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On the Nonlinearity of Layer Normalization

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Outline

- Background
- The Existence of Nonlinearity in LN
- Capacity of a Network with LN
- Amplify and Exploit the Nonlinearity of LN
- Conclusion

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Background

Input ↓

Linear Layer → **store** the main **parameters** of the neural network

↓

Non-Linear Layer → contains the main **expressive power**

↓

Normalization Layer →

Previous:

→ **stablizing** training and **accelerating** optimization

BN: $\hat{x} = \dfrac{x - \mu}{\sqrt{\sigma^2 + \epsilon}}$ → Optimization > Fitting

But?

↓

……

↓

Normalization Layer

↓

Linear Layer

Output ↓

Background

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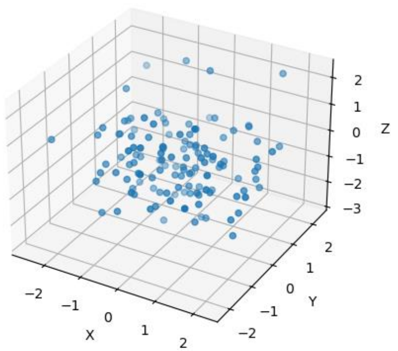
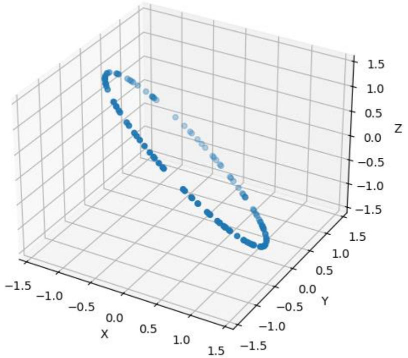
Layer Normalization



$$\hat{x}_i = \frac{x_i - \mu}{\sqrt{\sigma^2 + \epsilon}}$$

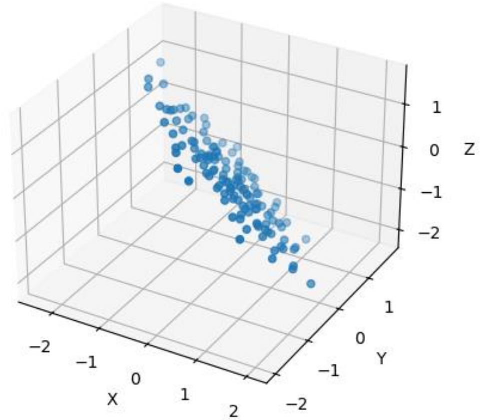


Centering

$$\bar{\boldsymbol{x}} = \boldsymbol{x} - \frac{\mathbf{1}}{\boldsymbol{d}}(\mathbf{1}_d^{\top} \boldsymbol{x}) \cdot \mathbf{1}_d$$

Projected onto the Hyperplane

$$\{\boldsymbol{x} \in \mathbb{R}^d : x_1 + \cdots + x_d = 0\}$$

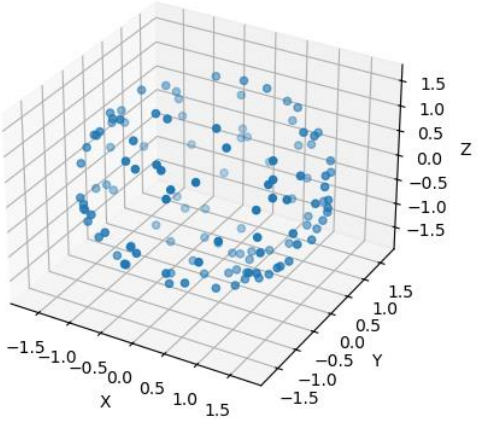


Scaling

$$\hat{\boldsymbol{x}} = \sqrt{d}\,\frac{\bar{\boldsymbol{x}}}{\|\bar{\boldsymbol{x}}\|_2}$$

