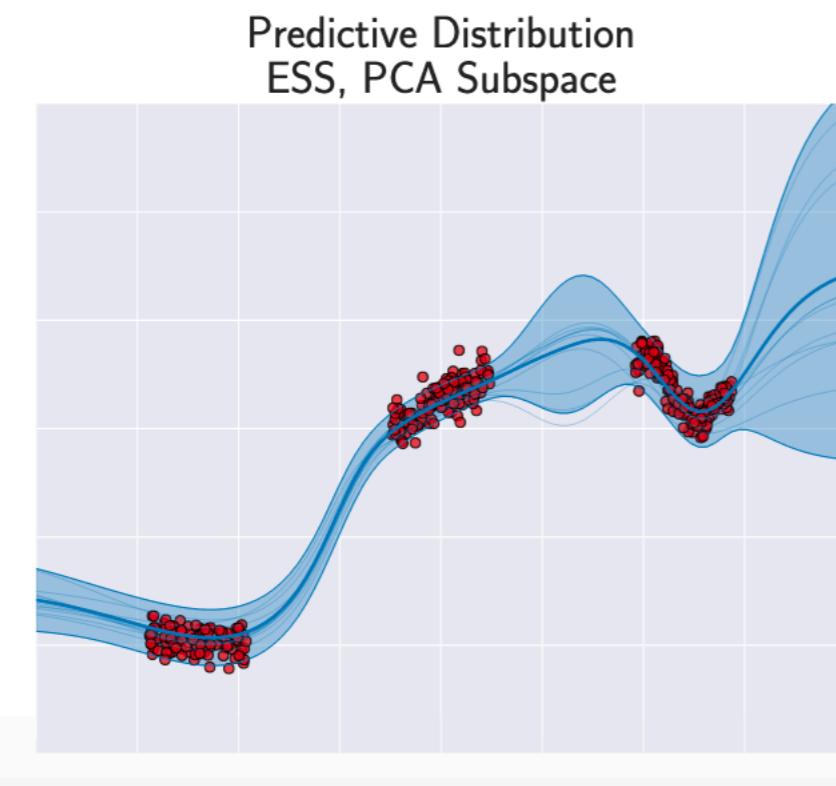
Posterior log-density
ESS, Random Subspace



WHICH SUBSPACE? (PCA OF THE SGD TRAJECTORY)

- ▶ Run SGD with high constant learning rate from a pre-trained solution
- ▶ Collect snapshots of weights
- ▶ Use SWA solution as shift
- ▶ $\{d_1, \dots, d_K\}$ – first K PCA components of vectors $\hat{w} - w_i$

