BML Lecture #7

Bayesian deep learning

Julyan Arbel

Bayesian deep learning

Bayesian neural networks

Introduction

- Bayesian model averaging, Maximum a posteriori = Regularized maximum likehood

Distribution properties

- Wide limits, Gaussian process, sub-Weibull units

Approximations

- Laplace approximation, Variational inference, Monte Carlo dropout

Some recent works

Implementation: Pyro & PyTorch

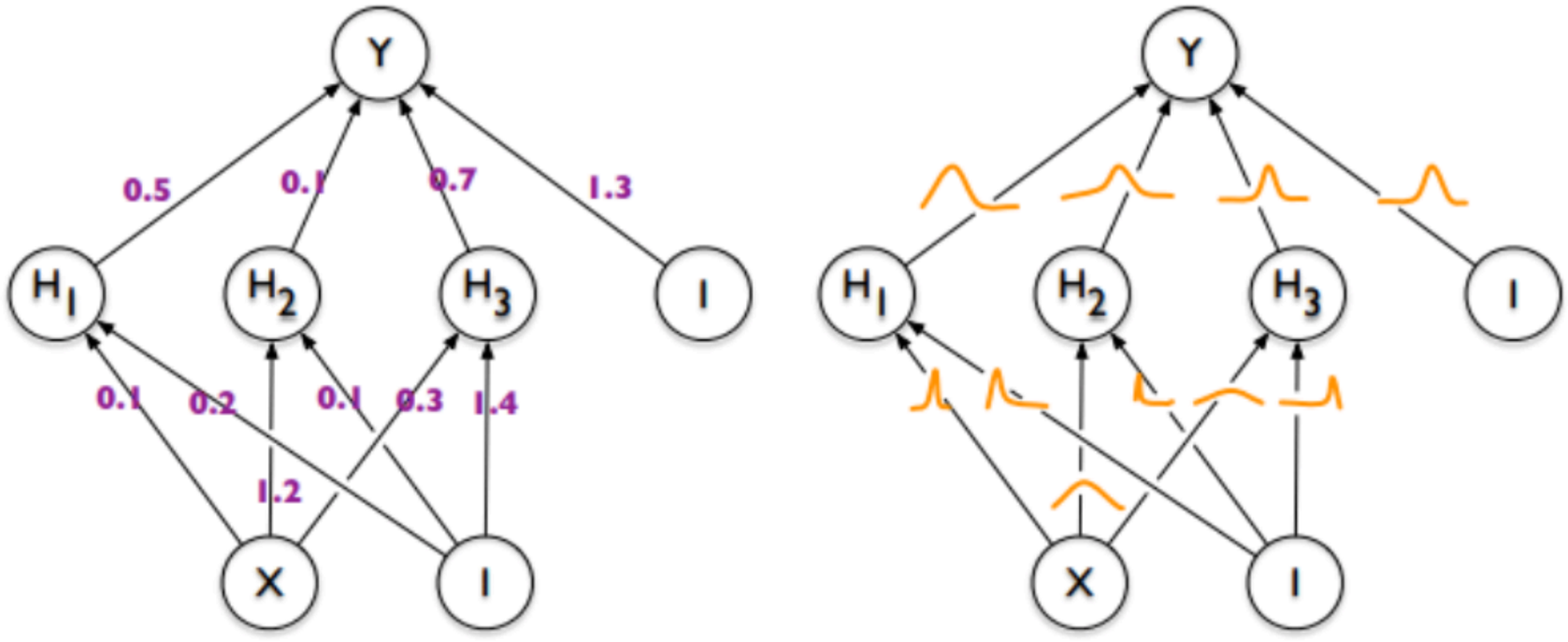
Bayesian deep learning

Bayesian neural networks: objectives

- Learn why Bayesian Neural networks are useful and exciting
- Understand how they're different from normal neural networks
- Appreciate how the uncertainty metrics you can obtain are a major advantage
- Install a library to start work with all things random

Introduction

- Bayesian model averaging
- Maximum a posteriori = Regularized maximum likehood



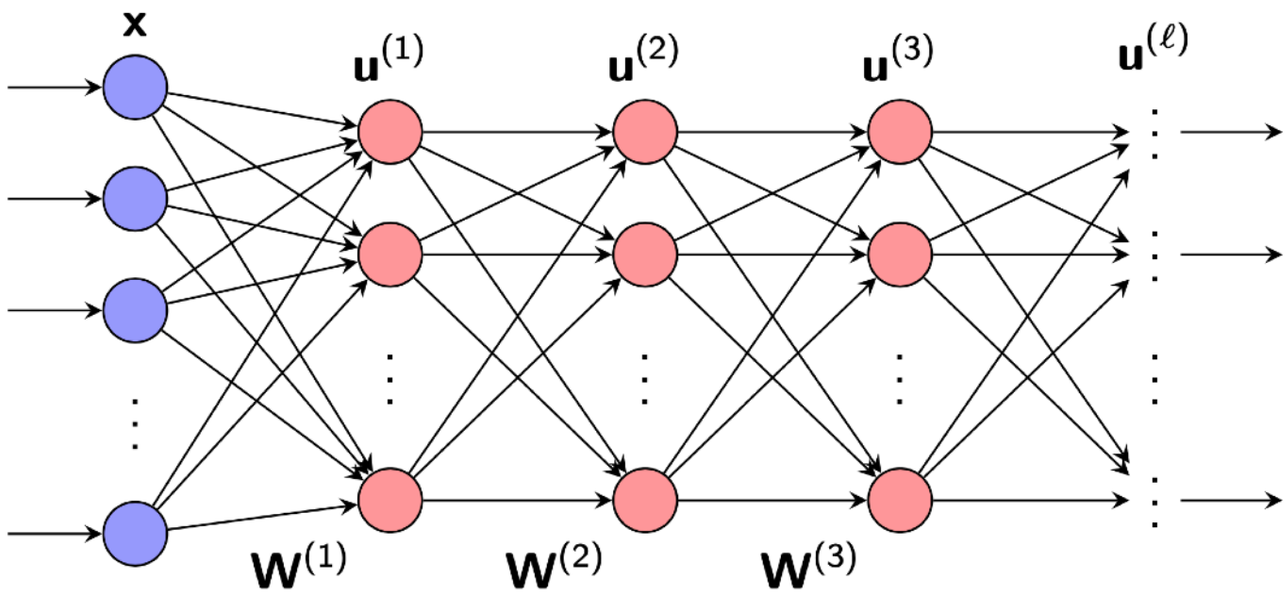
Standard DNN

Bayesian DNN

"Weight Uncertainty in Neural Networks" by Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, Daan Wierstra

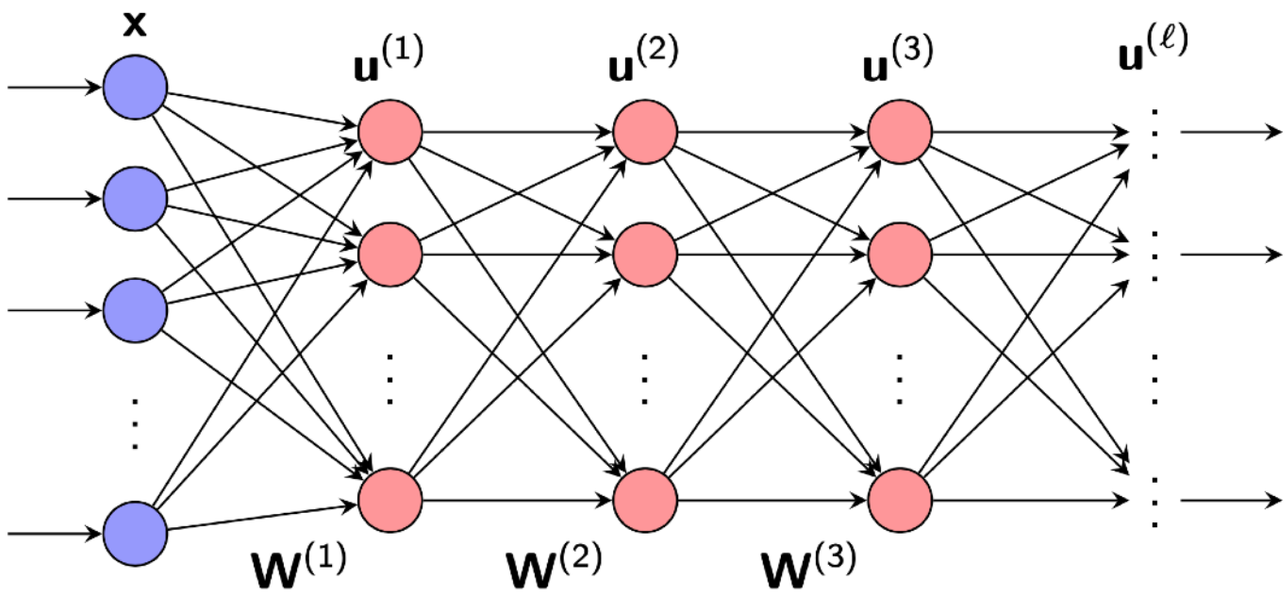
BAYESIAN NEURAL NETWORKS

DEEP NEURAL NETWORK



$$\boldsymbol{g}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{W}^{(\ell)}\boldsymbol{h}^{(\ell-1)}(\boldsymbol{x}),$$
$$\boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \phi(\boldsymbol{g}^{(\ell)}(\boldsymbol{x})).$$

DEEP NEURAL NETWORK



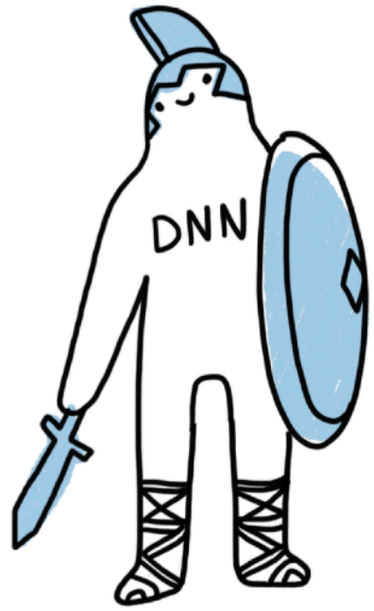
$$L(f(\mathbf{x}), \mathbf{y})$$

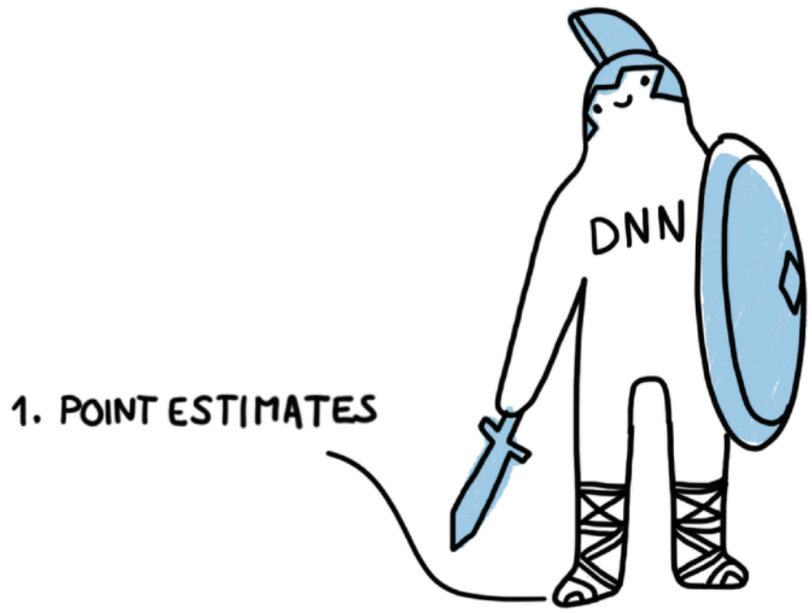
Forward pass:

$$\boldsymbol{g}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{W}^{(\ell)}\boldsymbol{h}^{(\ell-1)}(\boldsymbol{x}),$$
$$\boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \phi(\boldsymbol{g}^{(\ell)}(\boldsymbol{x})).$$

