NEURAL INFORMATION PROCESSING SYSTEMS

Critical Initialization of Wide and Deep Neural Networks using Partial Jacobians

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Paper

GitHub

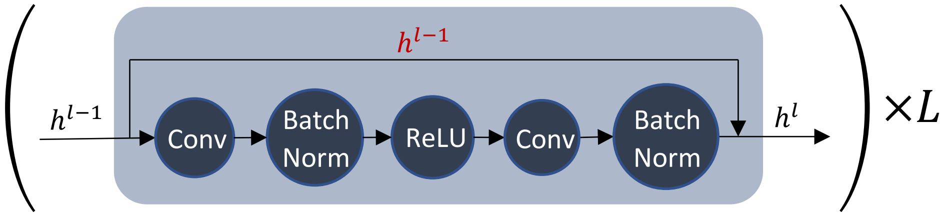
Overview

Deep neural networks need to be initialized at “criticality” to avoid exploding/vanishing gradients and ensure non-exponential scaling with depth.

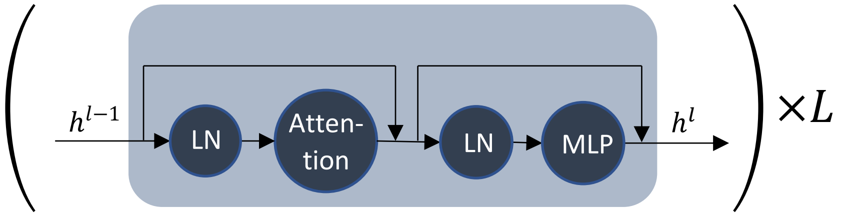
Key Contributions:

1. Novel diagnostic for critical initialization, **Averaged Partial Jacobian Norm (APJN)**, that is..
    - applicable to *general* feedforward architectures (Transformers, CNNs, MLPs etc.)
    - numerically cheap to estimate
    - analytically sound; equivalent to known theoretical measures

2. Identification and analysis of **everywhere-critical architectures**:
    - Architectures can be designed to be *critical regardless of their initialization*, by using specific combinations of normalization layers and residual connections

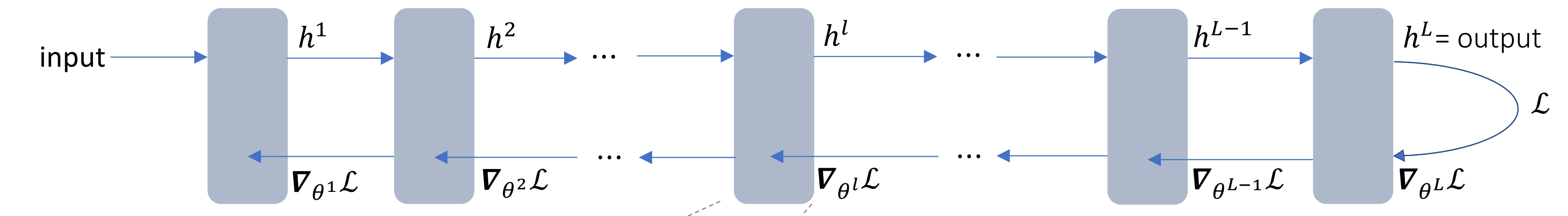


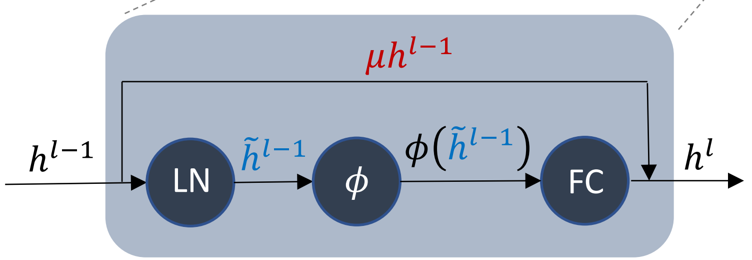
ResNet(V2)



Vision Transformer

Signal Propagation





$$\boldsymbol{h}^{l+1} = \boldsymbol{W}^{l+1}\phi(\tilde{\boldsymbol{h}}^{l}) + \boldsymbol{b}^{l+1} + \mu\boldsymbol{h}^{l}$$

$$\theta^{l+1} \coloneqq \{ W_{ij}^{l+1}\sim\mathcal{N}(0,\sigma_w^2/N_l);\quad b_i^{l+1}\sim\mathcal{N}(0,\sigma_b^2) \}$$