Projected onto the Hypersphere

$$\{\boldsymbol{x} \in \mathbb{R}^d : [x_1]^2 + \cdots + [x_d]^2 = \mathrm{d}\}$$



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The Existence of Nonlinearity in LN

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Find a linearly invariant index.

$$SS(\boldsymbol{X}_c) = \sum_{i=1}^{m} \|\boldsymbol{x}_{ci} - \overline{\boldsymbol{x}}_c\|^2$$

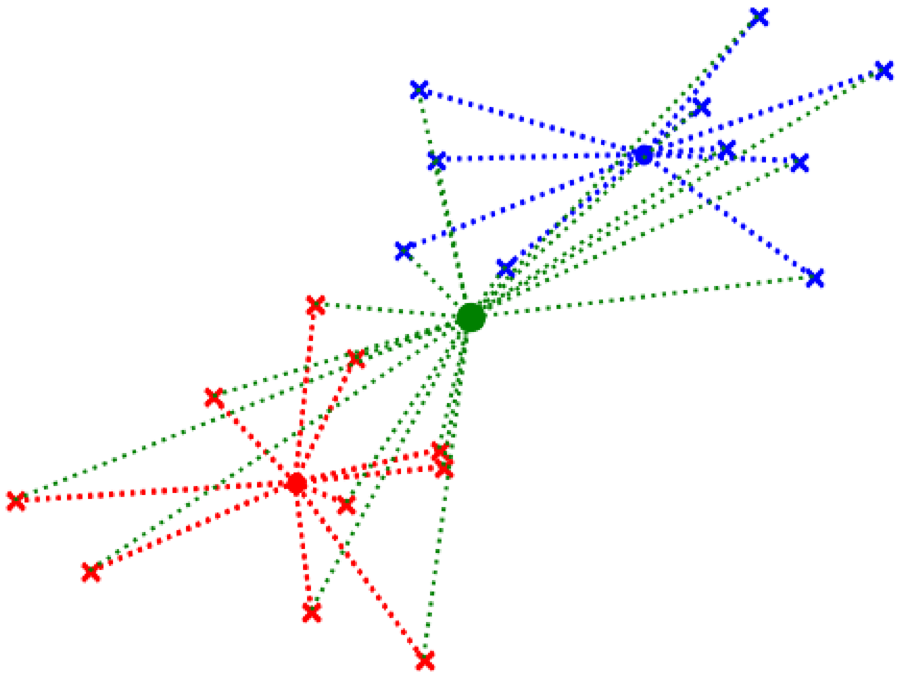
Intra distance

$$SSR(\boldsymbol{X}_1,\boldsymbol{X}_2) = \frac{\underline{SS(\boldsymbol{X}_1)} + SS(\boldsymbol{X}_2)}{\underline{SS([\boldsymbol{X}_1,\boldsymbol{X}_2])}}$$

Total distance

$$LSSR(\boldsymbol{X}_1,\boldsymbol{X}_2) = \inf_{\underline{\varphi \in \mathbb{D}_\varphi(d)}} SSR(\varphi(\boldsymbol{X}_1),\varphi(\boldsymbol{X}_2))$$

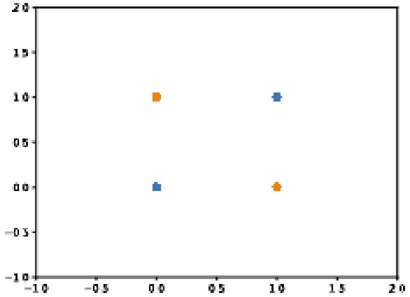
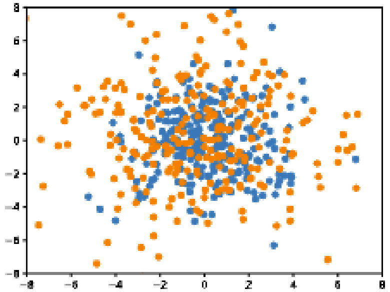
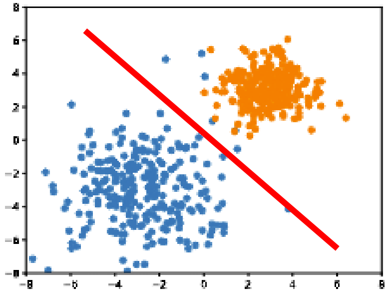
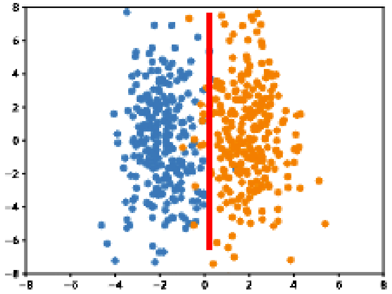
Linear Transformations