Back-propagation of the gradients:

$$\boldsymbol{\delta}^{(\ell)} = \frac{\partial L}{\partial \mathbf{h}^{(\ell)}} = \phi'(\mathbf{g}^{(\ell)})\boldsymbol{\delta}^{\ell+1}\mathbf{W}^{\ell+1},$$
$$\frac{\partial L}{\partial \mathbf{W}^{(\ell)}} = \boldsymbol{\delta}^{(\ell)}\phi(\mathbf{g}^{(\ell-1)})\,.$$


DNN


DNN
1. POINT ESTIMATES

DNN

BOXER

PUG

DALMATIAN

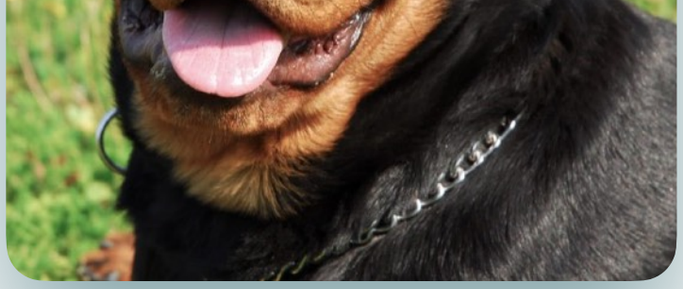
BULLDOG

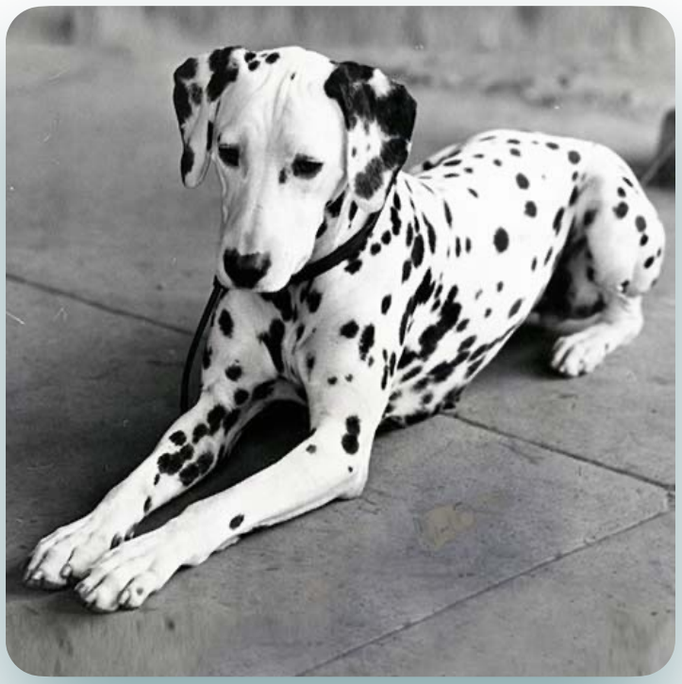
ROTTWEILER

LABRADOR

CHIHUAHUA

informatics mathematics





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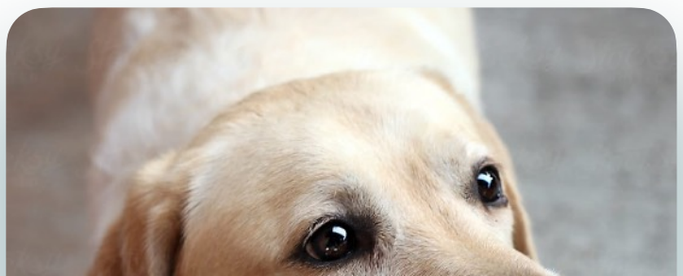

informatics mathematics
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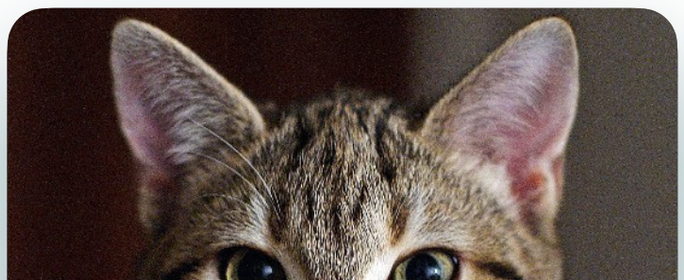

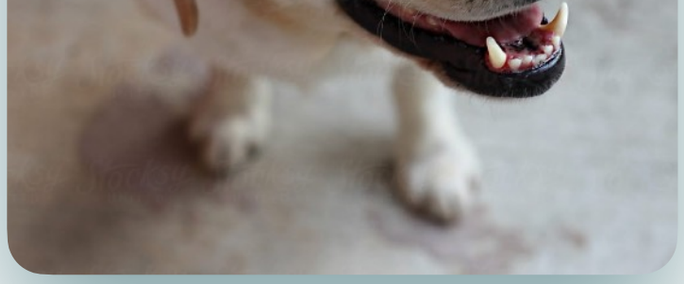

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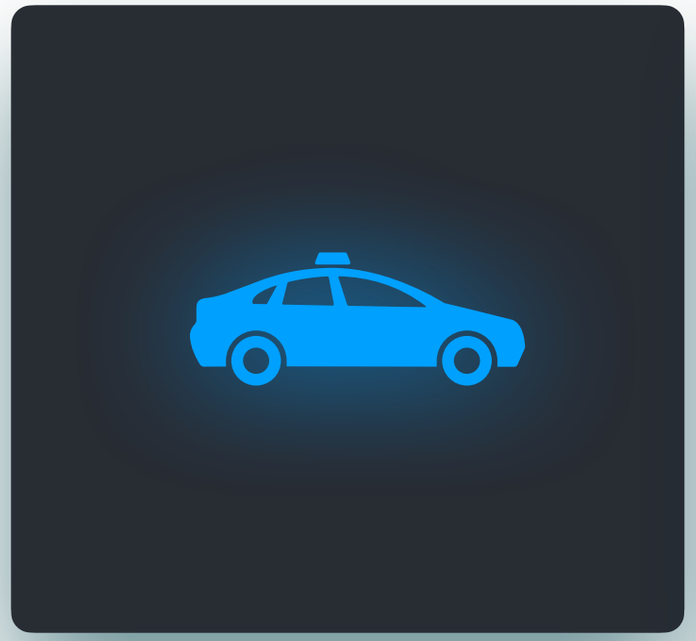
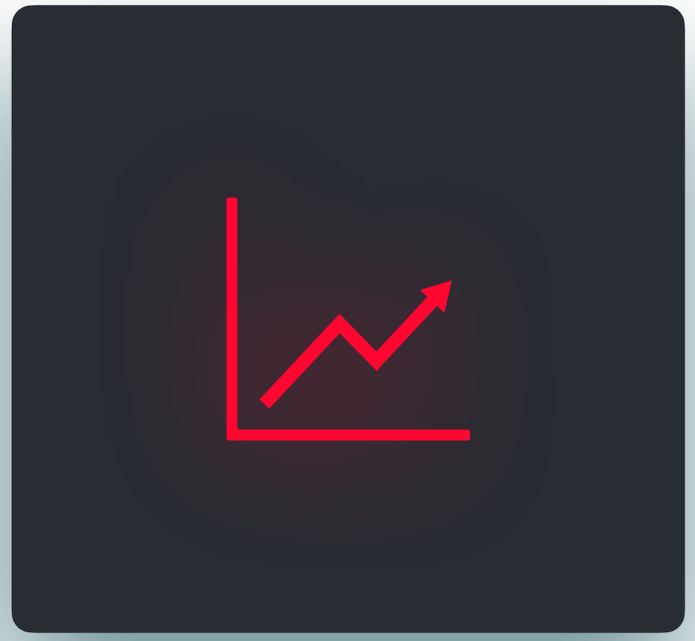
informatics mathematics





informatics mathematics

Solution: put a prior on weights, $w^{(i)} \sim \pi$

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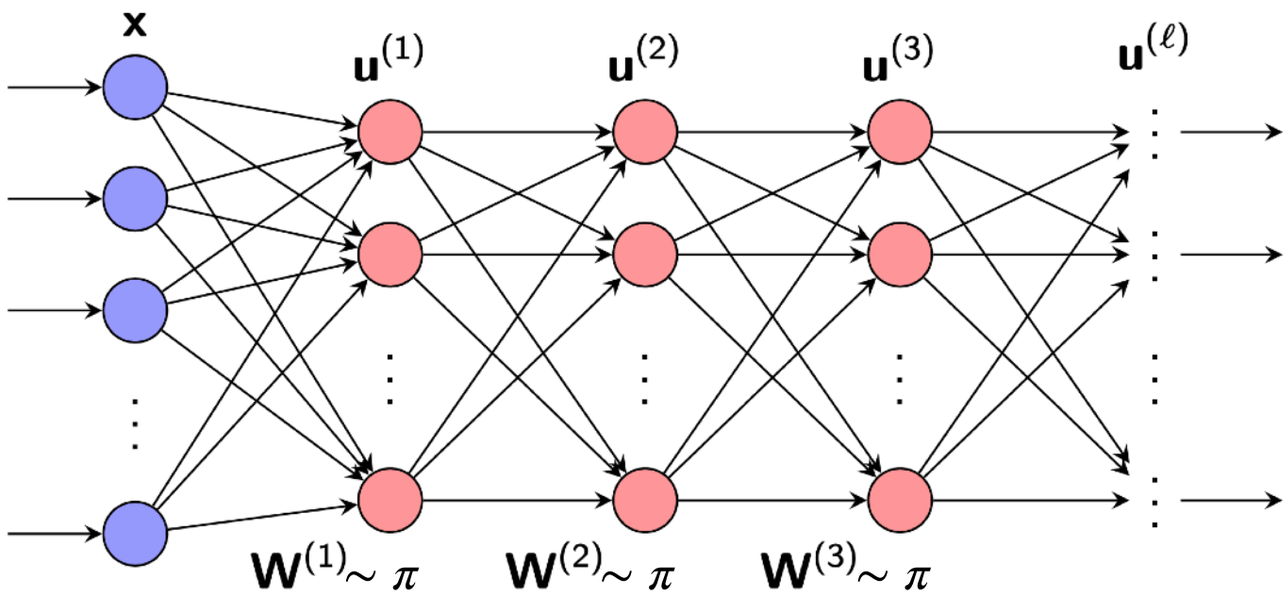
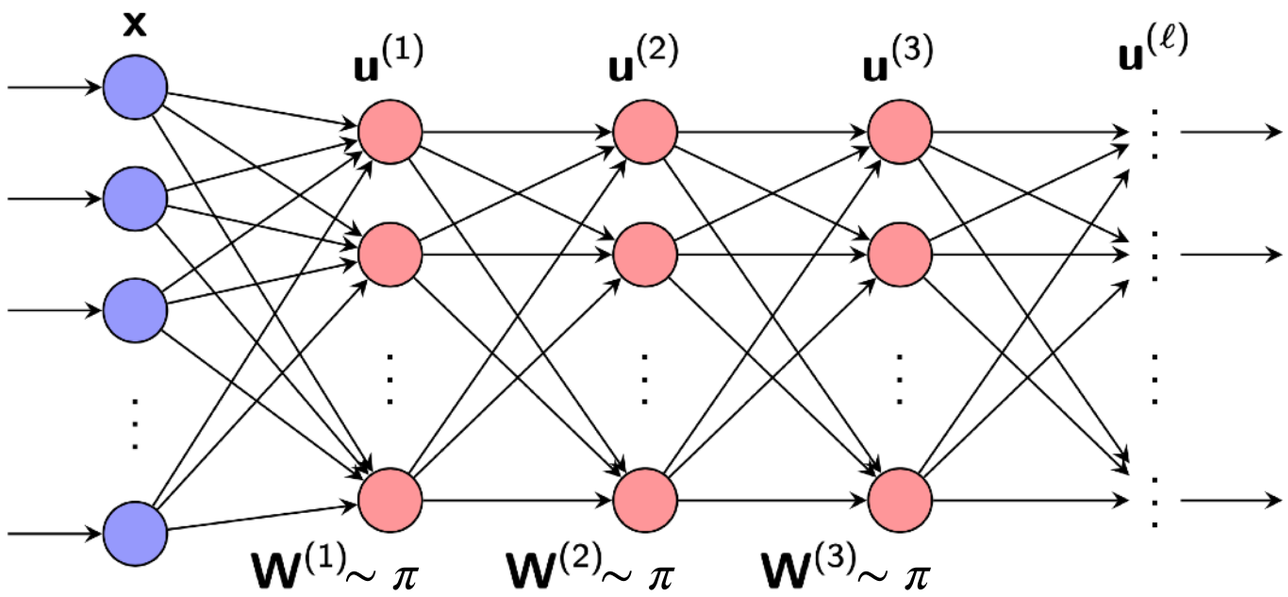