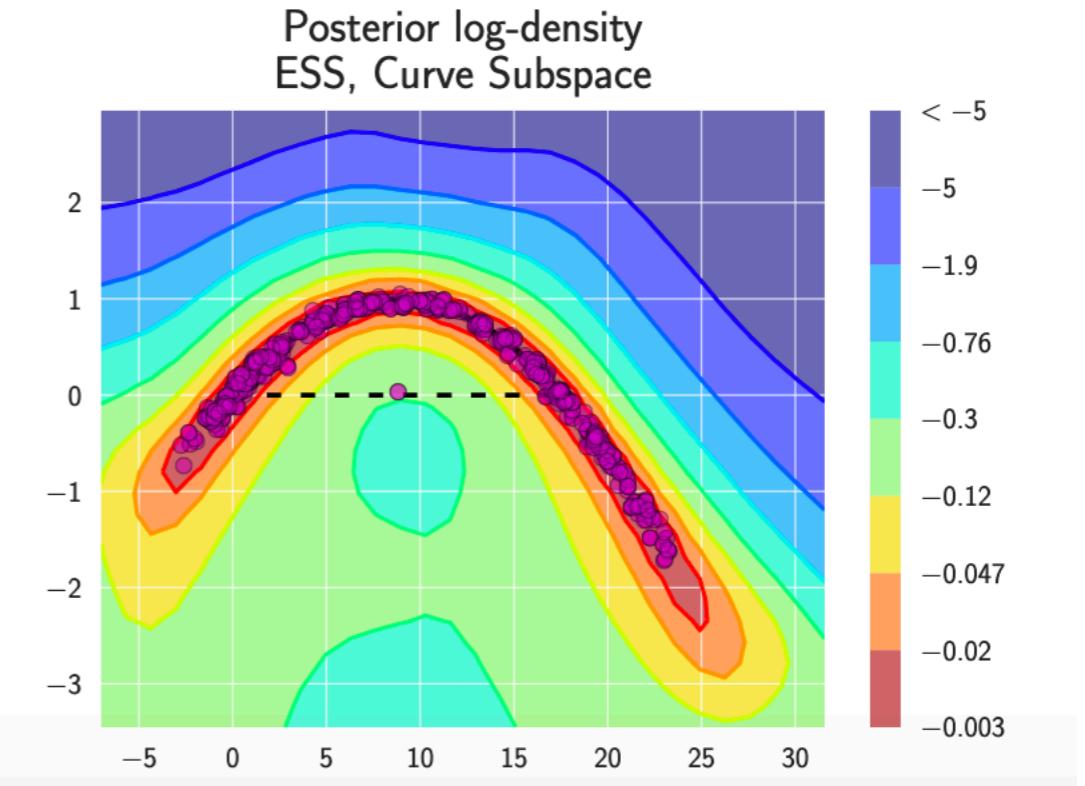
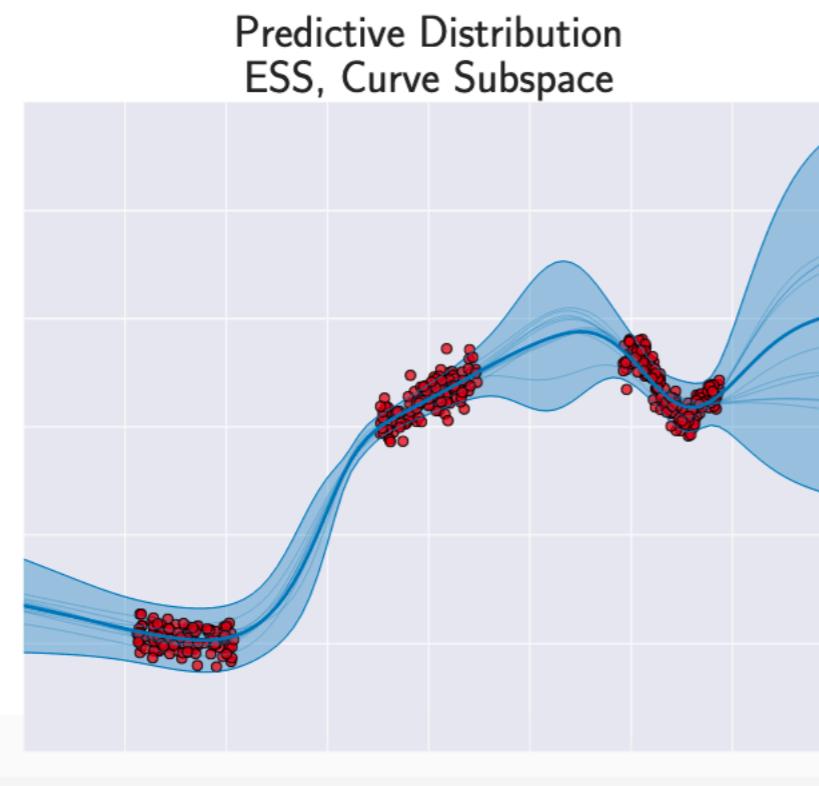
$$\hat{w} = \frac{1}{T} \sum_{i=1}^T w_i$$



WHICH SUBSPACE? (CURVES — GARIPOV ET AL, '18)