$N_l \to \infty$

$$h_i^l\sim\mathcal{N}(0,\mathcal{K}^l)$$

Critical Initializtion

To analyse the behaviour of gradients, we define APJN:

$$\mathcal{J}^{l_0,l} \coloneqq \mathbb{E}_\theta\left[\left\|\boldsymbol{\nabla}_{\boldsymbol{h}^{l_0}}\boldsymbol{h}^l\right\|_F^2 / N_l\right]$$

Gradients scale depends on scaling of APJN $\mathcal{J}^{l,L}$

$$\boldsymbol{\nabla}_{\theta^l}\mathcal{L} = \left(\boldsymbol{\nabla}_{h^L}\mathcal{L}\right)\left(\boldsymbol{\nabla}_{h^l}h^L\right)\left(\boldsymbol{\nabla}_{\theta^l}h^l\right)$$

$$\left\|\boldsymbol{\nabla}_{\theta^l}\mathcal{L}\right\|^2 \approx O\left(\left\|\boldsymbol{\nabla}_{\boldsymbol{h}^L}\mathcal{L}\right\|^2 \cdot \mathcal{J}^{l,L} \cdot \mathcal{K}^l\right)$$

In the limit $N_l \to \infty$, APJN can be written as a product of layer-to-layer APJNs:

$$\mathcal{J}^{l_0,l} = \mathcal{J}^{l_0,l_0+1}\,\mathcal{J}^{l_0+1,l_0+2}\cdots\mathcal{J}^{l-1,l}$$

$\mathcal{J}^{l-1,l}$ only depends on $\sigma_w^2, \sigma_b^2, \phi$ and μ.

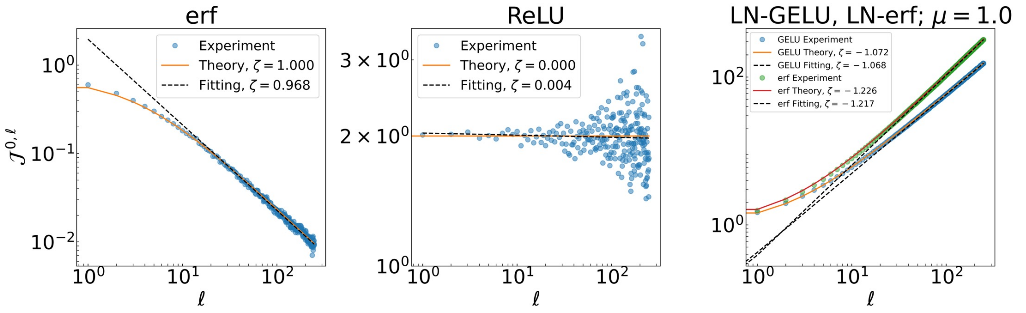
To avoid exploding/vanishing gradients, we want $\mathcal{J}^{l_0,l}$ to behave **non-exponentially** with l. This can be achieved by:

$$\left.\mathcal{J}^{l-1,l}\right|_{l\to\infty} = 1$$

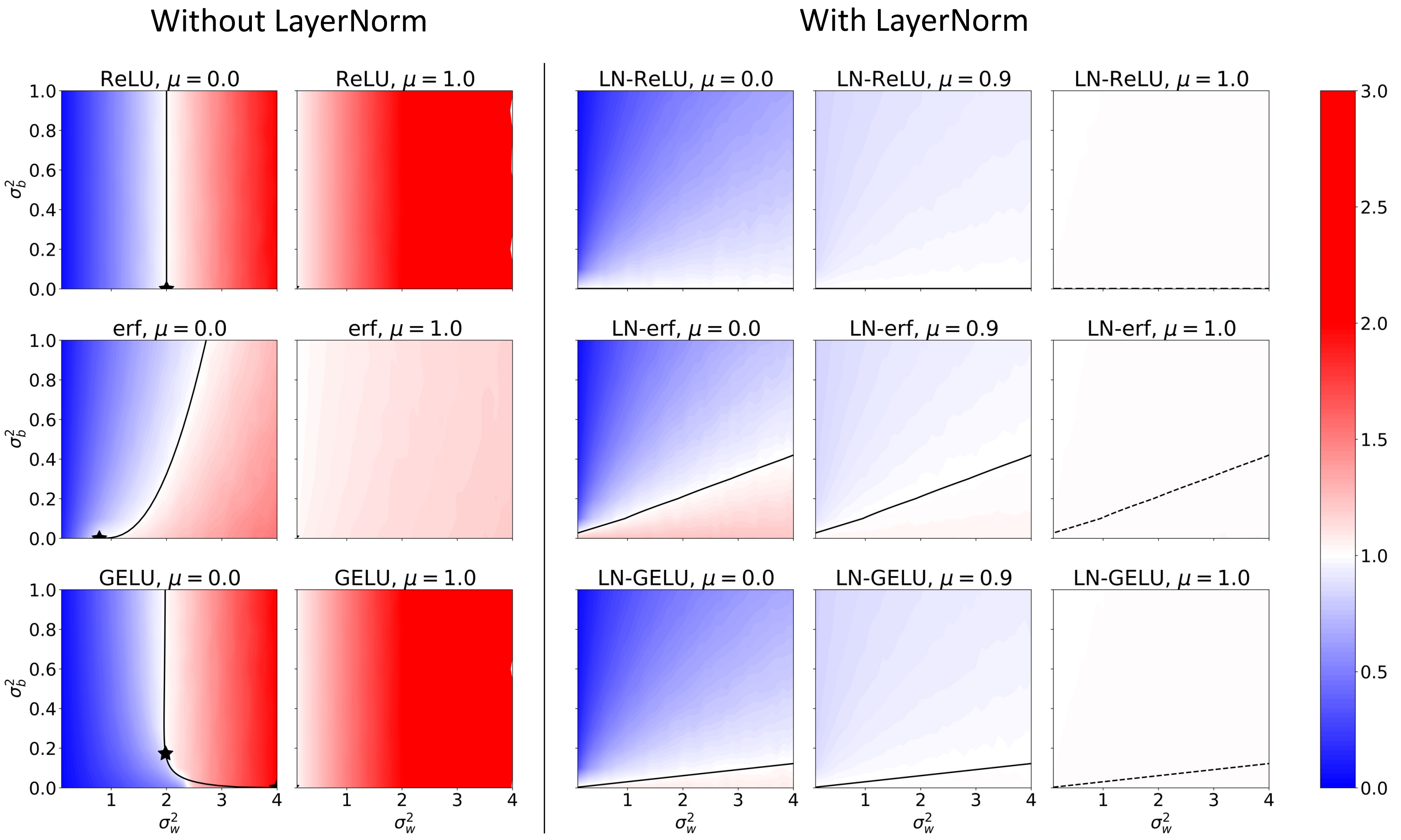
This gives us the **critical line** in the $\sigma_w - \sigma_b$ plane.

Without LayerNorm, demanding non-exponential behaviour of $\mathcal{K}^l$ gives us the **critical point** in the $\sigma_w - \sigma_b$ plane.

At the critical point, $\mathcal{J}^{l_0,l}$ scales algebraically with l : $\boxed{\mathcal{J}^{l_0,l} \sim l^{-\zeta}}$