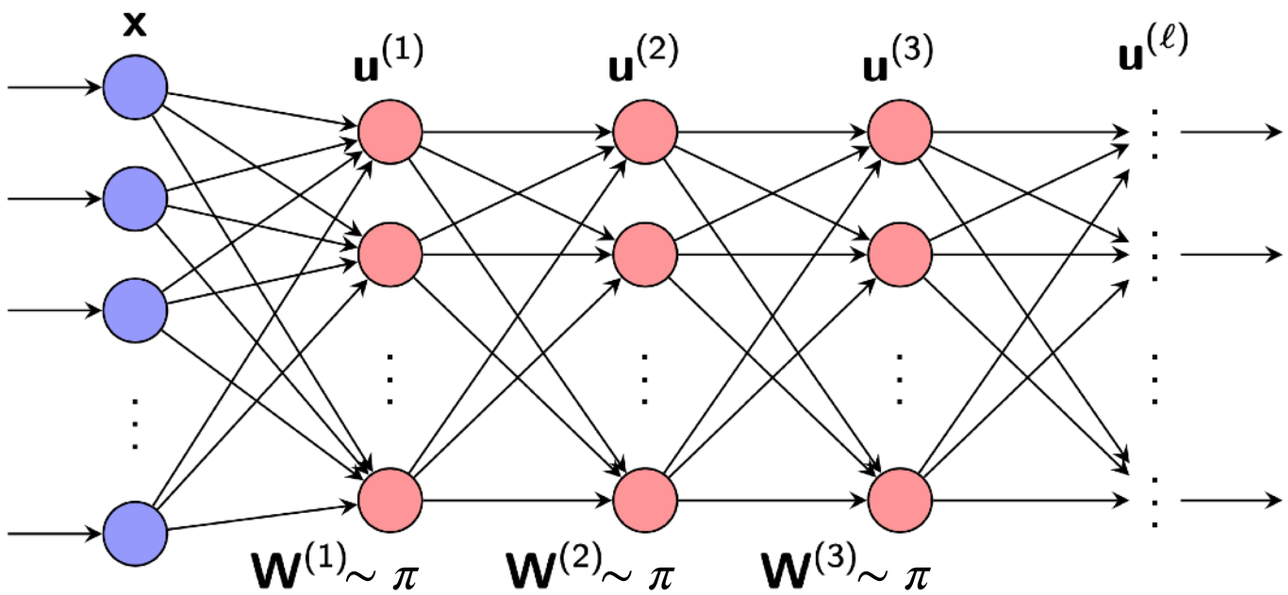
Solution: put a prior on weights, $\mathrm{w}^{(i)} \sim \pi$ ⟶ Bayesian Neural Networks



Posterior predictive

$$\pi(\mathbf{y} \mid \mathbf{x}, \mathscr{D})$$

Solution: put a prior on weights, $\mathrm{w}^{(i)} \sim \pi$ ⟶ Bayesian Neural Networks



Posterior predictive

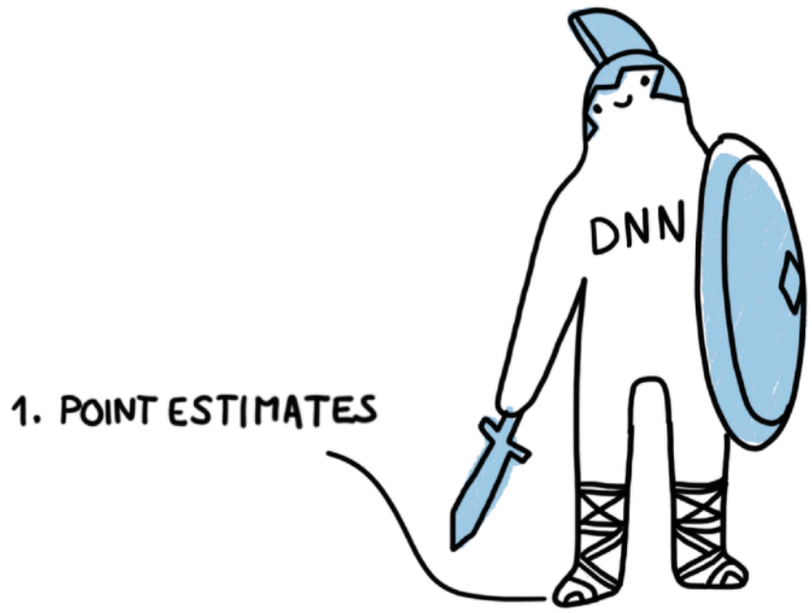
$$\pi(\mathbf{y} \mid \mathbf{x}, \mathscr{D})$$

Advantages:

- Allows to model uncertainty
- Represents a standard neural network

Problems:

- Intractable for large datasets
- Have to choose a prior


DNN
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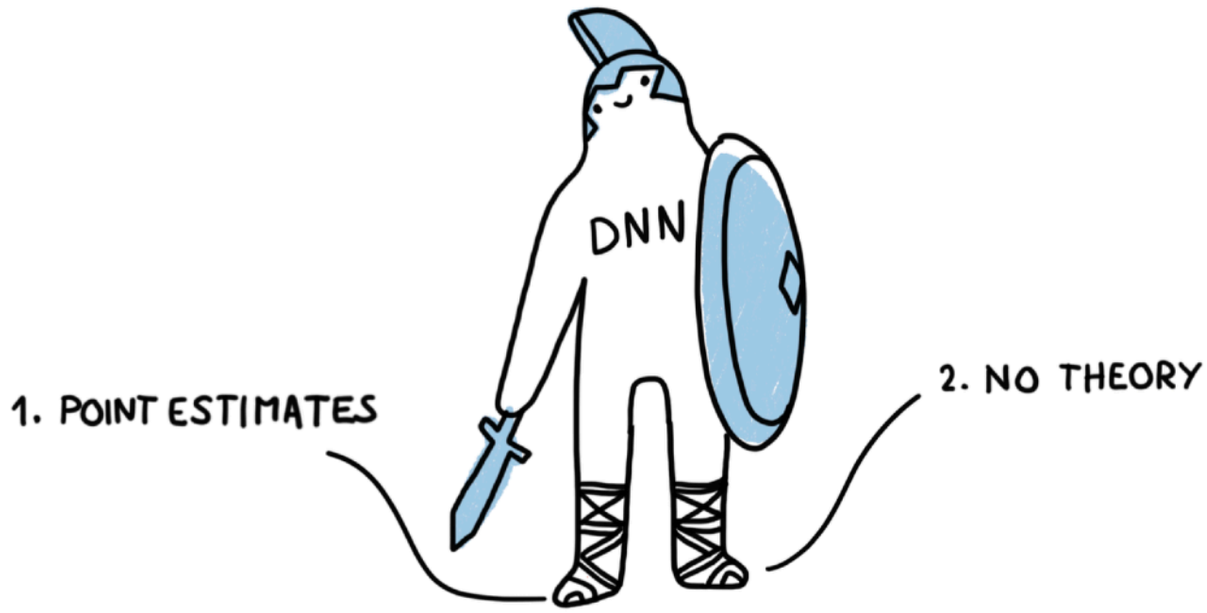
DNN
1. POINT ESTIMATES
2. NO THEORY

Distribution properties

- Wide limits
- Gaussian process limit
- Stable process limit
- Sub-Weibull units

WHAT DO WE WANT?

- To propagate information: avoid activations explosion/ collapse
- To back-propagate information: avoid gradients explosion/collapse

WHAT DO WE WANT?

- To propagate information: avoid activations explosion/ collapse
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We can try to tackle those problems at initialization!

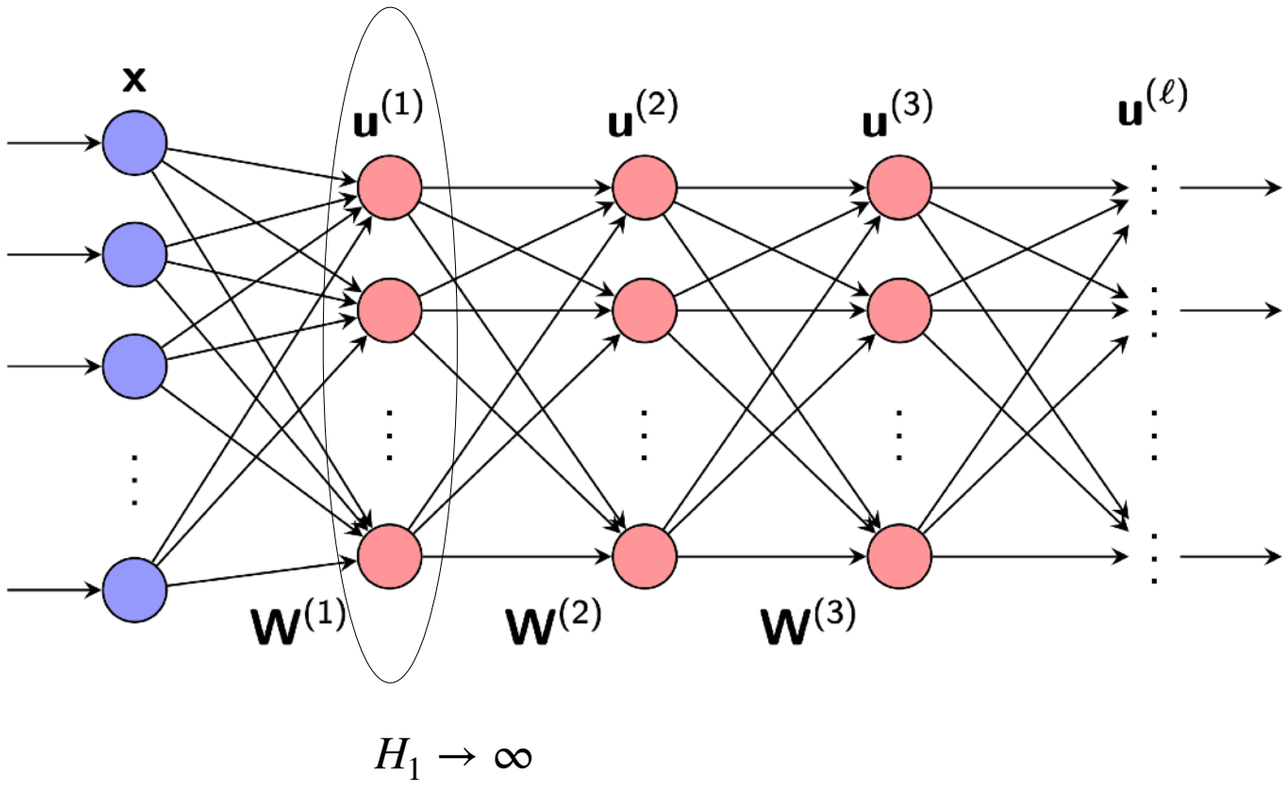
What are the good initializations techniques for $\mathbf{W}^{\ell}$?