The Existence of Nonlinearity in LN

SSR and LSSR

*XOR data

Data				
Linearly separable?	No	No	Yes	Yes
SSR	0.9963	0.9929	0.2304	**0.7365**
LSSR	0.9929	0.9859	**0.1312**	0.2157

LSSR is a better index to describe linear separability than SSR.

The Existence of Nonlinearity in LN

Proof Method

Taylor's Expansion $f(x) = f(x_0) + f'(x_0)(x - x_0) + o(x - x_0)$

A brief equation $$\underbrace{SSR\left(v^T\hat{X}_1, v^T\hat{X}_2\right)}_{\text{Linear+Scaling}} = \underbrace{LSSR(X_1, X_2)}_{\text{Lower Bound}} \boxed{-\frac{2(T_1 + T_2)}{T_3}t + o(t)}$$

$< \mathbf{0}$

Linear transformations with LN can break LSSR.

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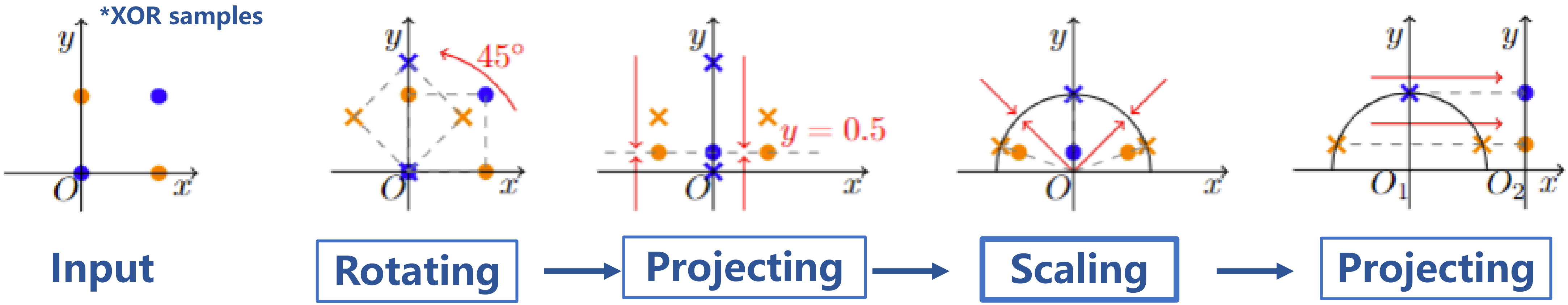
Capacity of a Network with LN

XOR



Classify XOR samples with linear transformations and scaling only.

※ **Hint:** Scaling can be represented by LN and linear transformations only.