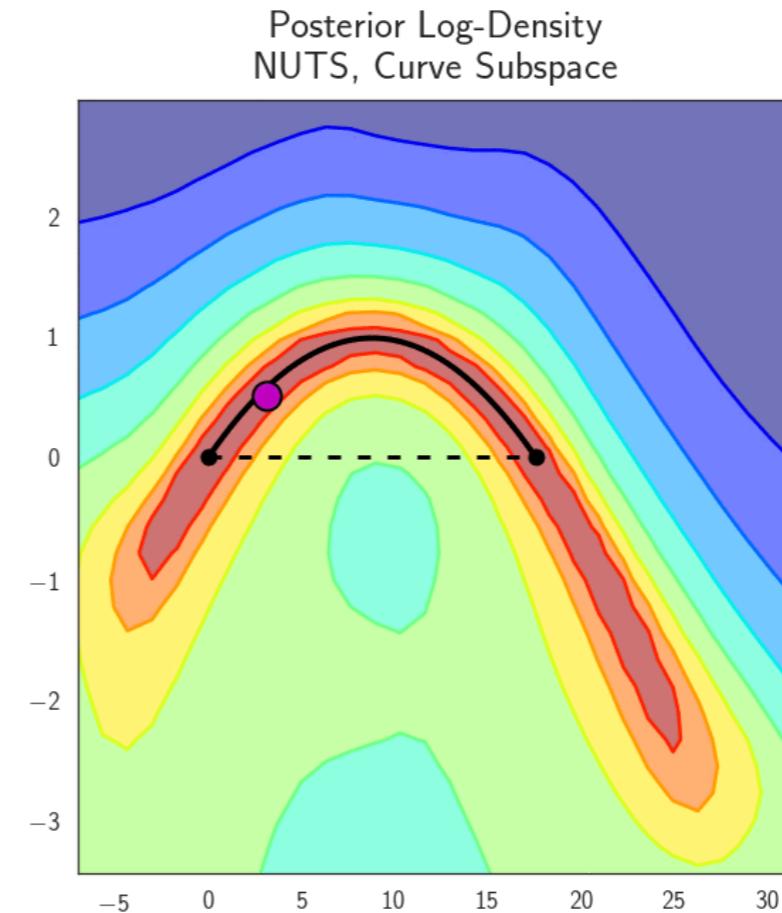
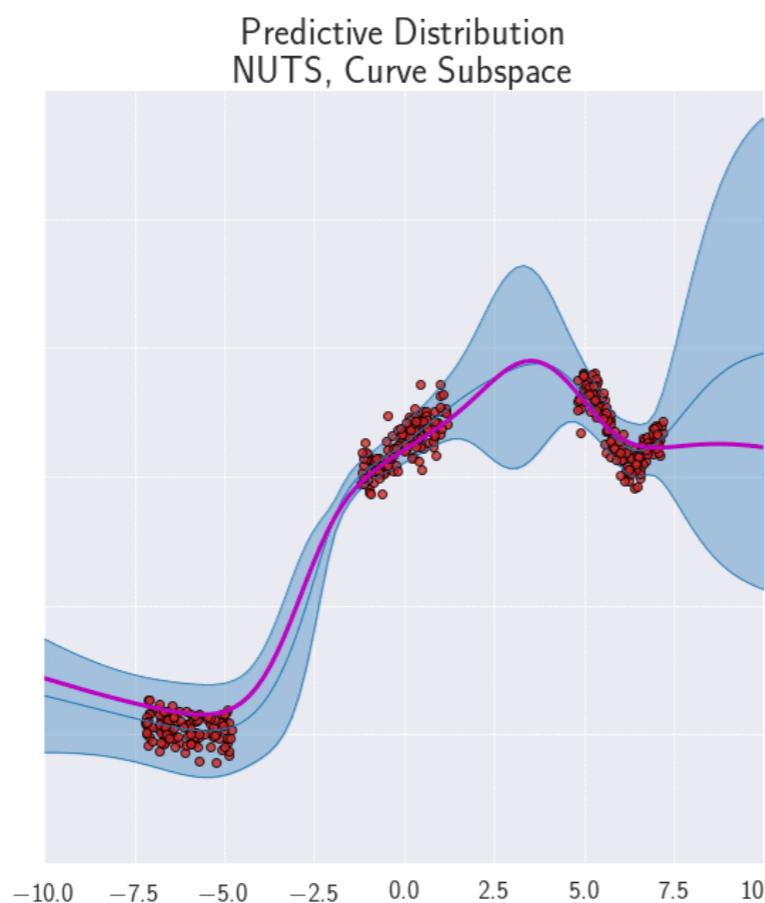
- ▶ Garipov et al, '18 proposed a method to find 2D subspaces containing a path of low loss between weights of two independently trained neural networks

$$\arg \min_{\theta} \mathbb{E}_{t \sim U(0,1)} (\mathcal{L}(\phi_{\theta}(t)))$$
$$\phi_{\theta}(t) = (1-t)^2 \hat{w}_1 + 2t(1-t)\theta + t^2 \hat{w}_2^2$$