Let’s study the behaviour of priors in BNNs and find a good prior distribution!

Get prior -> get initialization!

BNN AND GAUSSIAN PROCESS

WIDE REGIME = NUMBER OF HIDDEN UNITS TENDS TO INFINITY



Marginal prior distribution of $\mathbf{u}^{(1)}$ converges to a Gaussian process (CLT)

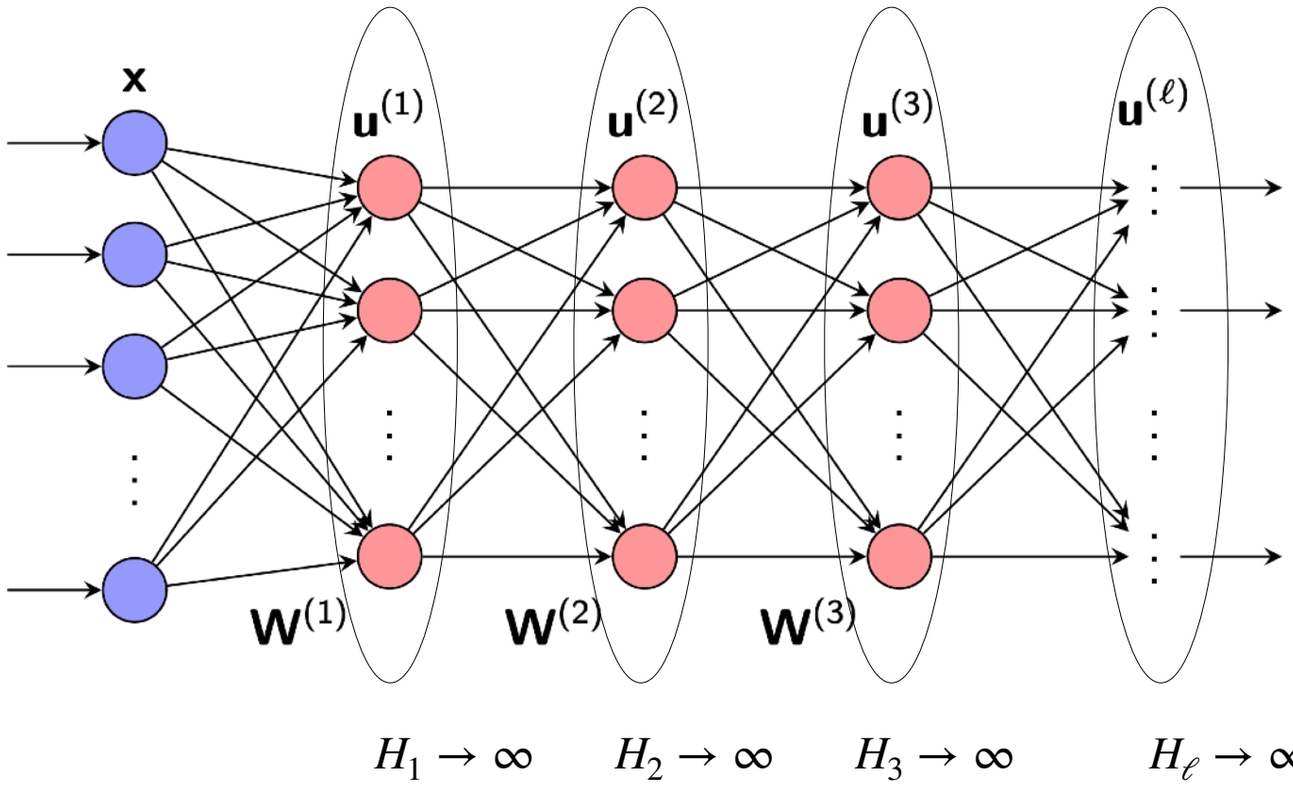
$\Rightarrow$ Distributions $u_i^{(2)}$ are dependent

Similar convergence for $\mathbf{u}^{(2)}$?

[R. Neal, PhD dissertation (1996)]

Gaussian distribution on weights: $\mathbf{W}^{(i)} \sim \mathcal{N}\left(0, \frac{\sigma_w^2}{H_i}\right)$

WIDE REGIME = NUMBER OF HIDDEN UNITS TENDS TO INFINITY



$\Rightarrow$

Marginal prior distribution of $\mathbf{u}^{(1)}$ converges to a Gaussian process

[R. Neal, PhD dissertation (1996)]

Marginal prior distribution of $\mathbf{u}^{(\ell)}$ converges to a Gaussian process

Matthews et al. (ICLR, 2018) Gaussian process behaviour in wide deep neural networks

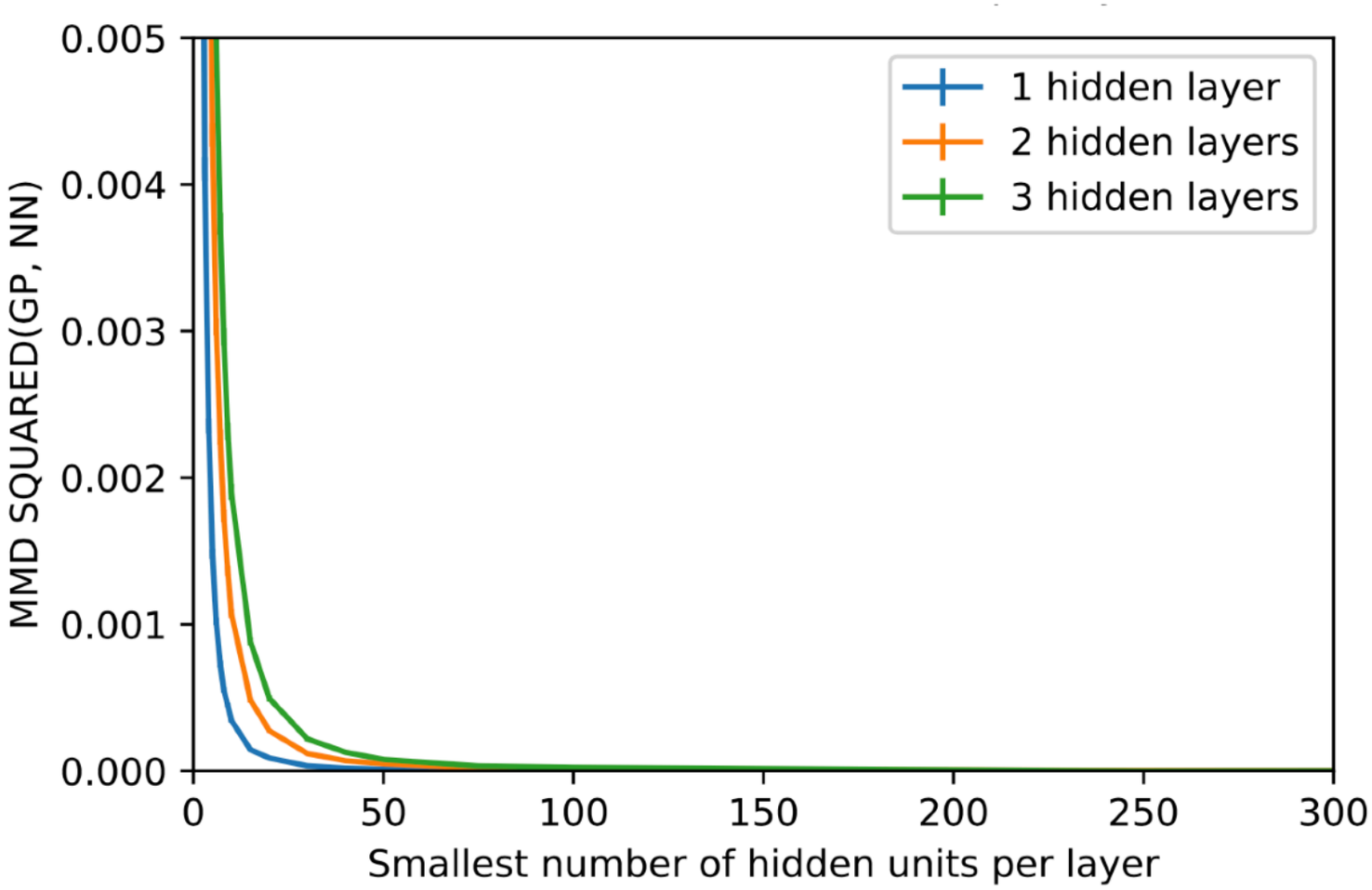
Lee et al. (ICLR, 2018) Deep neural networks as gaussian processes

Gaussian distribution on weights: $\mathbf{W}^{(i)} \sim \mathcal{N}\left(0, \frac{\sigma_w^2}{H_i}\right)$

BUT

KEEP IN MIND THE REALITY :

DEEPER IN NNs THE DISTANCE FROM GP IS INCREASING



[Matthews et al. (2018) Gaussian process behaviour in wide deep neural networks, ICLR]

Other choices of priors for BNNs

[Favaro et al, 2021. Stable behaviour of infinitely wide deep neural networks. arxiv]

- Considers stable priors St(α,σ) with stability parameter α and scale parameter σ. Very heavy tails, only moments of order less than α exist.
- Convergence in distribution of the infinitely wide limit to a stable process.
- Some open questions:
  - application to Bayesian inference
  - existence of a neural tangent kernel (NTK) in the stable regime
  - application to information propagation

INITIALIZATION TECHNIQUES

VARIANCE PRESERVATION

Additional assumptions:

- Inputs are random and i.i.d.
- Gradients are i.i.d. and independent from inputs

Ideas:

- Preserve the variance of the pre-activations during propagation
- Preserve the variance of the gradients during back-propagation

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$$\text{Var}(h^{(\ell)}) = \text{Var}(h^{(\ell+1)})$$

$$\text{Var}\left(\frac{\partial L}{\partial h^{(\ell+1)}}\right) = \text{Var}\left(\frac{\partial L}{\partial h^{(\ell)}}\right) \quad \Rightarrow \quad \begin{aligned} &\text{Var}(\phi(g^{(\ell)})) \approx H_{\ell-1}\text{Var}(\mathbf{W}^{(\ell)}) = 1 \\ &\text{Var}(\phi'(g^{(\ell)})\mathbf{W}^{(\ell)}) \approx H_{\ell}\text{Var}(W^{(\ell)}) = 1 \end{aligned}$$

GLOROT AND HE INITIALIZATIONS

Glorot's initialization

Arithmetic compromise between forward and backward variance preservations

$$\mathbf{W}^{\ell} \sim \mathcal{U}\left(-\frac{\sqrt{6}}{\sqrt{H_{\ell}+H_{\ell-1}}}, \frac{\sqrt{6}}{\sqrt{H_{\ell}+H_{\ell-1}}}\right)$$

$$\text{Var}(\mathbf{W}^{\ell}) = \frac{2}{H_{\ell}+H_{\ell-1}}$$

Glorot and Bengio (2010). Understanding the difficulty of training deep feedforward neural networks

He's initialization

- Preserves the variance in the forward pass ($\sqrt{2}$ for ReLU)
- No variance collapse/explosion in the backward pass

$$\mathbf{W}^{\ell} \sim \mathcal{N}\left(0, \left(\frac{\sqrt{2}}{\sqrt{H_{\ell-1}}}\right)^2\right)$$

He et al. (2015). Delving deep into rectifiers: Surpassing human-level performance on Imagenet classification.