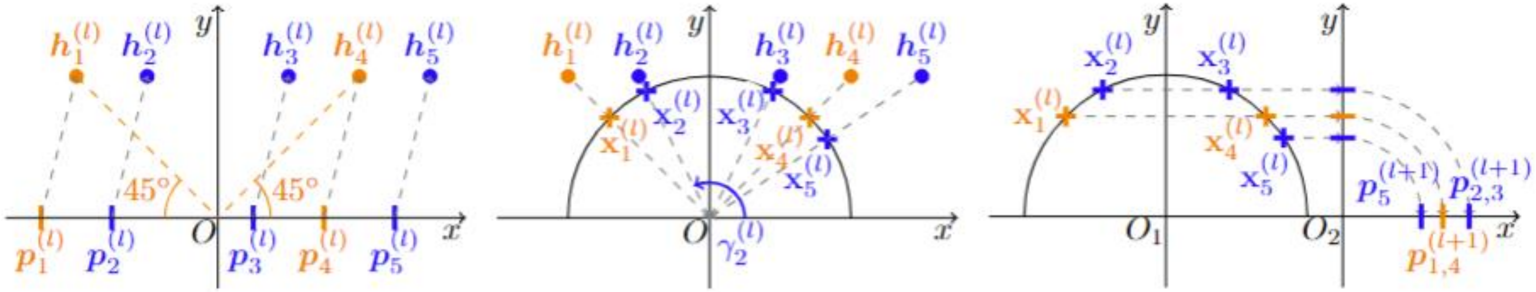
Capacity of a Network with LN

Binary Classification

Algorithm 1 Projection Merge Algorithm

input The initial input $\boldsymbol{P}^{(1)}$.
output The final output $\boldsymbol{P}^{(L)}$.

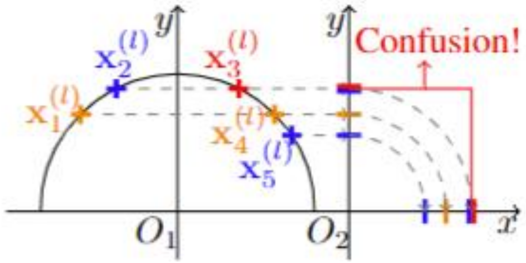
$l \leftarrow 1$;
$\mathbb{P} \leftarrow \{\boldsymbol{p}_1^{(l)}, \boldsymbol{p}_2^{(l)}, \cdots, \boldsymbol{p}_m^{(l)}\}$;
while $\mathbb{P} \neq \emptyset$ **do**
  $i \leftarrow \arg\min_k \{p_k^{(l)} : \boldsymbol{p}_k^{(l)} \in \mathbb{P}\}$;
  $\mathbb{J}_i \leftarrow \{\boldsymbol{p}_j^{(l)} \in \mathbb{P} : \boldsymbol{p}_j^{(l)} \neq \boldsymbol{p}_i^{(l)}, y_j = y_i\}$;
  if $\mathbb{J}_i \neq \emptyset$ **then**
    $j \leftarrow \arg\min_k \{p_k^{(l)} : \boldsymbol{p}_k^{(l)} \in \mathbb{J}_i\}$;
    for $k \leftarrow 1$ to m **do**
      $\boldsymbol{h}_k^{(l)} \leftarrow \boldsymbol{p}_k^{(l)} - \begin{bmatrix} p_i^{(l)} + p_j^{(l)} \\ p_i^{(l)} - p_j^{(l)} \end{bmatrix} / 2$;
      $\mathbf{x}_k^{(l)} \leftarrow \boldsymbol{h}_k^{(l)} / \|\boldsymbol{h}_k^{(l)}\|$;
      $\boldsymbol{p}_k^{(l+1)} \leftarrow \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \mathbf{x}_k^{(l)}$;
    end for
    $l \leftarrow l + 1$;
    $\mathbb{P} \leftarrow \{\boldsymbol{p}_1^{(l)}, \boldsymbol{p}_2^{(l)}, \cdots, \boldsymbol{p}_m^{(l)}\}$;
  else
    remove $\boldsymbol{p}_j^{(l)}$ from $\mathbb{P}$, as long as $\boldsymbol{p}_j^{(l)} = \boldsymbol{p}_i^{(l)}$;
  end if
end while
return $\boldsymbol{P}^{(l)}$;



Projecting → **Scaling** → **Projecting**

Binarily classify any m samples with linear transformations and scaling only.

