基于信息瓶颈理论的神经元竞争初始化策略

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Neuron Campaign for Initialization Guided by Information Bottleneck Theory

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Background

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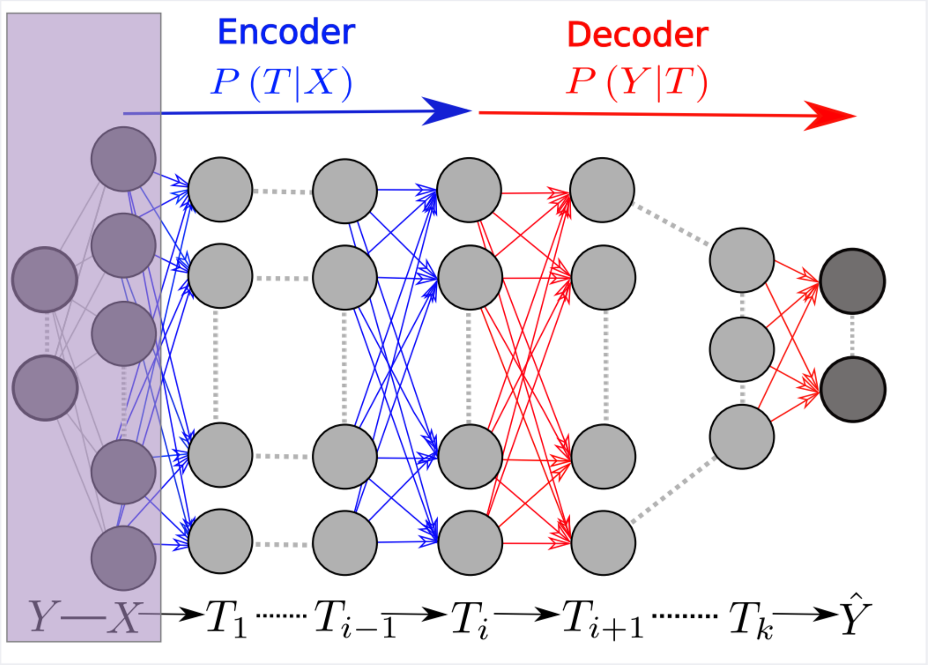
Information Bottleneck Theory

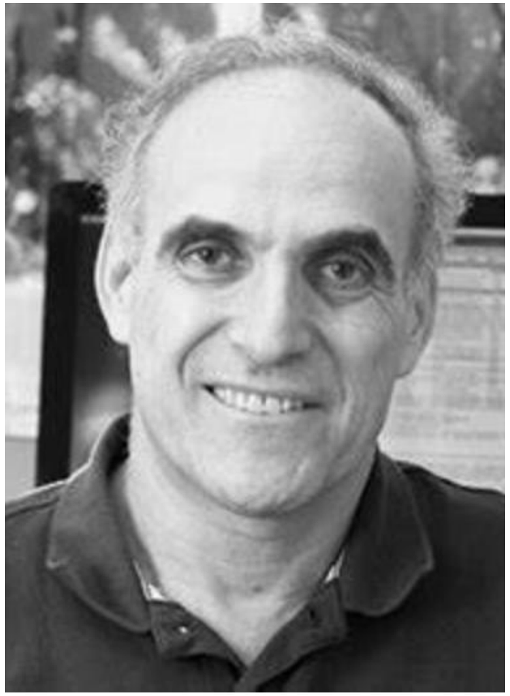
Information Bottleneck

- Tishby et al. believes that DNN training is actually optimizing the following objective:

$$\min_{\Theta} I(X;T) - \beta I(T;Y)$$

where T is the feature of each layer, X is the input and Y is the label

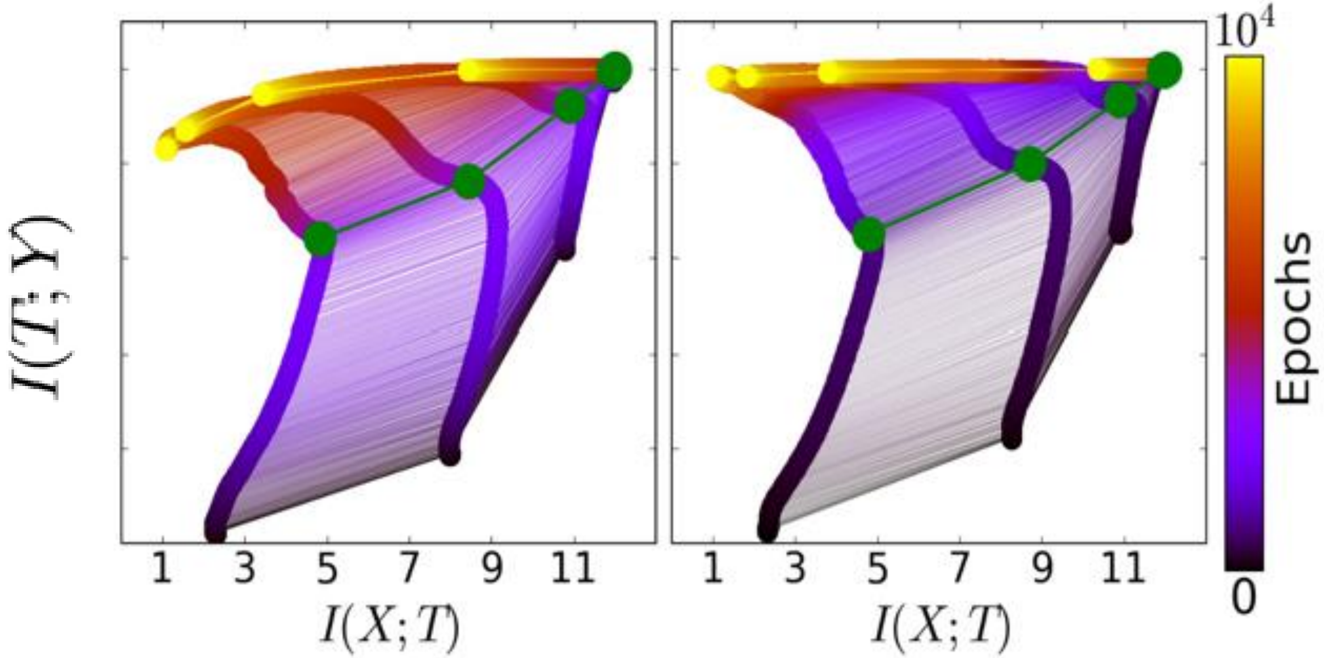




[1] Opening the Black Box of Deep Neural Networks via Information. Arxiv: 1703.00810