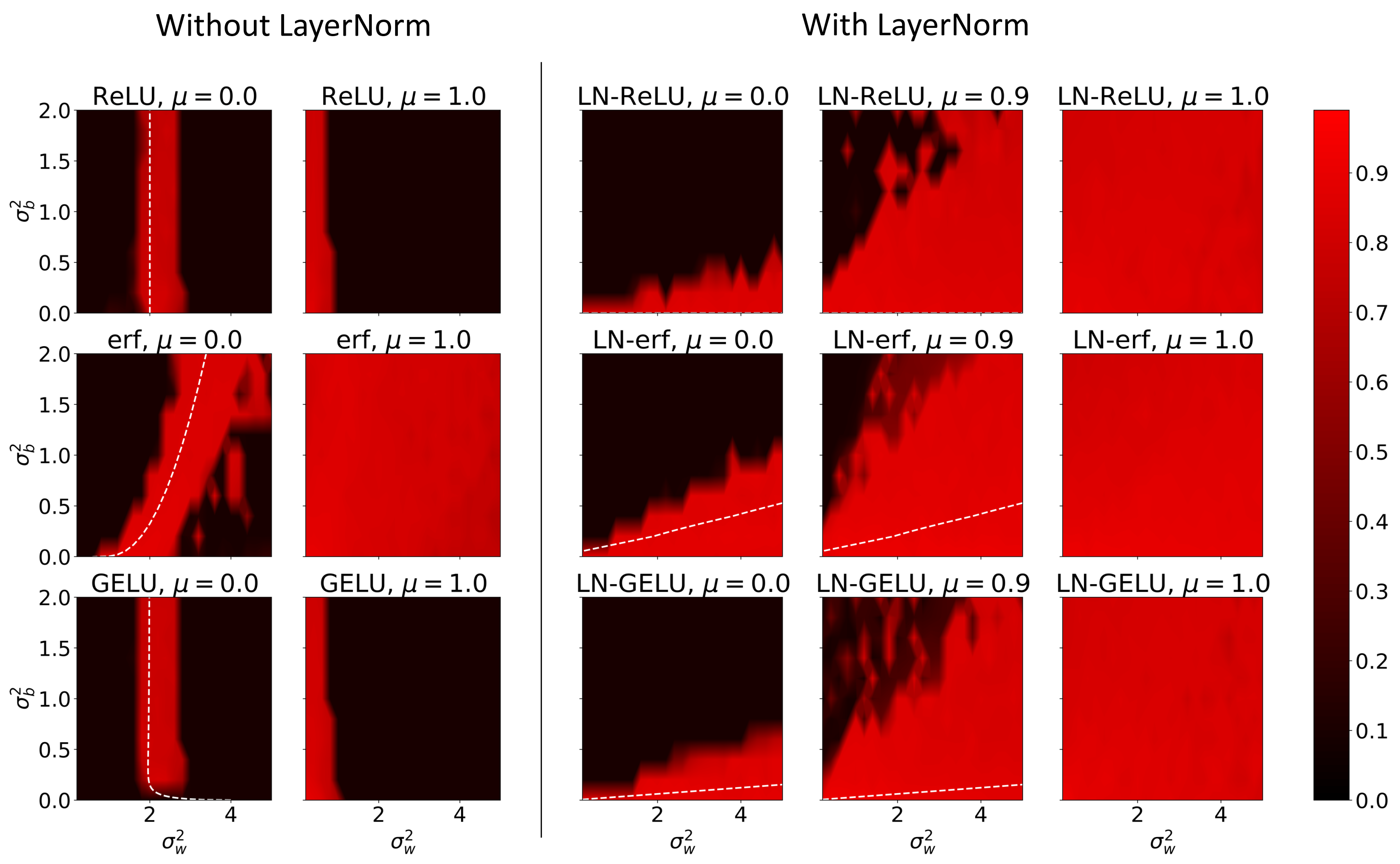
APJN Phase Diagrams



$\mathcal{J}^{l-1,l}$ phase diagrams of MLP ReLU, erf and GELU activations

- For real, finite width networks, we use numerical estimates for APJN; utilizing backward pass.
- Networks with **pre**-LayerNorm and $\mu = 1$ are **everywhere critical**!
  In this case, $\mathcal{J}^{l_0,l} \sim l^{-\zeta}$ where ζ depends on σ_w, σ_b.
- Bounded activations, with $\mu = 1$ *without* LayerNorm are **semi-critical**.
  In this case, $\mathcal{J}^{l_0,l} \sim e^{\sqrt{l/\lambda}}$, where λ depends on σ_w, σ_b.

Training Results



Training accuracy of $L = 50$ MLP on FashionMNIST dataset.