Multiclass Classification



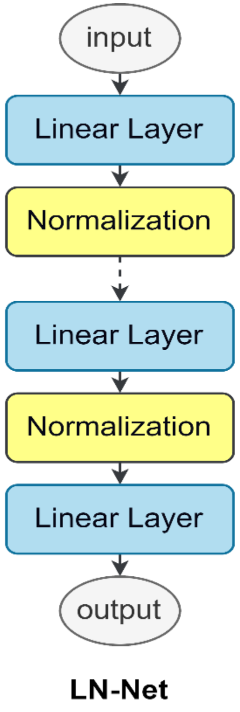
Difference: Confusion is possible.

Solution: Breaking Parallelization.

Capacity of a Network with LN

▶ The first to discuss about the expressive power of layer normalization.

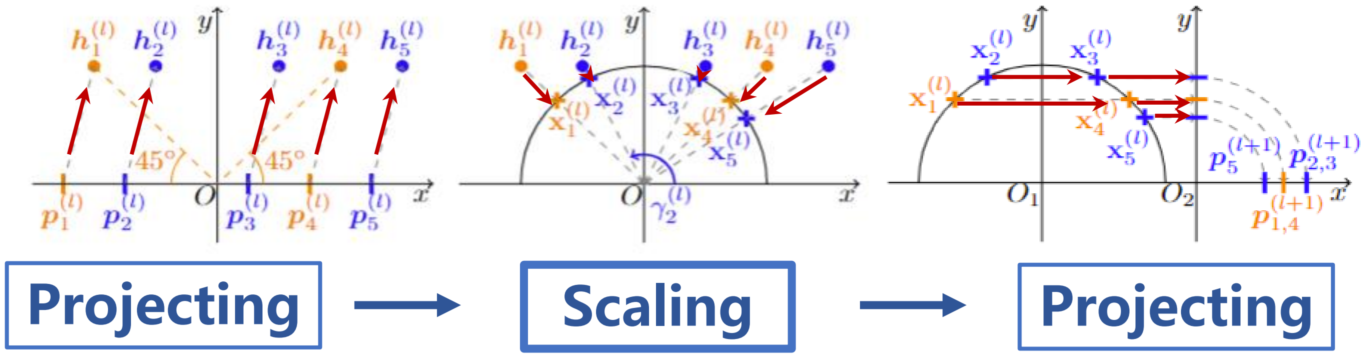
Universal Approximation Theory of LN-Net



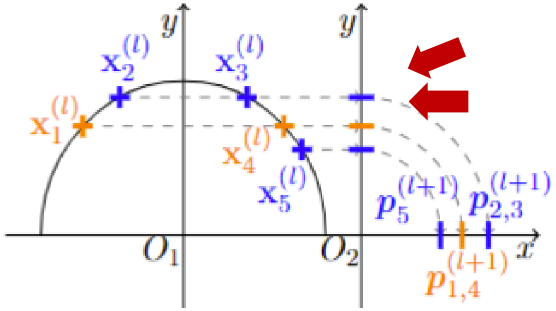
An infinitely deep LN-Net can classify any given m samples correctly.

Computation Operation ⇒ **Merging Operation**

Universal Approximation ⇒ **Universal Classification**



VC dimension



Samples with the same label: at least two are merged with each LN.
Samples with different labels: none are merged.
Width: at least 3.

▶ Given an LN-Net $f_\theta(\cdot)$ with width 3 and depth L its VC dimension $VCdim(f_\theta(\cdot))$ is lower bounded by $L+2$.

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Amplify and Exploit the Nonlinearity of LN

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Group based LN (LN-G) has stronger nonlinearity than LN

Measurement of Nonlinearity

Hessian: $\mathcal{H}(f;x) = \sum_{i=1}^{d} \left\| \left| \frac{\partial^2 y_i}{\partial x^2} \right| \right\|_F^2$

Noted that $\mathcal{H}(f;x) \geq 0$, and $\mathcal{H}(f;x) = 0$ if and only if f is linear.