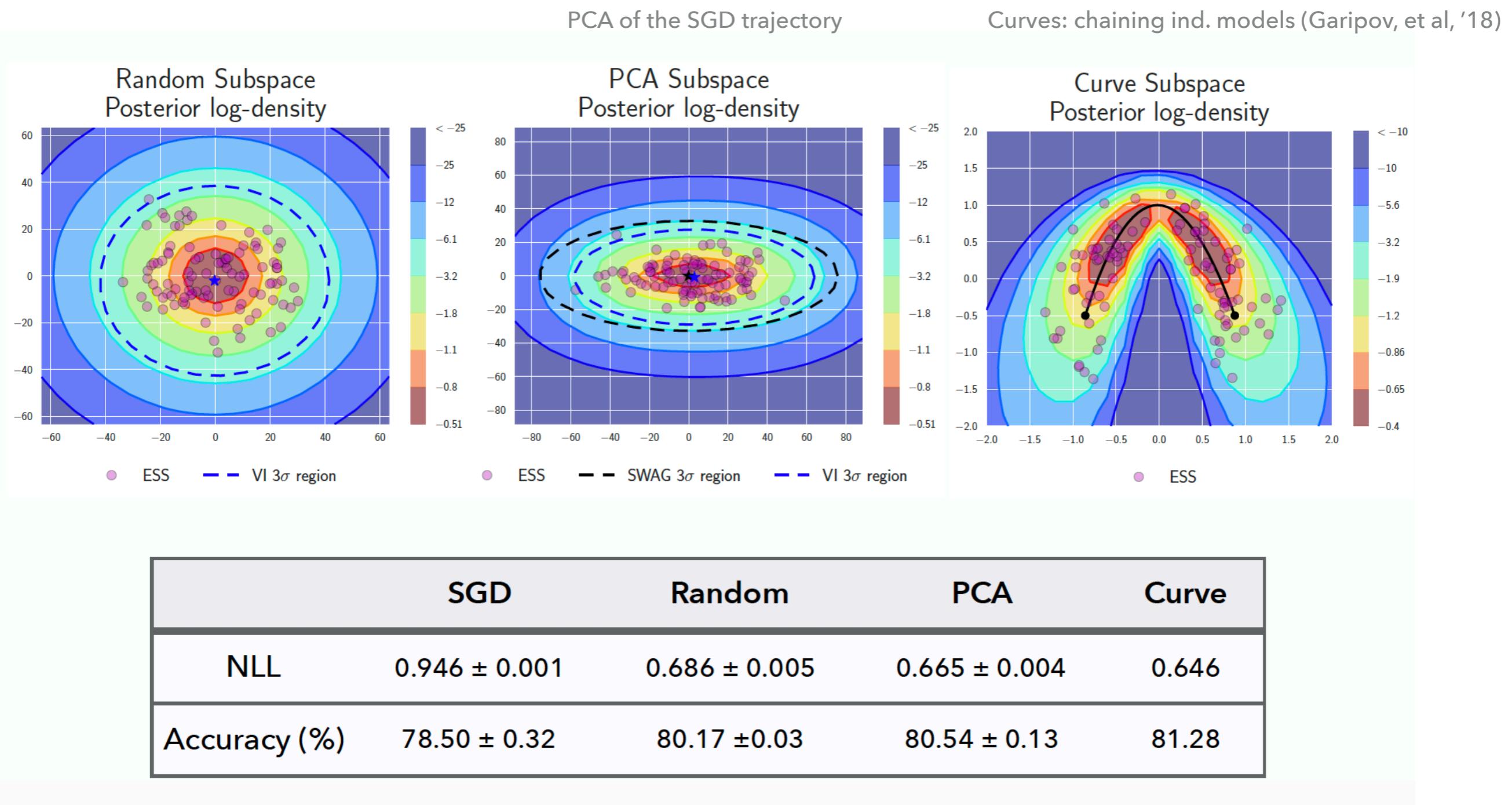


WHICH SUBSPACE? (CURVES — GARIPOV ET AL, '18)