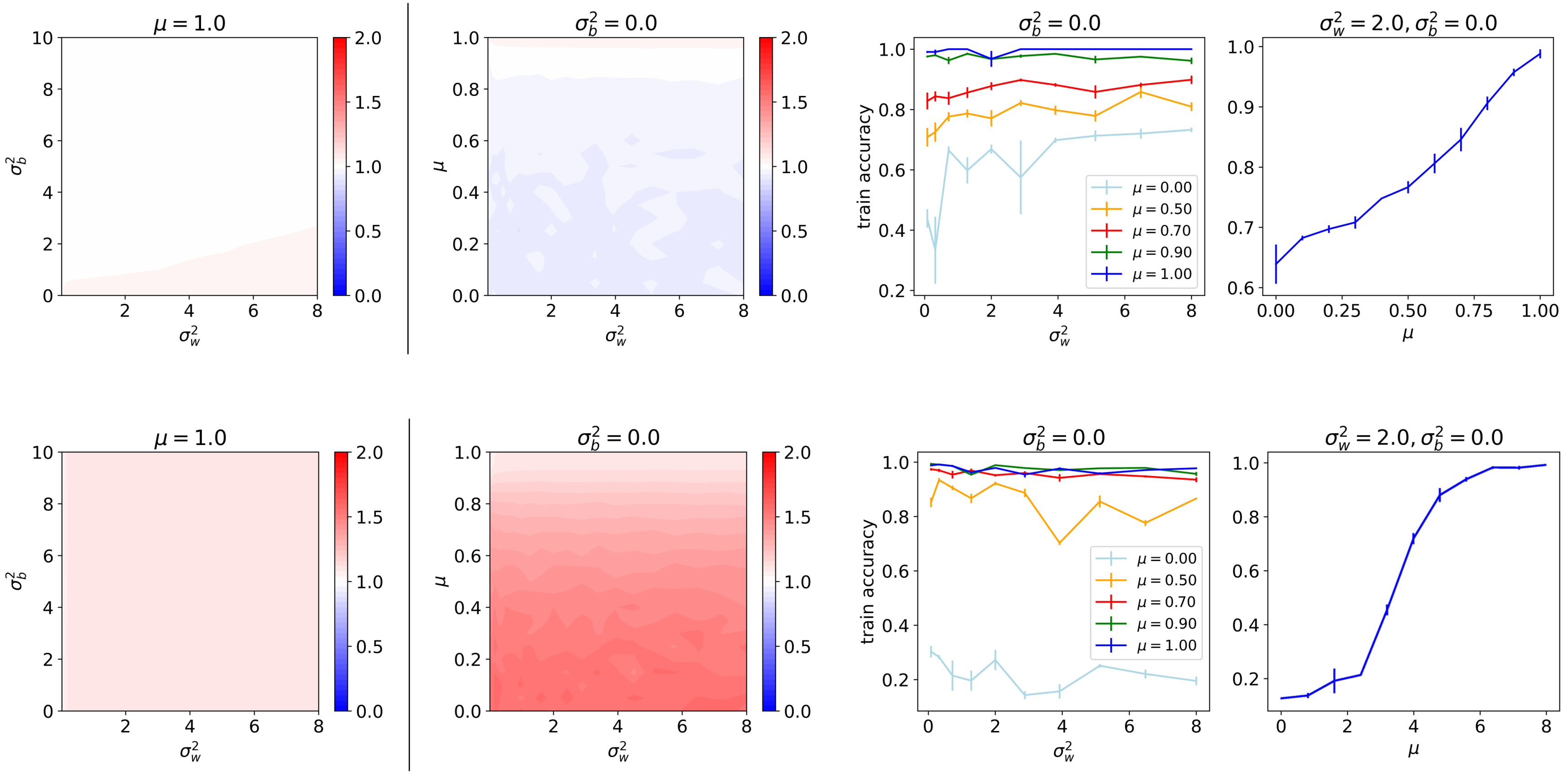
- Training results are in excellent agreement with APJN phase diagrams.
- Networks with Pre-LayerNorm and $\mu = 1$ are, in fact, **everywhere trainable**!
- Network with erf, $\mu = 1$ and no LayerNorm has enhanced trainability.

ResNet110 V2

$\mathcal{J}^{l-1,l}$ phase diagrams for $(\sigma_w - \sigma_b)$ and $(\sigma_w - \mu)$; training accuracies on CIFAR10.