$\rightarrow$ We ***assume*** that the larger $\mathcal{H}(f;x)$, the more nonlinearity f contains.

Amplifying Nonlinearity by Group

Proposition: Given $g \leq d/3$, we have $\frac{\mathcal{H}(\psi_G(g;\cdot);x)}{\mathcal{H}(\psi_L(\cdot);x)} \geq 1$. When $g = d/4$, $\frac{\mathcal{H}(\psi_G(g;\cdot);x)}{\mathcal{H}(\psi_L(\cdot);x)} \geq \frac{d}{8}$.

※ $\psi_G(g;\cdot)$ denotes LN-G on $\mathbb{R}^d$ with group number g, $\psi_L(\cdot)$ denotes LN on $\mathbb{R}^d$.

$\rightarrow$ LN-G can amplify the nonlinearity of LN by using appropriated group number.

Amplify and Exploit the Nonlinearity of LN

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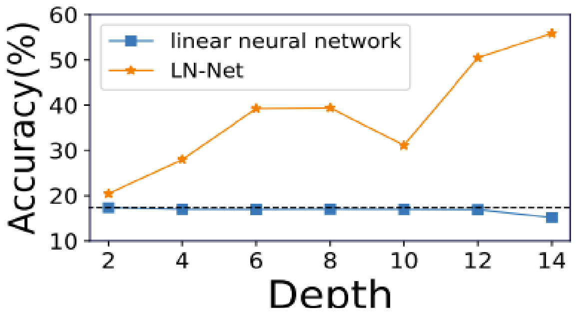
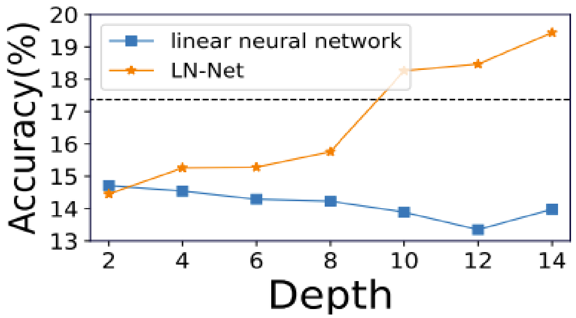
Comparison of Representation Capacity by Fitting Random Labels

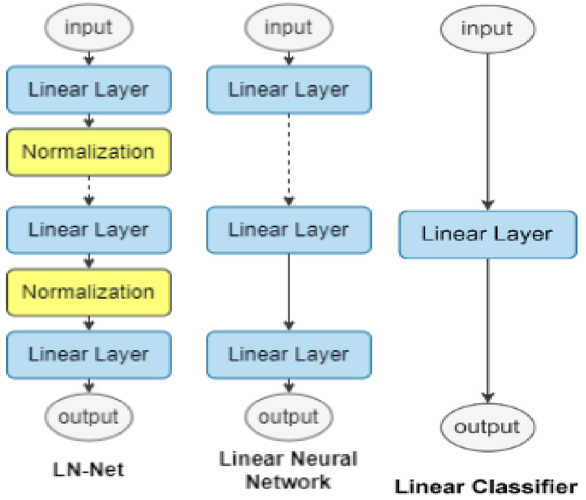
LN-Net & linear neural network & linear classifier



(a) CIFAR-10-RL.

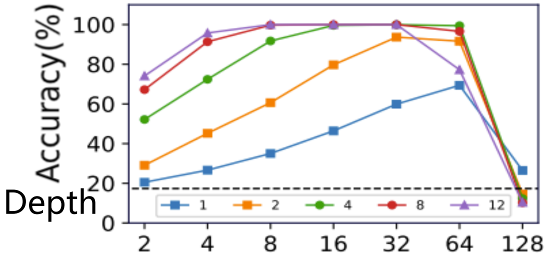


(b) MNIST-RL.