DEEP INFORMATION PROPAGATION

- Propagation of deterministic inputs
- Correlation between two data points across a neural network

Ideas:

- Study the variance of a pre-activation for a given data point a

$$q_{aa}^{\ell} = \mathbb{E}\left[\left(g^{\ell}(a)\right)^2\right]$$

- Study the covariance between pre-activations for given two different data-points a and b

$$q_{ab}^{\ell} = \mathbb{E}\left[g^{\ell}(a), g^{\ell}(b)\right]$$

DEEP INFORMATION PROPAGATION

Assumptions:

- Pre-activations are Gaussian (= close to wide regime)
- Gaussian initialization: $\mathbf{W}^{(\ell)} \sim \mathcal{N}\left(0, \frac{\sigma_w^2}{H_\ell}\right), \quad \mathbf{b}^{(\ell)} \sim \mathcal{N}(0, \sigma_b^2)$

Reccurence relations of $q_{aa}^{\ell} = \mathbb{E}\left[\left(g^{\ell}(a)\right)^2\right]$ and $q_{ab}^{\ell} = \mathbb{E}\left[g^{\ell}(a), g^{\ell}(b)\right]$:

$$q_{aa}^{\ell} = \sigma_w^2 \int \phi^2\left(\sqrt{q_{aa}^{\ell-1}}\, g\right) \mathfrak{D}g + \sigma_b$$

$\mathfrak{D}g \sim \mathcal{N}(0,1)$ (Gaussian assumption)

Discribes the evolution of a single input a through a neural network!

Poole et al. (2016). Exponential expressivity in deep neural networks through transient chaos, NIPS
Schoenholz et al. (2017). Deep information propagation, ICLR

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$\mathfrak{D}g \sim \mathcal{N}(0,1)$ (Gaussian assumption)

Describes the evolution of a single input a through a neural network!

For any choice of σ_w and σ_b with bounded ϕ, there is a fixed point $q^* = \lim_{\ell \to \infty} q_{aa}^{\ell}$

Poole et al. (2016). Exponential expressivity in deep neural networks through transient chaos, NIPS
Schoenholz et al. (2017). Deep information propagation, ICLR

DEEP INFORMATION PROPAGATION

Recurrence relations of $q^{\ell}_{aa} = \mathbb{E}\left[\left(g^{\ell}(a)\right)^2\right]$ and $q^{\ell}_{ab} = \mathbb{E}\left[g^{\ell}(a), g^{\ell}(b)\right]$:

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$$q^{\ell}_{ab} = \sigma_w^2 \int \phi(z_1)\phi(z_2)\mathfrak{D}g_1 \mathfrak{D}g_2 + \sigma_b$$

Propagation of two signals through a neural network!

$\mathfrak{D}g \sim \mathcal{N}(0,1)$ Gaussian

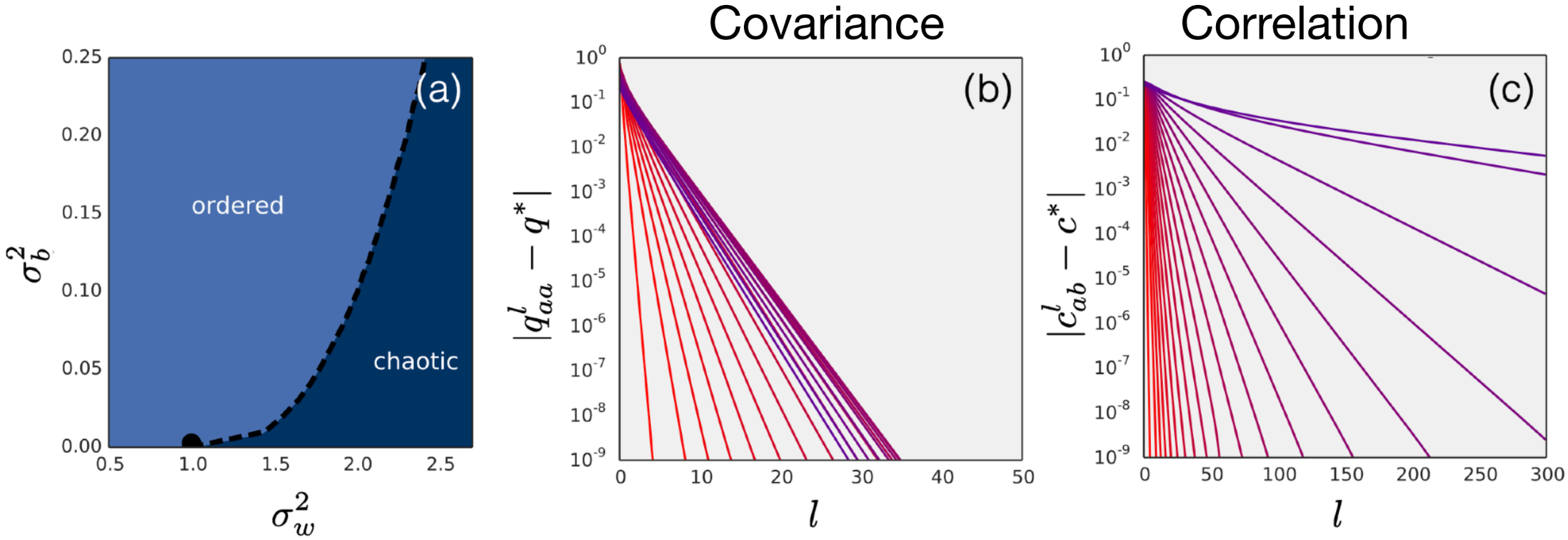
$c^{\ell}_{ab} = \dfrac{q^{\ell}_{ab}}{\sqrt{q^{\ell}_{aa} q^{\ell}_{bb}}}$ distributions correlation

$z_1 = \sqrt{q^{\ell-1}_{aa}}\, g \quad z_2 = \sqrt{q^{\ell-1}_{bb}}\, g \left(c^{\ell}_{ab} g_1 + \sqrt{1 - (c^{\ell}_{ab})^2}\, g_2\right)$

Gaussian approximations to the pre-activations

Poole et al. (2016). Exponential expressivity in deep neural networks through transient chaos, NIPS
Schoenholz et al. (2017). Deep information propagation, ICLR

EDGE OF CHAOS INITIALIZATION



There is a critical line separating an ordered phase (in which c* = 1 and all inputs end up asymptotically correlated) and a chaotic phase (in which c* < 1 and all inputs end up asymptotically decorrelated).

$$q_{aa}^{\ell} = \sigma_w^2 \int \phi^2\left(\sqrt{q_{aa}^{\ell-1}}\, g\right) \mathfrak{D}g + \sigma_b$$

$$q_{ab}^{\ell} = \sigma_w^2 \int \phi(z_1)\phi(z_2) \mathfrak{D}g_1 \mathfrak{D}g_2 + \sigma_b$$

$$c_{ab}^{\ell} = \frac{q_{ab}^{\ell}}{\sqrt{q_{aa}^{\ell} q_{bb}^{\ell}}}$$

Poole et al. (2016). Exponential expressivity in deep neural networks through transient chaos, NIPS

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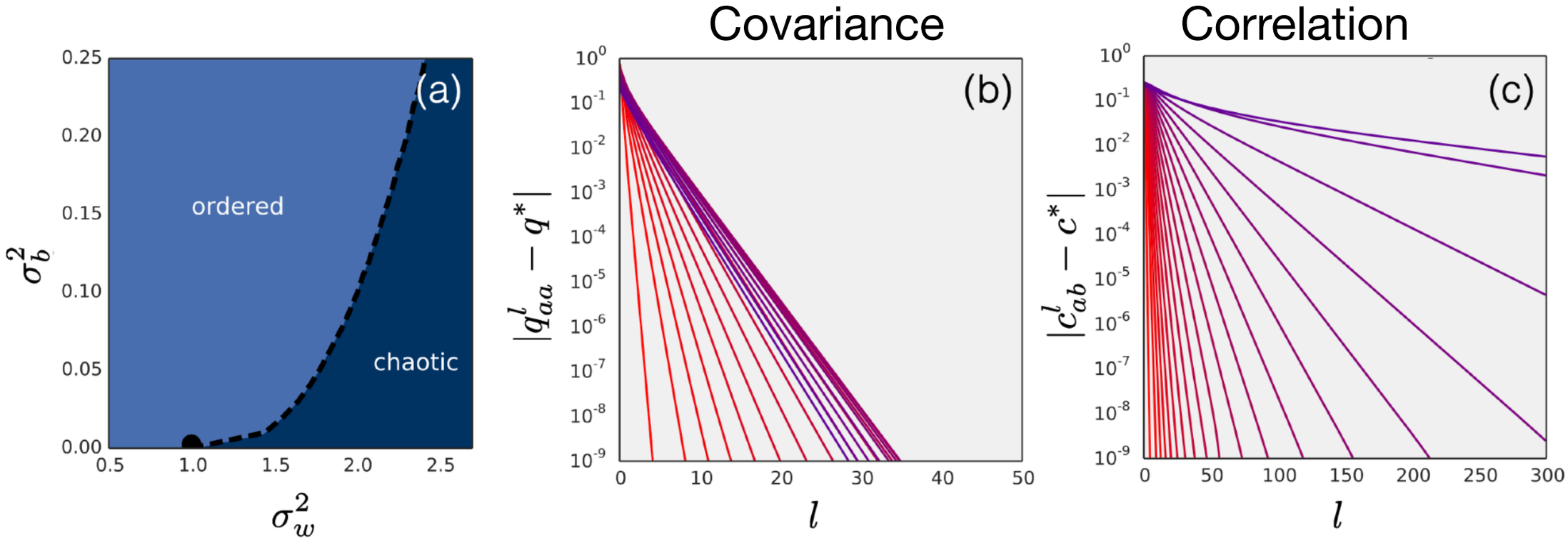

$\mathbf{W}^{(\ell)} \sim \mathcal{N}\left(0, \frac{\sigma_w^2}{H_\ell}\right)$, $\mathbf{b}^{(\ell)} \sim \mathcal{N}(0, \sigma_b^2)$, where σ_w and σ_b are chosen from the separating line (Edge of Chaos) Deeper propagates the information!

Schoenholz et al. (2017). Deep information propagation, ICLR

BUT

KEEP IN MIND THE REALITY :

$$q^{\ell}_{aa} = \sigma_w^2 \int \phi^2 \left(\sqrt{q^{\ell-1}_{aa}} g \right) \mathfrak{D}g + \sigma_b$$

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Gaussian approximations to the pre-activations

=

Wide Regime!

