Understanding Priors in Bayesian Neural Networks at the Unit Level

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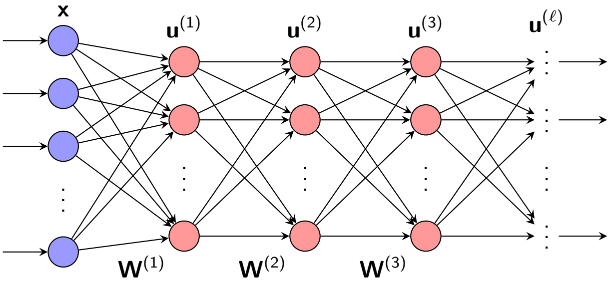
Bayesian neural networks: why?

Neal [1996], MacKay [1992]

- Prior on weights, $w \sim N(\mu, \sigma^2)$
- Allows to model uncertainty
- Represents a standard neural network



Outline

Recent works on distributional properties

Sub-Weibull distributions

Main result: Prior on units gets heavier-tailed with depth

Regularization interpretation

Wide regime: infinite number of hidden units in the layer

Theorem (Neal [1996])

Consider a Bayesian neural network with (A1) iid Gaussian priors on the weights
(A2) with bounded variances and
(A3) ReLU activation function. Then conditional on input $\mathbf{x}$*,*
the marginal prior distribution of a unit $u^{(2)}$ *of 2-nd hidden layer converges to a Gaussian process in a wide regime.*

Proof.
Components of $\mathbf{u}^{(1)}$ are iid $\Rightarrow$ CLT ☐

Wide regime: infinite number of hidden units in the layer

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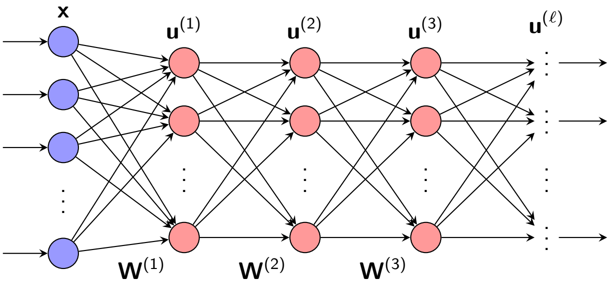

Wide regime: infinite number of hidden units in the layer

Theorem (Matthews et al. [2018], Lee et al. [2018])

Conditional on input $\mathbf{x}$*, the marginal prior distribution of a unit* $u^{(\ell)}$ *of* ℓ*-nd hidden layer converges to a Gaussian process in a wide regime.*

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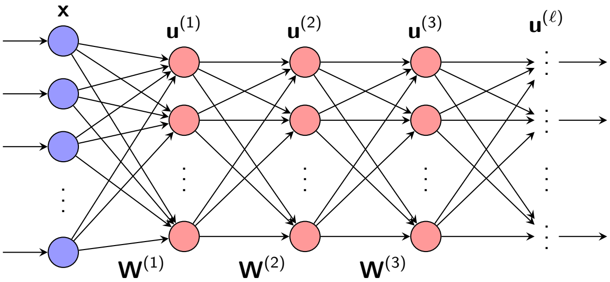

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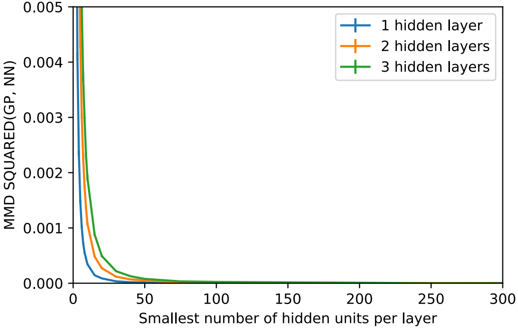


Alexander G de G Matthews, Mark Rowland, Jiri Hron, Richard E Turner, and Zoubin Ghahramani. "Gaussian Process Behaviour in Wide Deep Neural Networks." ICLR (2018).

Jaehoon Lee, Jascha Sohl-dickstein, Jeffrey Pennington, Roman Novak, Sam Schoenholz, and Yasaman Bahri. "Deep neural networks as Gaussian processes." ICLR (2018).

Gaussian process approximation

Samuel S. Schoenholz, Justin Gilmer, Surya Ganguli, Jascha Sohl-Dickstein. "Deep Information Propagation." ICLR (2017).

- Prior on weights, $w \sim N(0, \sigma^2)$ iid
- Initialisation is a crucial step in deep NN
- "Edge of Chaos" initialization can lead to good performances

Soufiane Hayou, Arnaud Doucet, and Judith Rousseau. "On the Impact of the Activation Function on Deep Neural Networks Training." ICML (2019).