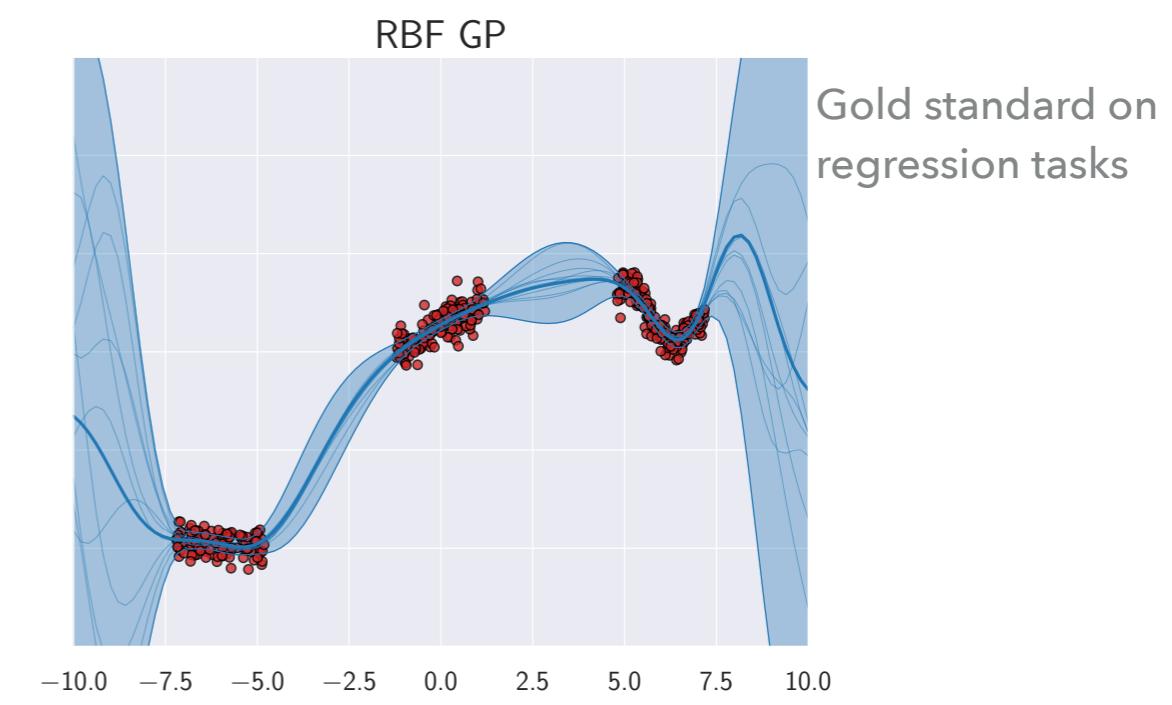
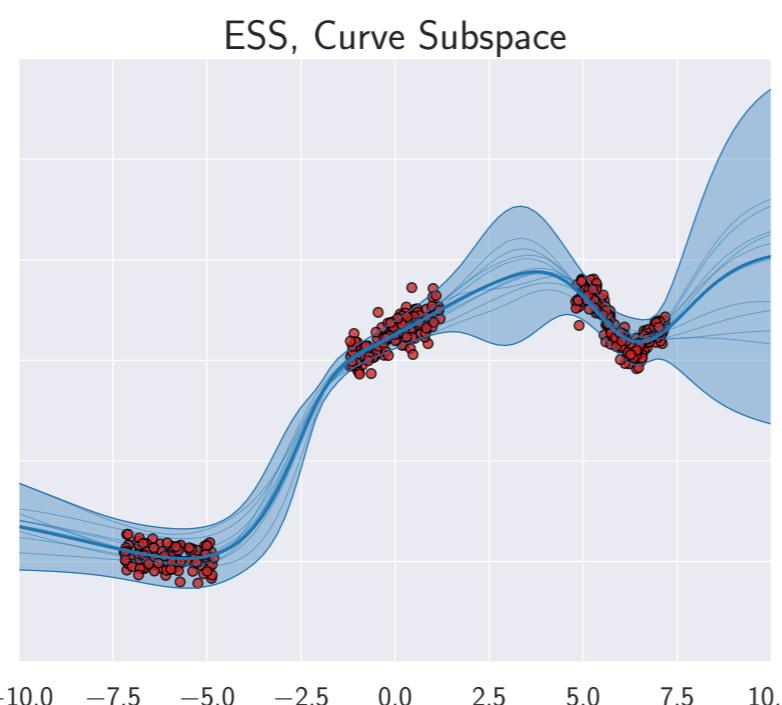
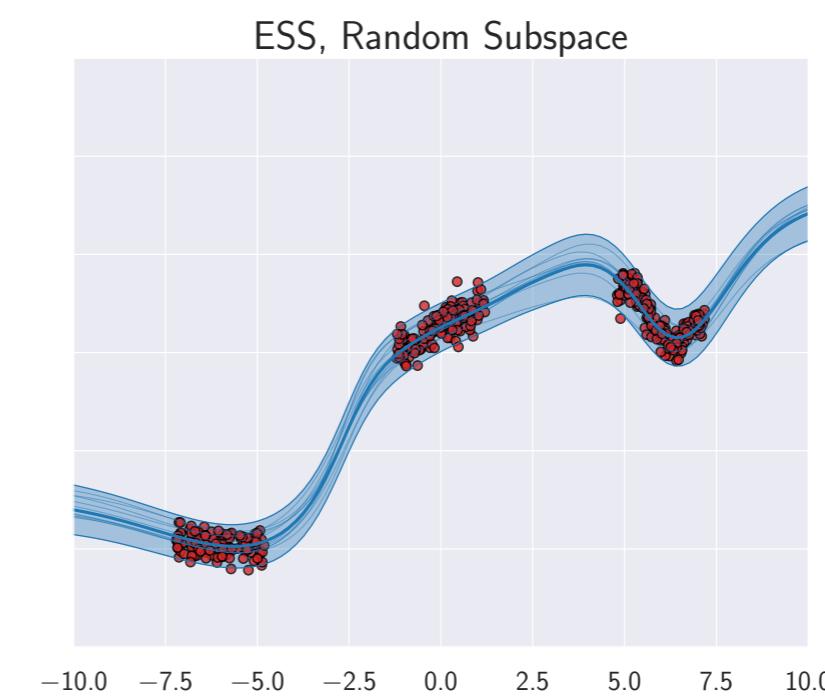