LayerNorm

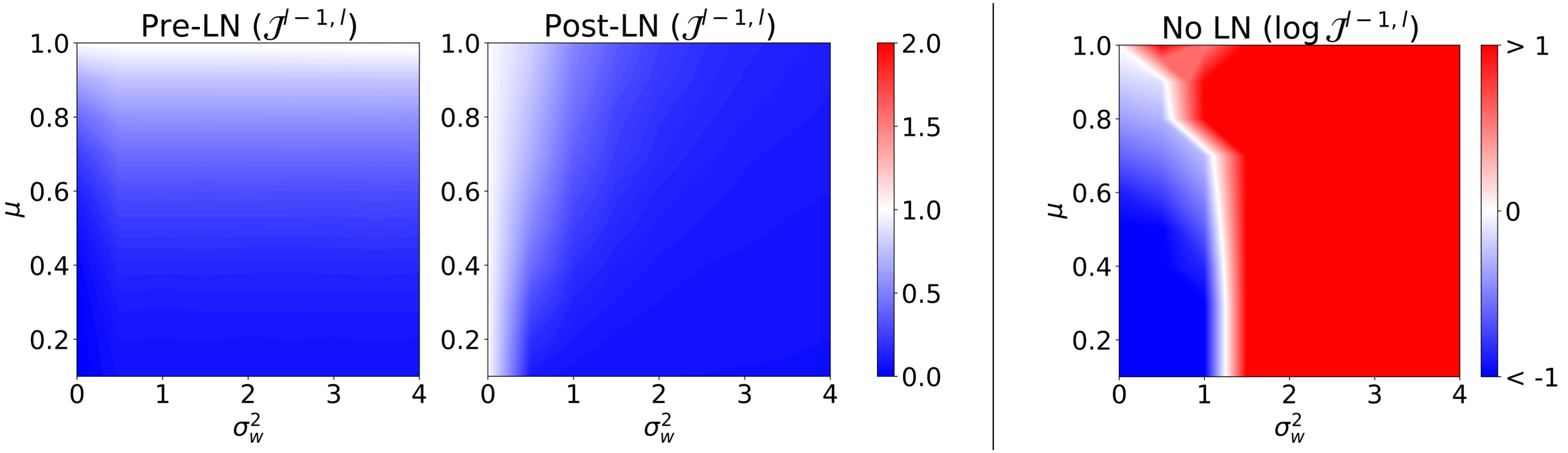
BatchNorm



- In both cases, the architecture is everywhere-critical with $\mu = 1$.
- $\mu < 1$ cases are drastically different for LayerNorm and BatchNorm.

Vision Transformer

$\mathcal{J}^{l-1,l}$ phase diagrams for $(\sigma_w - \mu)$, with pre-LN, post-LN and no LN.

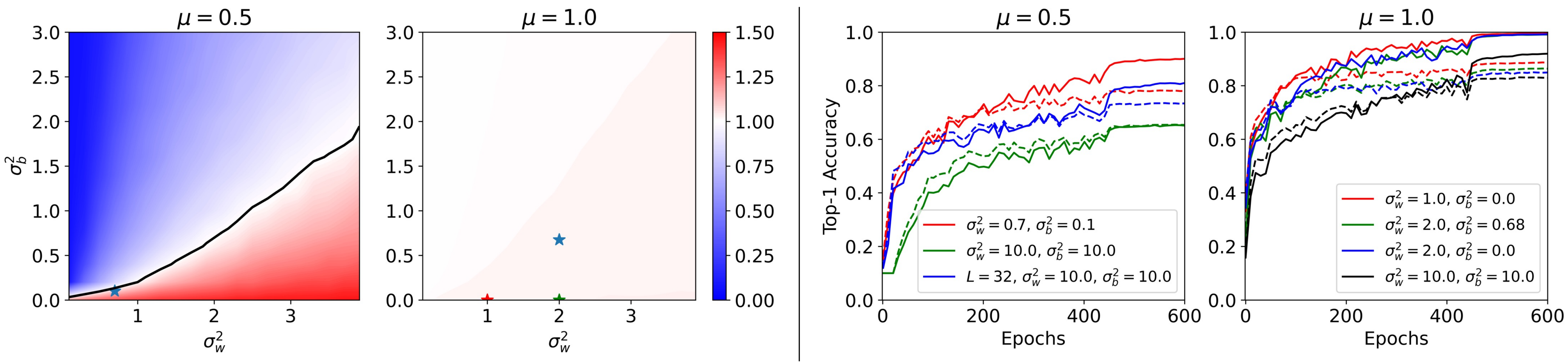


- In the pre-LN case, $\mu = 1.0$ is *everywhere-critical*.
- Post-LN and no LN cases do not feature everywhere-criticality.
- The advantage of Pre-LN Transformer is empirically known in literature.

Xiong et al. "On Layer Normalization in the Transformer Architectures". (2020)

MLP-Mixer

$\mathcal{J}^{l-1,l}$ phase diagrams for $\mu = 1.0$ and $\mu = 0.5$; training accuracies on CIFAR10.



- $\mu = 1.0$ case is *everywhere-critical*; while $\mu = 0.5$ is not.
- As a result, $\mu = 1.0$ trained well for all initializations; whereas $\mu = 0.5$ deteriorates far from the critical line.

Thank you!

Questions + comments?

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