- Prior on weights, $w \sim N(0, \sigma^2)$ iid
- Gaussian process approximation $u^\ell \approx \mathcal{GP}(0, K^\ell)$ marginally
- "Edge of Chaos" initialization

Results:

- Smooth activation functions (e.g. ELU) are better than ReLU activation, especially if ℓ is large
- "Edge of Chaos" accelerates the training and improves performances

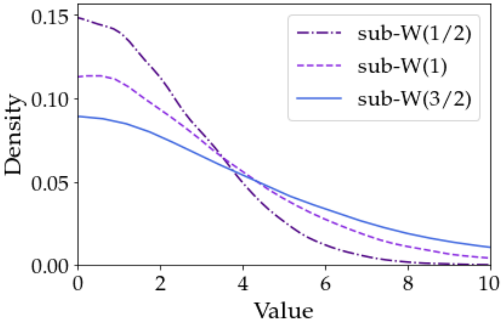
Outline

Distribution families with respect to tail behavior

Vershynin [2018] – subG, subE;
Kuchibhotla and Chakrabortty [2018]; Vladimirova and Arbel [2019] – subW

For all $k \in \mathbb{N}$, k-th row moment: $\|X\|_k = \left(\mathbb{E}|X|^k\right)^{1/k}$

Distribution	Tail	Moments
Sub-Gaussian	$\overline{F}(x) \leq \mathrm{e}^{-\lambda x^2}$	$\|X\|_k \leq C\sqrt{k}$
$\subset$ Sub-Exponential	$\overline{F}(x) \leq \mathrm{e}^{-\lambda x}$	$\|X\|_k \leq Ck$
Sub-Weibull	$\overline{F}(x) \leq \mathrm{e}^{-\lambda x^{1/\theta}}$	$\|X\|_k \leq Ck^\theta$



- $\theta > 0$ called tail parameter
- $\|X\|_k \asymp k^\theta \implies X \sim \mathrm{subW}(\theta)$, θ called optimal
- $\mathrm{subW}(1/2) = \mathrm{subG}$, $\mathrm{subW}(1) = \mathrm{subE}$

Outline

Assumptions on neural network

We analyze Bayesian neural networks which satisfy the following assumptions

(A1) Parameters. The weights w have i.i.d. Gaussian prior

$$w \sim \mathcal{N}(\mu, \sigma^2)$$

(A2) Nonlinearity. ReLU-like with envelope property: exist $c_1, c_2, d_2 \geq 0$, $d_1 > 0$ s.t.

$$\begin{aligned} |\phi(u)| &\geq c_1 + d_1|u| \quad \text{for all } u \in \mathbb{R}_+ \text{ or } u \in \mathbb{R}_-, \\ |\phi(u)| &\leq c_2 + d_2|u| \quad \text{for all } u \in \mathbb{R}. \end{aligned}$$

- Examples: ReLU, ELU, PReLU etc, but no compactly supported like sigmoid and tanh.
- Nonlinearity does not harm the distributional tail:

$$\|\phi(X)\|_k \asymp \|X\|_k, \quad k \in \mathbb{N}$$

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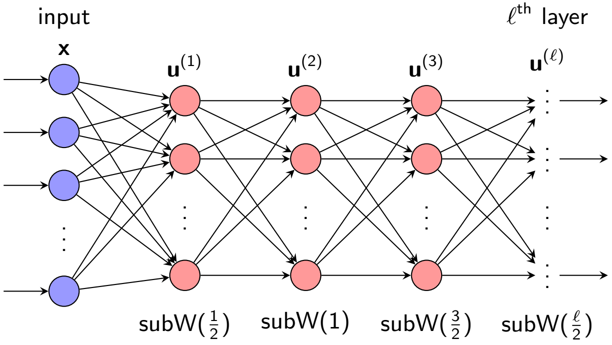
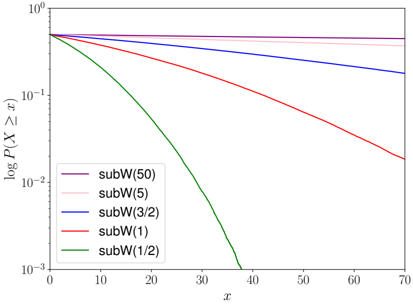
Main theorem

Consider a Bayesian neural network with (A1) i.i.d. Gaussian priors on the weights and (A2) nonlinearity satisfying envelope property.