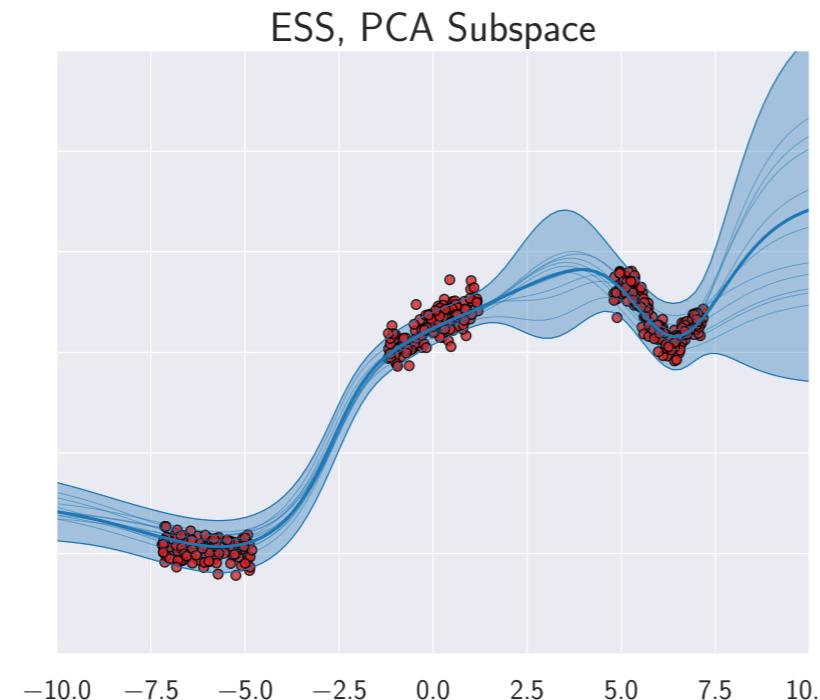
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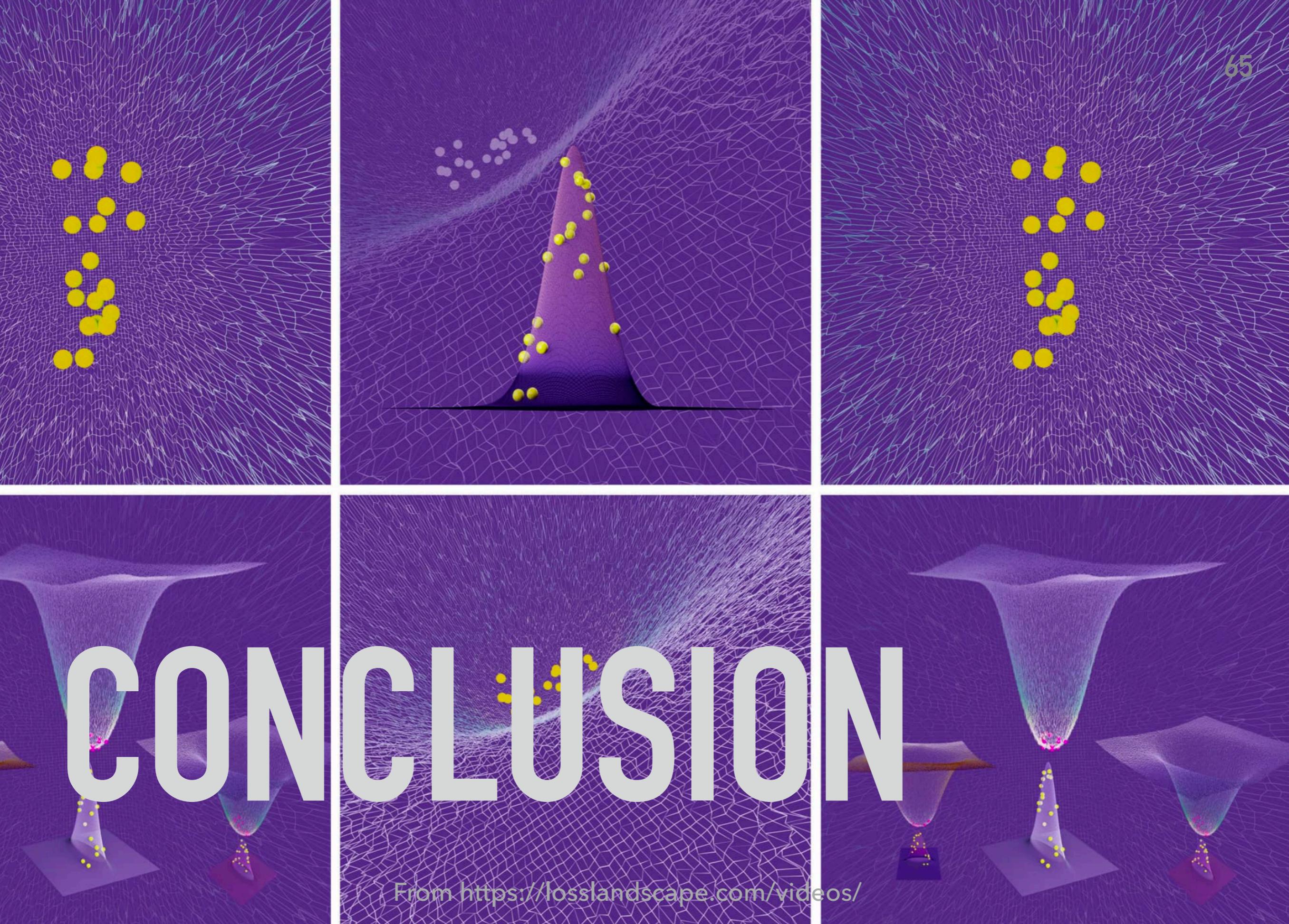