PRIORS AT THE UNIT LEVEL

SUB-WEIBULL RANDOM VARIABLE

A random variable X, such that

$$\mathbb{P}(|X| \geq x) \leq \exp\left(-x^{1/\theta}/K\right)$$

for all $x \geq 0$ and for some $K > 0$, is called a **sub-Weibull** random variable with tail parameter $\theta > 0$:

$$X \sim \mathsf{subW}(\theta).$$

Vladimirova, M., Girard, S., Nguyen, H. and Arbel, J. (2020). Sub-Weibull distributions: generalizing sub-Gaussian and sub-Exponential properties to heavier-tailed distributions, Stat Journal

SUB-WEIBULL RANDOM VARIABLE

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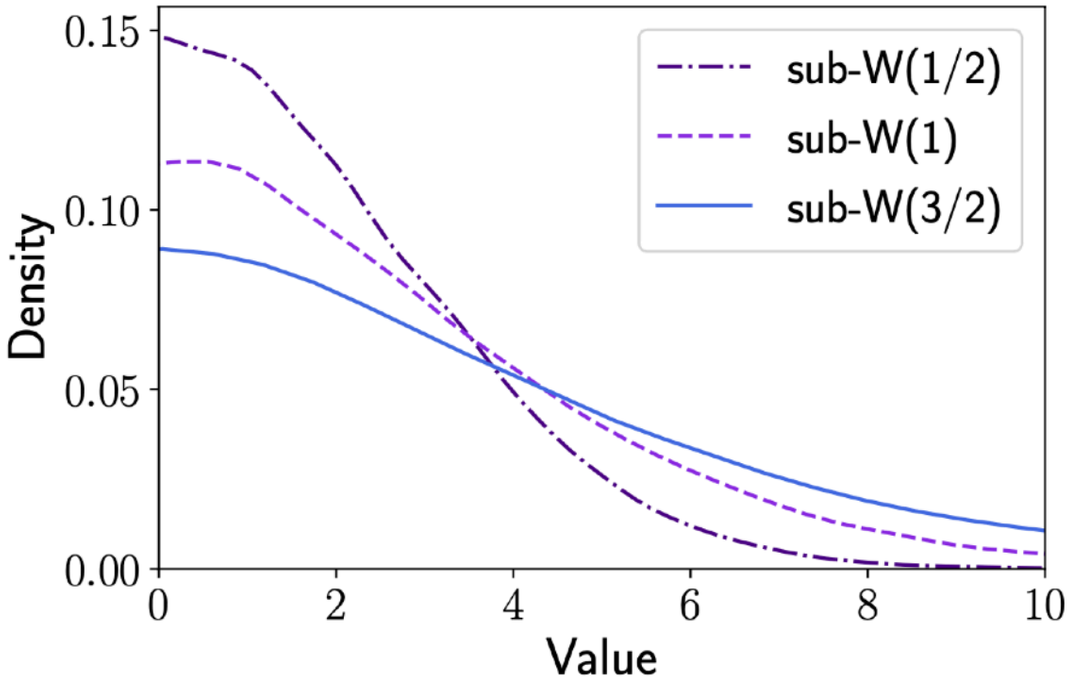
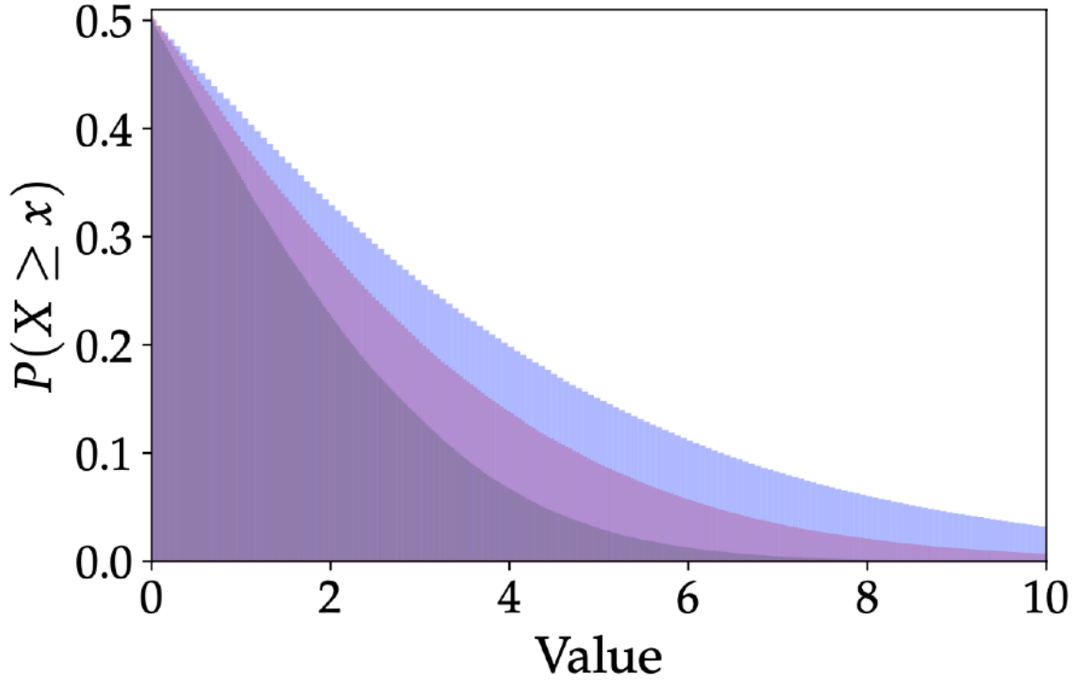
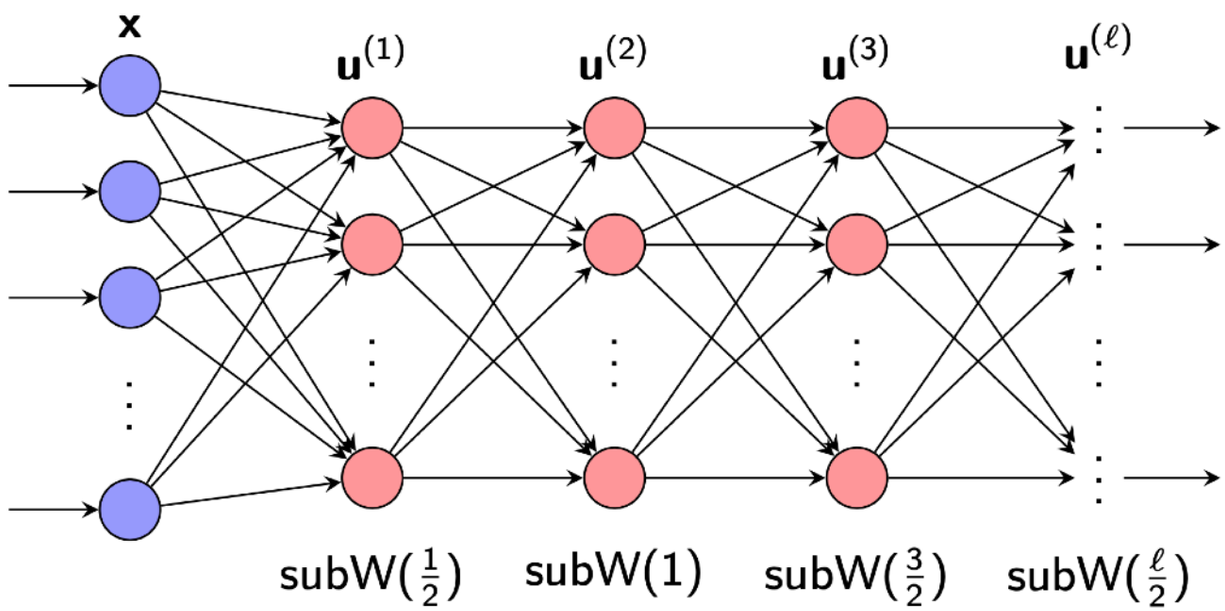




Vladimirova, M., Verbeek, J., Mesejo, P., and Arbel, J. (2019). Understanding Priors in Bayesian Neural Networks at the Unit Level, ICML

OUR RESULT: BNNS BECOME HEAVIER-TAILED WITH DEPTH



$$X \sim \mathsf{subW}(\theta) \quad \Leftrightarrow \quad \mathbb{P}(|X| \geq x) \leq \exp\left(-x^{1/\theta}/K\right)$$

Vladimirova, M., Verbeek, J., Mesejo, P., and Arbel, J. (2019). Understanding Priors in Bayesian Neural Networks at the Unit Level, ICML

OUR RESULT: BNNS BECOME HEAVIER-TAILED WITH DEPTH

Main Theorem

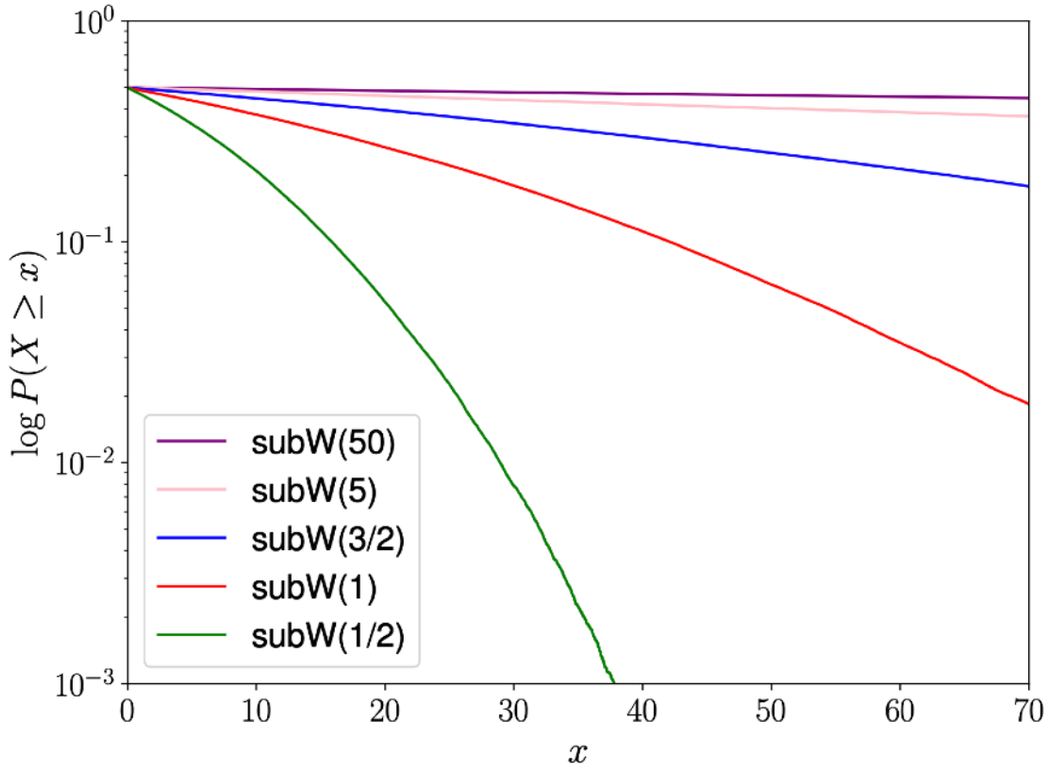
The ℓ-th hidden layer units $U^{(\ell)}$ (pre-activation $g^{(\ell)}$ or post-activation $h^{(\ell)}$) of a feed-forward Bayesian neural network with:

- **Gaussian priors** on weights and
- **extended envelope condition** activation function ϕ

have **sub-Weibull marginal prior distribution** with tail parameter $\theta = \ell/2$, conditional on the input $\boldsymbol{x}$:

$$U^{(\ell)} \sim \mathsf{subW}(\ell/2),$$

Priors for 100-layer BNN



Vladimirova, M., Verbeek, J., Mesejo, P., and Arbel, J. (2019). Understanding Priors in Bayesian Neural Networks at the Unit Level, ICML

POSSIBLE REGULARIZATION INTERPRETATION

POSSIBLE REGULARIZATION INTERPRETATION

Maximum a Posterior (MAP)
Is a Regularized Problem

$$\max_{\mathbf{W}} \pi(\mathbf{W}|\mathcal{D}) \propto \mathcal{L}(\mathcal{D}|\mathbf{W})\pi(\mathbf{W})$$

$$\min_{\mathbf{W}} -\log \mathcal{L}(\mathcal{D}|\mathbf{W}) - \log \pi(\mathbf{W})$$

$$\min_{\mathbf{W}} L(\mathbf{W}) + \lambda R(\mathbf{W})$$

Loss function

Regularizer

POSSIBLE REGULARIZATION INTERPRETATION

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Loss function — Regularizer

Example:

Gaussian Prior $\Leftrightarrow$ Weight Decay (L2) Regularization

$$\pi(\mathbf{W}) = \prod_{\ell=1}^{L} \prod_{i,j} \mathrm{e}^{-\frac{1}{2}(W_{i,j}^{(\ell)})^2} \qquad R(\mathbf{W}) = \sum_{\ell=1}^{L} \sum_{i,j} (W_{i,j}^{(\ell)})^2 = \|\mathbf{W}\|_2^2$$

POSSIBLE REGULARIZATION INTERPRETATION

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Loss function

Regularizer

Gaussian
Prior on
Weights

$$\pi(\mathbf{W}) = \prod_{\ell=1}^{L} \prod_{i,j} \mathrm{e}^{-\frac{1}{2}(W_{i,j}^{(\ell)})^2}$$

$$\pi(w) \approx e^{-w^2}$$

Sub-Weibull
Prior on Units

$$\mathbb{P}(|U_m^{(\ell)}| \geq u) \leq \exp\left(-u^{2/\ell}/K_1\right) \quad \text{for all } u \geq 0$$

$$\pi_m^{(\ell)}(u) \approx \mathrm{e}^{-|u|^{2/\ell}/K_1}$$

POSSIBLE REGULARIZATION INTERPRETATION

Maximum a Posterior (MAP)
Is a Regularized Problem

$$\max_{\mathbf{W}} \pi(\mathbf{W}|\mathcal{D}) \propto \mathcal{L}(\mathcal{D}|\mathbf{W})\pi(\mathbf{W})$$

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Loss function — Regularizer

Gaussian
Prior on
Weights

$$\pi(\mathbf{W}) = \prod_{\ell=1}^{L} \prod_{i,j} \mathrm{e}^{-\frac{1}{2}(W_{i,j}^{(\ell)})^2}$$

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$$\pi_m^{(\ell)}(u) \approx \mathrm{e}^{-|u|^{2/\ell}/K_1}$$

Sklar's theorem: $$\pi(\boldsymbol{U}) = \prod_{\ell=1}^{L} \prod_{m=1}^{H_\ell} \pi_m^{(\ell)}(U_m^{(\ell)})\, C(F(\boldsymbol{U})),$$

where C represents the copula of $\mathbf{U}$
(all the dependences between the units)

POSSIBLE REGULARIZATION INTERPRETATION

Maximum a Posterior (MAP)
Is a Regularized Problem

$$\max_{\mathbf{W}} \pi(\mathbf{W}|\mathcal{D}) \propto \mathcal{L}(\mathcal{D}|\mathbf{W})\pi(\mathbf{W})$$

$$\min_{\mathbf{W}} -\log \mathcal{L}(\mathcal{D}|\mathbf{W}) - \log \pi(\mathbf{W})$$

$$\min_{\mathbf{W}} L(\mathbf{W}) + \lambda R(\mathbf{W})$$

Loss function — Regularizer

Weight distribution $\pi(w) \approx e^{-w^2}$ $\Rightarrow$ ℓ-th layer unit distribution $\pi^{(\ell)}(u) \approx e^{-u^{2/\ell}}$

Layer	Penalty on $\mathbf{W}$	Penalty on $\mathbf{U}$	
1	$\|\mathbf{W}^{(1)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(1)}\|_2^2$	$\mathcal{L}^2$ (weight decay)
2	$\|\mathbf{W}^{(2)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(2)}\|$	$\mathcal{L}^1$ (Lasso)
ℓ	$\|\mathbf{W}^{(\ell)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(\ell)}\|_{2/\ell}^{2/\ell}$	$\mathcal{L}^{2/\ell}$

BUT

POSSIBLE REGULARIZATION INTERPRETATION

Weight distribution
$\pi(w) \approx e^{-w^2}$

$\Rightarrow$

ℓ-th layer unit distribution
$\pi^{(\ell)}(u) \approx e^{-u^{2/\ell}}$

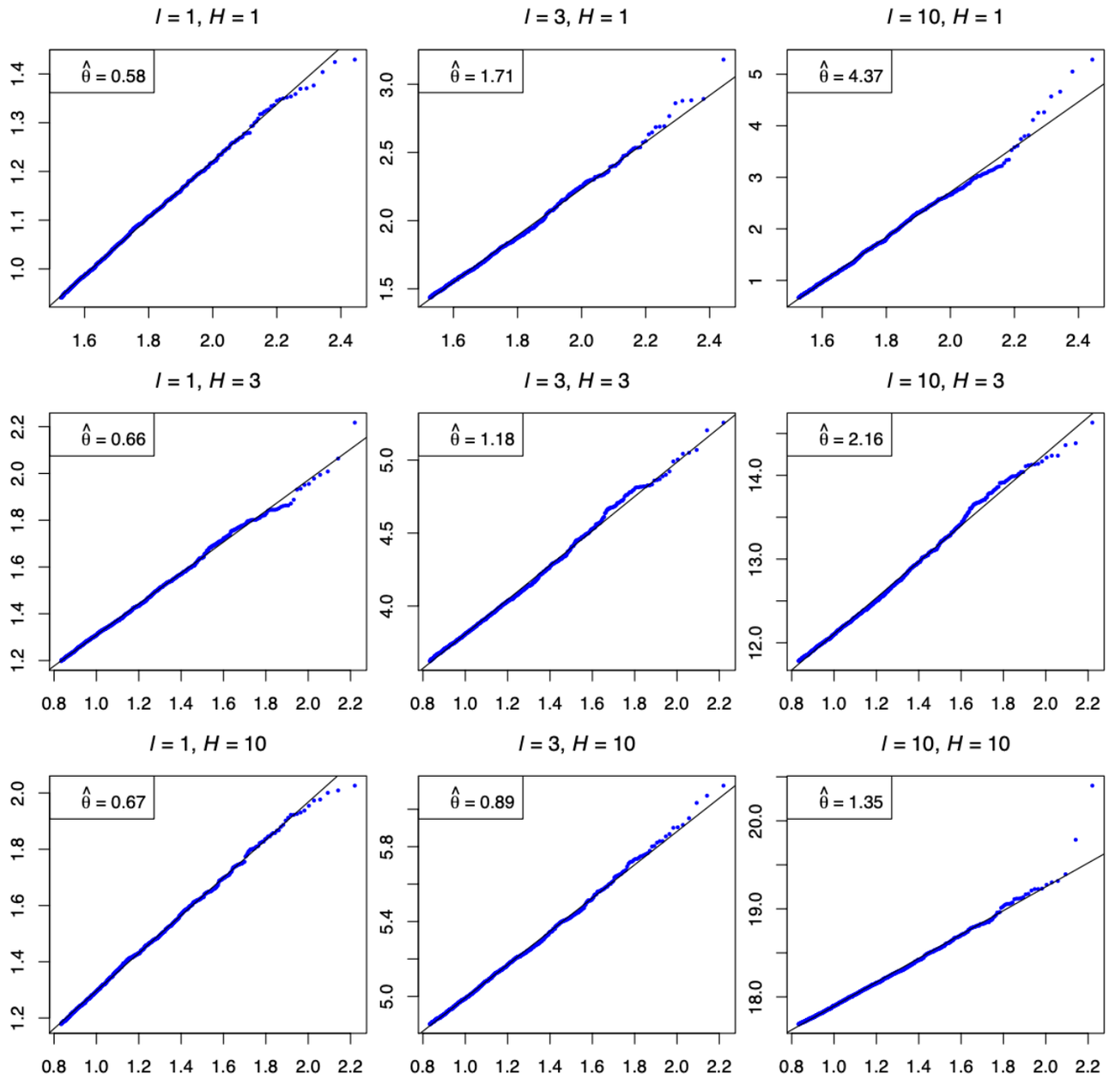
Layer	Penalty on **W**	Penalty on **U**	
1	$\|\mathbf{W}^{(1)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(1)}\|_2^2$	$\mathcal{L}^2$ (weight decay)
2	$\|\mathbf{W}^{(2)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(2)}\|$	$\mathcal{L}^1$ (Lasso)
ℓ	$\|\mathbf{W}^{(\ell)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(\ell)}\|_{2/\ell}^{2/\ell}$	$\mathcal{L}^{2/\ell}$

Two approximations:

- Unit distribution by its tails,
- Joint distribution by Sklar's theorem

$$\pi(\boldsymbol{U}) = \prod_{\ell=1}^{L} \prod_{m=1}^{H_\ell} \pi_m^{(\ell)}(U_m^{(\ell)})\, C(F(\boldsymbol{U}))$$

TAIL COEFFICIENT ESTIMATION



Depth L equals 1, 3 and 10

Width H equals 1, 3 and 10 (for all considered layers L)

Theoretical:

$\theta = \ell/2$ for finite H

$\theta = 1/2$ for infinite H

Vladimirova, M., Girard, S., Nguyen, H. and Arbel, J. (2020). Sub-Weibull distributions: generalizing sub-Gaussian and sub-Exponential properties to heavier-tailed distributions, Stat Journal

Approximations

- Laplace approximation (MacKay, 1992, Neur. Comp.)
- Variational inference (Hinton and van Kamp, 1993, Barber & Bishop, 1998, NIPS, Blundell et al, 2015, ICML)
- Monte Carlo dropout (Gal & Ghahramani, 2016, ICML)

Bayesian NN under a Laplace approximation

Chap 5.7 of Bishop

Univariate regression $t \in \mathbb{R}$

Goussian $p(t \mid x)$ to be Goussian

the mean $= y(x, w)$ output of NN

input, weight

variance β^{-1} β precision

Data $\mathcal{D} = \{(x_n, t_n), n = 1 \dots N\}$

$$\begin{cases} \text{Model} & p(t \mid x) = \mathcal{N}(t \mid y(x, w), \beta^{-1}) \\ \text{Prior} & p(w \mid \alpha) = \mathcal{N}(w \mid 0, \alpha^{-1} I) \end{cases}$$

$$\text{Posterior} \quad p(w \mid \mathcal{D}, \alpha, \beta) \propto \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(x_n, w), \beta^{-1}) \, p(w \mid \alpha)$$

w_{MAP} : numerically find local optimum.

$$\log p(w \mid \mathcal{D}, \alpha, \beta) = \underbrace{-\frac{\alpha}{2} w^T w}_{\text{penalty to the MLE.}} - \frac{\beta}{2} \sum_{n=1}^{N} (y(x_n, w) - t_n)^2 + c^t$$