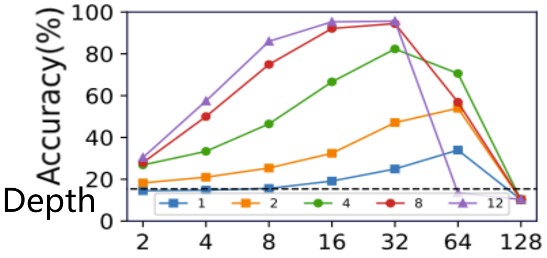


→ LN can break the bound of linearity.

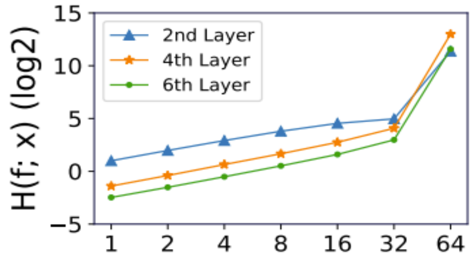
LN-Net (LN-G)



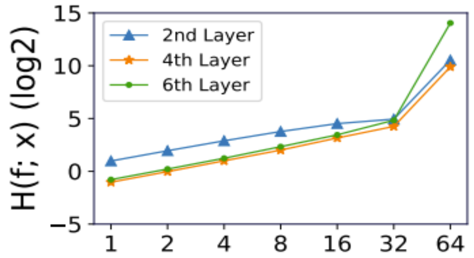
(a) Accuracy on CIFAR-10-RL.



(b) Accuracy on MNIST-RL.



(c) $\mathcal{H}(f;\mathbf{x})$ on CIFAR-10-RL.



(d) $\mathcal{H}(f;\mathbf{x})$ on MNIST-RL.

Amplify and Exploit the Nonlinearity of LN

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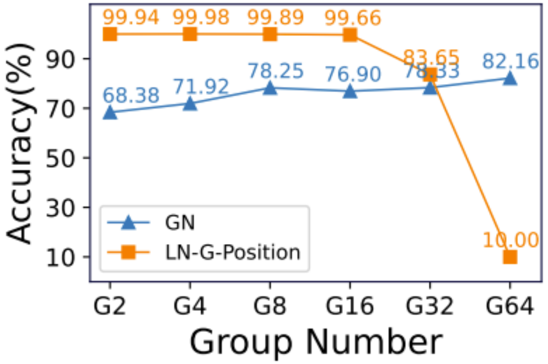
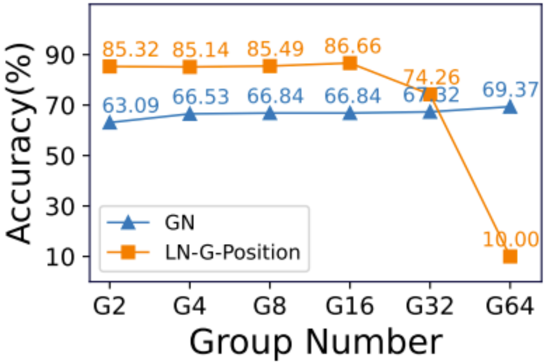
Inspiration for Neural Architecture Design

ResNet without ReLU on CIFAR-10



(a) Training.



(b) Test.

Normalization methods	Train Acc(%)	Test Acc(%)
IN	10	10
BN	36.0	39.3
LN	59.5	62.85
GN	82.16	69.37
LN-G-Position	99.66	86.66

Transformer

fairseq-py on IWSLT14 De-EN:(BLEU) LN: 35.01 ± 0.10 ; LN-G: 35.23 ± 0.07

Tiny-ViT on CIFAR-10*: (test Acc)* LN: 88.81% ; LN-G: 89.26%

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Conclusion

- Mathematically demonstrated that LN is a nonlinear transformation.
- Theoretically showed the representation capacity of an LN-Net in correctly classifying samples with any label assignment.
- Call for reconsidering the analyses of the representation capacity of a network with normalization layer.

Thanks for your attention!