RESULTS (PRERESNET164, CIFAR100)



RESULTS - REGRESSION





BAYESIAN DEEP LEARNING: CHALLENGES

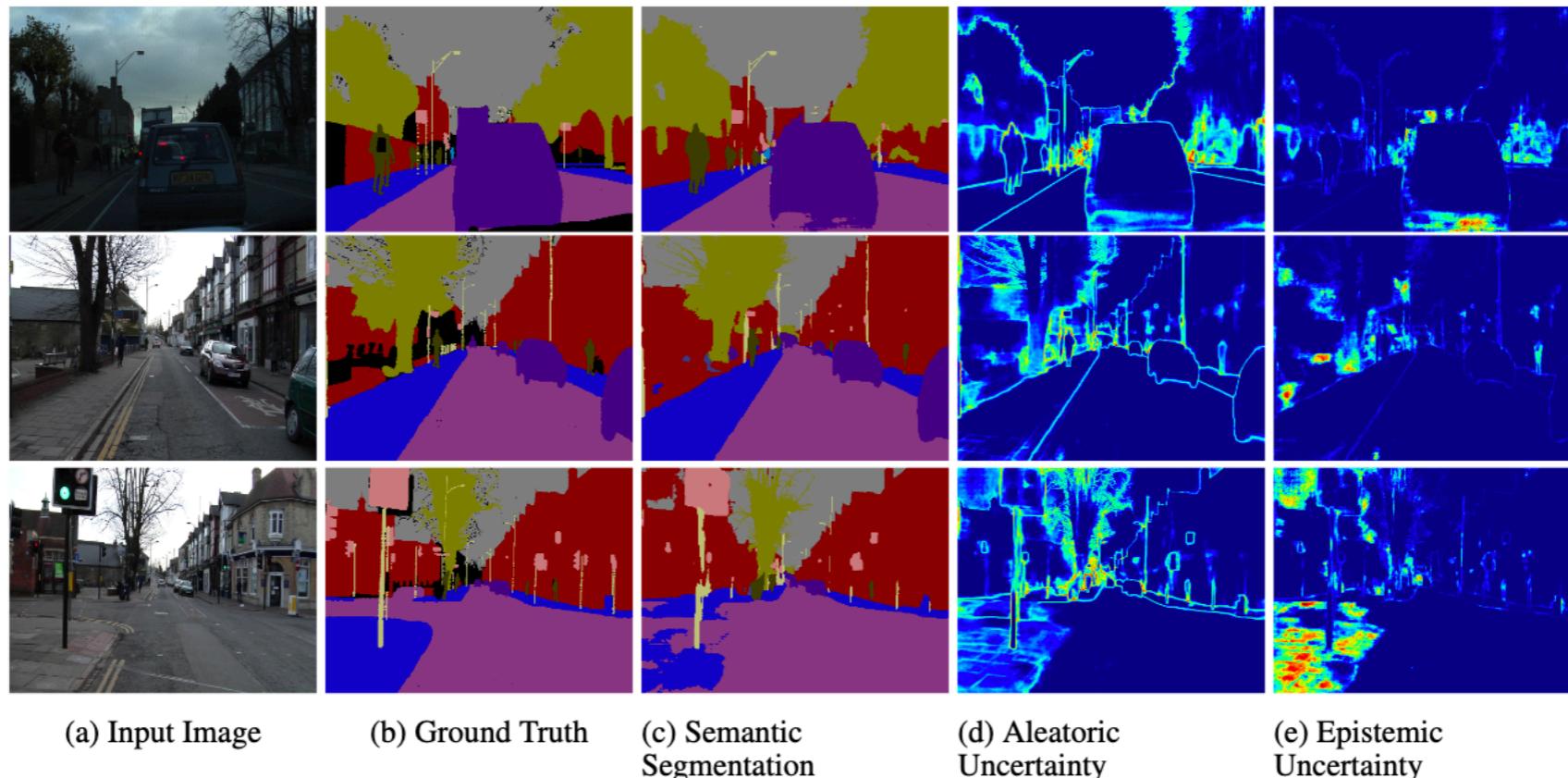
Bayesian inference for deep neural networks is extremely challenging

- ▶ Posterior is intractable Is the likelihood correct? Probably
- ▶ Millions of parameters What do these parameters mean? Care about functions instead
- ▶ Large datasets Can we run MCMC for 1 million steps on ImageNet?? We don't need to
- ▶ Unclear which priors to use Is the prior correct? Probably

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int_{w'} p(D|w')p(w')dw'}$$

BAYESIAN DEEP LEARNING: SUCCESSES

- ▶ But it doesn't mean we shouldn't try...



Again from Kendall & Gal, "What Uncertainties do we need for bayesian deep learning for computer vision?"

BAYESIAN DEEP LEARNING: PRIOR CHOICE

- ▶ Typically use a iid Gaussian prior $\mathcal{N}(0, \alpha^2 I)$
- ▶ Choices may not be adversarial...
- ▶ But also not fantastic...