Laplace approx. of the posterior:

$$q(w \mid \mathcal{D}, \alpha, \beta) = N(w \mid w_{MAP}, A^{-1})$$

$$A = -\nabla\nabla \log p = \alpha I + \beta H \text{, with } H = \text{Hess}(SSE)$$

approx. predictive

$$p(t \mid x, \mathcal{D}) = \int_w \underbrace{p(t \mid x, w)}_{N(t \mid y(x,w), \beta^{-1})} q(w \mid \mathcal{D}, \alpha, \beta) \, dw \quad (*)$$

Taylor approximation for NN :

$$y(x,w) \approx y(x, w_{MAP}) + g^T (w - w_{MAP})$$

$$g = \nabla_w y(x,w) \big|_{w=w_{MAP}}$$

$$p(t \mid x, w, \beta) \approx N\left(t \mid y(x, w_{MAP}) + g^T (w - w_{MAP}), \beta^{-1}\right)$$

plug this in (*) :

Plus use $\begin{cases} p(x) = N(x \mid \mu, \Lambda^{-1}) \\ p(y \mid x) = N(y \mid Ax + b, L^{-1}) \end{cases}$

$$\Rightarrow p(y) = N(y \mid A\mu + b, \underbrace{L^{-1} + A\Lambda^{-1}A^T})$$

$$p(t \mid x, \mathcal{D}, \alpha, \beta) \approx N(t \mid y(x, w_{MAP}), \sigma^2(x))$$

$$\sigma^2(x) = \underbrace{\beta^{-1}}_{\text{aleatoric}} + \underbrace{g^T A^{-1} g}_{\text{x-dependent : epistemic.}}$$

α, β hyperparameters

Marginal likelihood $p(\mathcal{D} \mid \alpha, \beta)$, aka evidence

$\rightsquigarrow$ w is integrated out.

$$(\hat{\alpha}, \hat{\beta}) = \underset{(\alpha,\beta)}{\operatorname{argmax}}\, p(\mathcal{D} \mid \alpha, \beta).$$

$$p(\mathcal{D} \mid \alpha, \beta) = \int p(\mathcal{D} \mid w, \beta)\, p(w \mid \alpha)\, dw$$

Laplace approximation: z_0 argmax, $A = -\nabla\nabla \log f(z)\big|_{z=z_0}$

$$\int f(z)\, dz = f(z_0) \int \exp\left(-\frac{1}{2}(z - z_0)^T A (z - z_0)\right) dz$$

$$= f(z_0)\, \frac{(2\pi)^{M/2}}{|A|^{1/2}} \qquad M = \#(z)$$

$$\Rightarrow \log p(\mathcal{D} \mid \alpha, \beta) = \underbrace{-E(w_{MAP})}_{\text{regularized SSE}} - \frac{1}{2}\log|A| + \frac{W}{2}\log\alpha + \frac{N}{2}\log\beta + \underbrace{\frac{\alpha}{2} w_{MAP}^T w_{MAP} + \frac{\beta}{2}\sum_{n=1}^{N}\left(y(x_n, w_{MAP}) - t_n\right)^2}_{\text{pen.}}$$

optimization in (α, β) is done by analogy with linear regression. → Bishop 5.7.

Other techniques for practical BNN:

variational inference: with various assumptions on approx family.

VI (Blundell, 2015)

parameters are weights $w = (w_1, \dots, w_{\bar{w}})$

Approximate family : Gaussian : $N(\mu, \sigma^2)$

w_i approximated by $\theta_i = (\mu_i, \sigma_i^2)$, $i = 1, \dots, \bar{w}$

$$q_\theta(w) = \prod_{i=1}^{\bar{w}} N(w_i \mid \mu_i, \sigma_i^2)$$

$$Q = \{ q_\theta(w), \ \mu_i \in \mathbb{R}, \ \sigma_i > 0 \}$$

$$KL\left(q_\theta(w) \,\|\, p(w \mid X, Y) \right) \qquad X, Y \begin{cases} X = (X_i) \\ Y = (Y_i) \end{cases} \quad i = 1 \dots N$$

$$= \int q_\theta(w) \log \left(\frac{q_\theta(w)}{p(w \mid X, Y)} \right) dw$$

$$= \int q_\theta(w) \log \left(\frac{q_\theta(w)\, p(Y \mid X)}{p(w)\, p(Y \mid w, X)} \right) dw$$

Some recent works

Other choices of priors for BNNs

[Fortuin et al, 2021. Bayesian Neural Network Priors Revisited. arxiv]

- Questions the use of iid Gaussian priors for weights in Bayesian Neural Networks
- Shows suboptimality of Gaussian priors essentially through the lens of the cold posterior effect
- Compares w/ other priors including Laplace, Student-t and Multivariate Gaussian with Matern covariance

Bayesian Neural Network Priors Revisited

When performing inference in Bayesian models, we can temper the posterior by a positive temperature T, giving

$$\log p(w|x,y)^{\frac{1}{T}} = \frac{1}{T}[\log p(y|w,x) + \log p(w)] + Z(T)$$

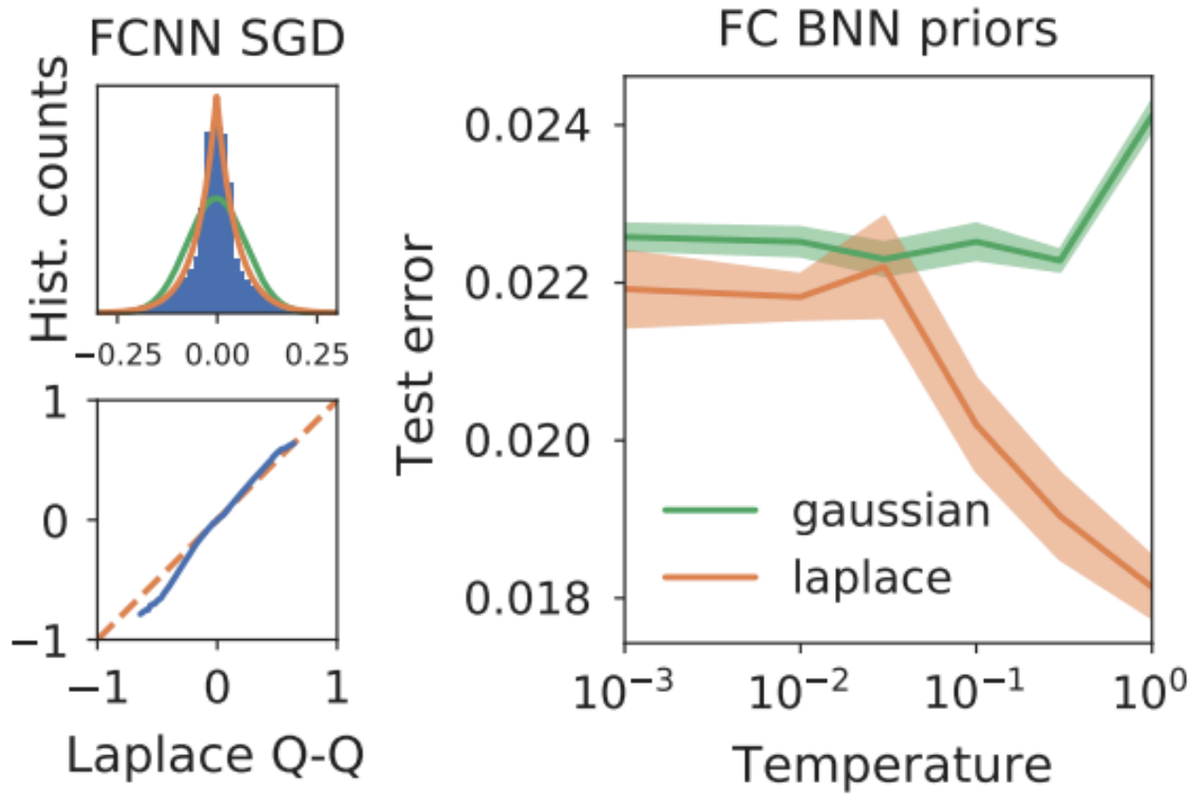


Figure 1: The weights of SGD-trained neural networks on MNIST follow a distribution that is more heavy-tailed than a Gaussian, and better approximated by a Laplace. When using a Laplace prior instead of a Gaussian prior for a BNN on the same task, the performance is improved and the cold posterior effect inverted, such that now the true Bayes posterior ($T = 1$) performs best.

[Fortuin et al, 2021. Bayesian Neural Network Priors Revisited. arxiv]

Bayesian Neural Network Priors Revisited

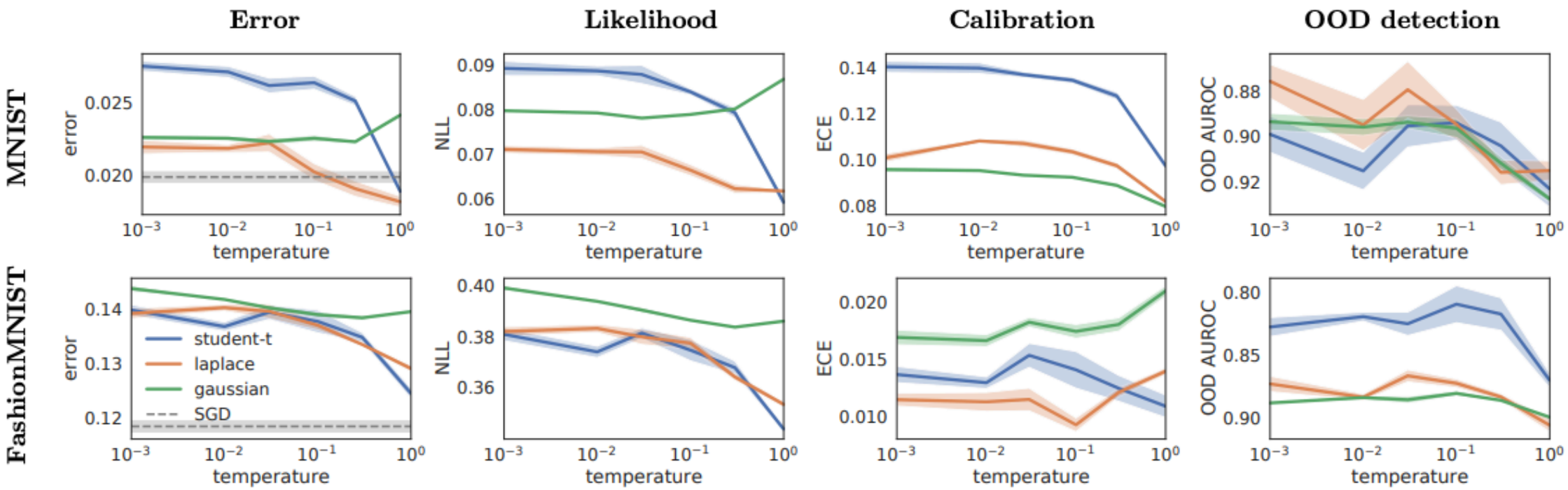


Figure 6: Performances of fully connected BNNs with different priors on MNIST and FashionMNIST (see Sec. 4.2). The heavy-tailed priors generally perform better, especially at higher temperatures, and lead to a less pronounced cold posterior effect. Note the reversed y-axis for OOD detection on the right to ensure that lower values are better in all plots.

[Fortuin et al, 2021. Bayesian Neural Network Priors Revisited. arxiv]

Bayesian deep learning

Pyro example on Bayesian neural networks

- Demonstrates how to use NUTS to do inference on a simple (small) Bayesian neural network with two hidden layers.