Then conditional on input $\mathbf{x}$, the marginal prior distribution of a unit $u^{(\ell)}$ of ℓ-th hidden layer is sub-Weibull with optimal tail parameter $\theta = \ell/2$: $\pi^{(\ell)}(u) \sim \text{subW}(\ell/2)$





Proof sketch I

Recall. $X \sim \text{subW}(\theta) \iff \exists C > 0, \|X\|_k = \left(\mathbb{E}|X|^k\right)^{1/k} \leq Ck^\theta, \quad \text{for all } k \in \mathbb{N}.$

Notations. $\phi(\cdot)$ — nonlinearity, $\mathbf{g}$ — pre-nonlinearity, $\mathbf{h}$ — post-nonlinearity

$$\mathbf{g}^{(1)}(\mathbf{x}) = \mathbf{W}^{(1)}\mathbf{x}, \quad \mathbf{h}^{(1)}(\mathbf{x}) = \phi(\mathbf{g}^{(1)}),$$

$$\mathbf{g}^{(\ell)}(\mathbf{x}) = \mathbf{W}^{(\ell)}\mathbf{h}^{(\ell-1)}(\mathbf{x}), \quad \mathbf{h}^{(\ell)}(\mathbf{x}) = \phi(\mathbf{g}^{(\ell)}), \quad \ell = \{2, \dots, L\}.$$

Goal. By induction with respect to hidden layer depth ℓ we want to show that

$$\|h^{(\ell)}\|_k \asymp k^{\ell/2}.$$

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Proof sketch II

1. Base step: weights $w_i^{(1)}$ are iid Gaussian $\Rightarrow \|w\|_k \asymp k^{1/2}$; for 1st layer

$$\|g^{(1)}\|_k = \left\| \sum_{i=1}^{H_1} w_i^{(1)} x_i \right\|_k \asymp k^{1/2}$$

   From nonlinearity ϕ assumption

$$\|h^{(1)}\|_k = \|\phi(g^{(1)})\|_k \asymp \|g^{(1)}\|_k \asymp k^{1/2}$$

2. Induction step: if $g^{(\ell-1)}, h^{(\ell-1)} \sim subW((\ell-1)/2)$, then for ℓ-th layer

$$\|g^{(\ell)}\|_k = \left\| \sum_{i=1}^{H} w_i^{(\ell)} h_i^{(\ell-1)} \right\|_k \overset{(\star)}{\asymp} k^{1/2} \cdot k^{(\ell-1)/2} = k^{\ell/2}$$

   2.1 Lower bound for $(\star)$ by positive covariance result: $\forall s, t$, $\mathrm{Cov}\left[\left(h^{(\ell-1)}\right)^s, \left(\tilde{h}^{(\ell-1)}\right)^t\right] \geq 0$
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Interpretation: shrinkage effect

Maximum a Posteriori (MAP) is a Regularized problem

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

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

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

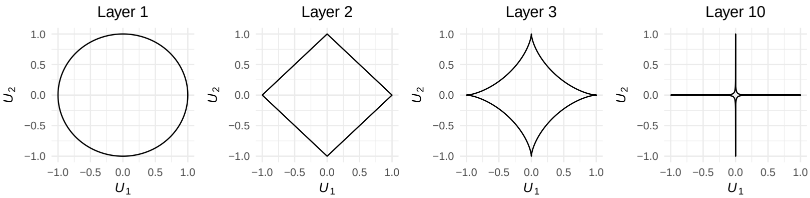
$L(\mathbf{W})$ is a loss function,
$R(\mathbf{W})$ is a norm on $\mathbb{R}^p$, regularizer.

Gaussian prior on the weights:

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

Equivalent to the *weight decay* penalty ($\mathcal{L}^2$):

$$R(\mathbf{W}) = \sum_{\ell=1}^{L}\sum_{i,j}(W_{i,j}^{(\ell)})^2 = \|\mathbf{W}\|_2^2,$$



Interpretation: shrinkage effect

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

Sklar's representation theorem:

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

where C represents the copula of $\mathbf{U}$ (which characterizes all the dependence between the units).

Regularizer:

$$R(\mathbf{U}) = -\sum_{\ell=1}^{L} \sum_{m=1}^{H_\ell} \log \pi_m^{(\ell)}(U_m^{(\ell)}) - \log C(F(\mathbf{U})),$$

$$\approx \|\mathbf{U}^{(1)}\|_2^2 + \|\mathbf{U}_1^{(2)}\|_1 + \cdots + \|\mathbf{U}^{(L)}\|_{2/L}^{2/L} - \log C(F(\mathbf{U})).$$

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	$\|\mathbf{W}^{(\ell)}\|_2^2$, $\mathcal{L}^2$	$\|\mathbf{U}^{(\ell)}\|_{2/\ell}^{2/\ell}$	$\mathcal{L}^{2/\ell}$

Conclusion

(i) We define the notion of sub-Weibull distributions, which are characterized by tails lighter than (or equally light as) Weibull distributions.

(ii) We proved that the marginal prior distribution of the units are heavier-tailed as depth increases.

(iii) We offered an interpretation from a regularization viewpoint.

Future directions:

- prove the Gaussian process limit of sub-Weibull distributions in the wide regime using Kuchibhotla and Chakrabortty [2018];
- investigate if the described regularization mechanism induces sparsity at the unit level.

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