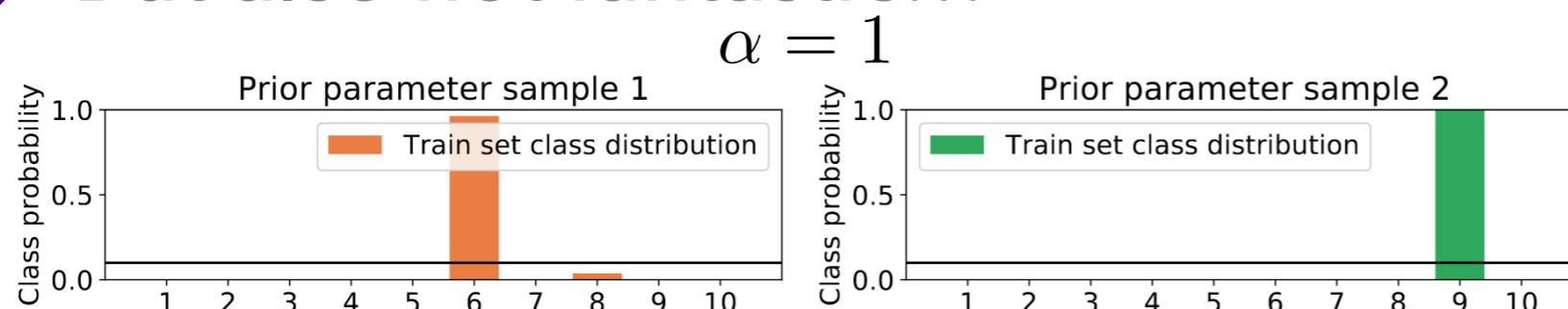


Figure 7. ResNet-20/CIFAR-10 typical prior predictive distributions for 10 classes under a $\mathcal{N}(0, I)$ prior averaged over the entire training set, $\mathbb{E}_{x \sim p(x)}[p(y|x, \theta^{(i)})]$. Each plot is for one sample $\theta^{(i)} \sim \mathcal{N}(0, I)$ from the prior. Given a sample $\theta^{(i)}$ the average training data class distribution is highly concentrated around the same classes for all x .

Figure 7 of Wenzel et al, '20 <https://arxiv.org/pdf/2002.02405.pdf>

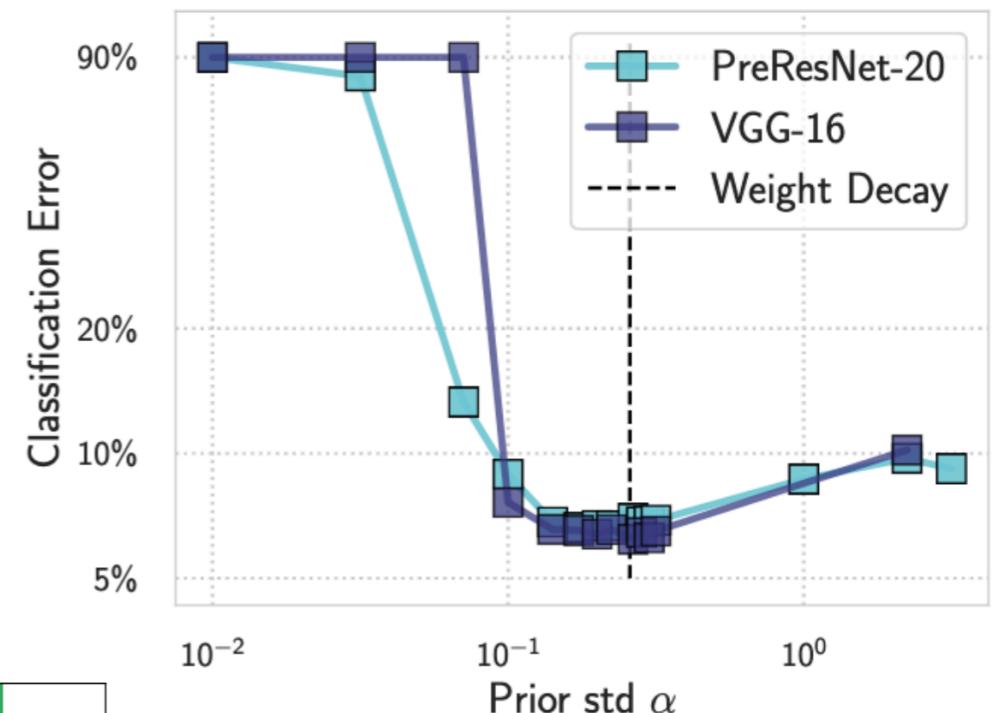


Figure 10g of Wilson & Izmailov '20

<https://arxiv.org/pdf/2002.08791.pdf>

BAYESIAN DEEP LEARNING: COMPARISONS

Method	Accuracy	Calibration	Train time	Test time	Code
Ensembles (Lakshminarayanan et al, '17)	high	Often more overconfident	K times standard training	K times slower	Train K models
Swag (Maddox et al, '19)	Slightly better than MAP	Less overconfident	Standard training	K times slower	Store models at train time
Dropout (Gal & Gharamani, '16)	About the same as MAP	Slightly less overconfident	Standard training	K times slower	Apply dropout at test time
VOGN (Osawa et al, '19)	Slightly worse than MAP?*	Less overconfident	2x standard training	K times slower	Modify Adam

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*: see figure 4, table 1 of Osawa et al, '19 (<https://arxiv.org/pdf/1906.02506.pdf>)

QUESTIONS?

Slides at https://wjmaddox.github.io/assets/BNN_tutorial_CILVR.pdf

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REFERENCE (VARIATIONAL INFERENCE)

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Li, Yingzhen, and Yarin Gal. "Dropout inference in Bayesian neural networks with alpha-divergences." *Proceedings of the 34th International Conference on Machine Learning-Volume 70*. JMLR.org, 2017.

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Li, Yingzhen, and Yarin Gal. "Dropout inference in Bayesian neural networks with alpha-divergences." *Proceedings of the 34th International Conference on Machine Learning-Volume 70*. JMLR.org, 2017.

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