[2] Talk by Prof. Tishby: https://www.youtube.com/watch?v=bLqJHjXihK8&t=262s

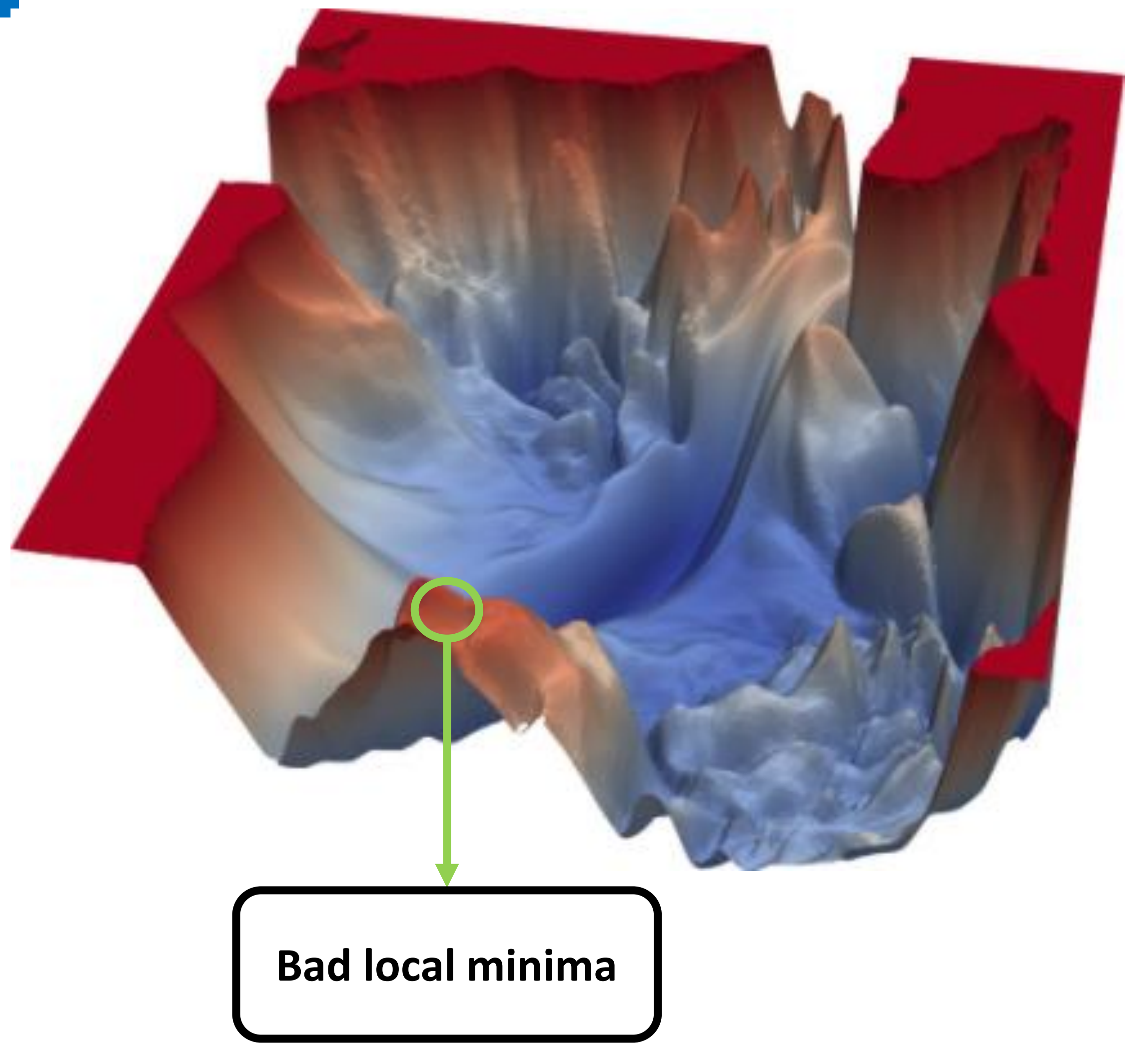
Information Bottleneck



- Phase 1: $I(X;\ T)$ and $I(T;\ Y)$ both increases, which indicates the network memorizes the information about the input
- Phase 2: $I(X;\ T)$ decrease while $I(T;\ Y)$ increases, which indicates that the network drops unimportant information to generalize.

Initialization Strategy

Background



- Training a DNN is to find a good local minima.
- A bad initialization may lead to stuck in a bad local minima.

Gradient vanish/explode

Random Initialization

$W \sim N(0, 0.01^2)$

```
x = torch.randn(512)

for i in range(100):
    a = torch.randn(512,512) * 0.01
    x = a @ x
x.mean(), x.std()
```

```
(tensor(0.), tensor(0.))
```

$W \sim N(0, 1)$

```
x = torch.randn(512)

for i in range(100):
    a = torch.randn(512,512)
    x = a @ x
    if torch.isnan(x.std()): break
i
```

```
28
```

Reason for it

- Gradient Exposure and vanish
  - Forward

$$y = W_3 * W_2 * W_1 * x$$

  - Backward

$$\nabla W_1 = \boxed{\frac{\partial Loss}{\partial f_3}} * \boxed{\frac{\partial f_3}{\partial z_3} * \frac{\partial f_2}{\partial z_2} * \frac{\partial f_1}{\partial z_1}} * \boxed{W_3 * W_2} * X$$

Glorot condition

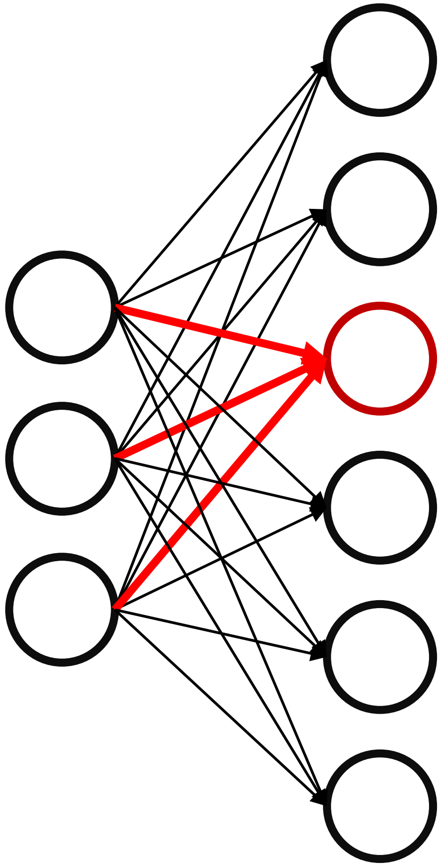
- The variance of the outputs of different hidden layer should be similar
- The variance of gradient from different layer should be similar

Xavier Initialization

$$y_l = W_l x_l + b_l$$

- *Assumptions*
  - *Linear activation function*
  - *The expectation of input and weight are all 0*
  - W_l *are mutually independent and share the same distribution*
  - x_l *are mutually independent and share the same distribution*
  - x_l *and* W_l *are independent of each other*
- Final form

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}\right]$$



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Variance scaling Initialization strategy

- He initialization (for Relu activation function)

$$W \sim N\left(0, \sqrt{\frac{2}{n_j}}\right)$$

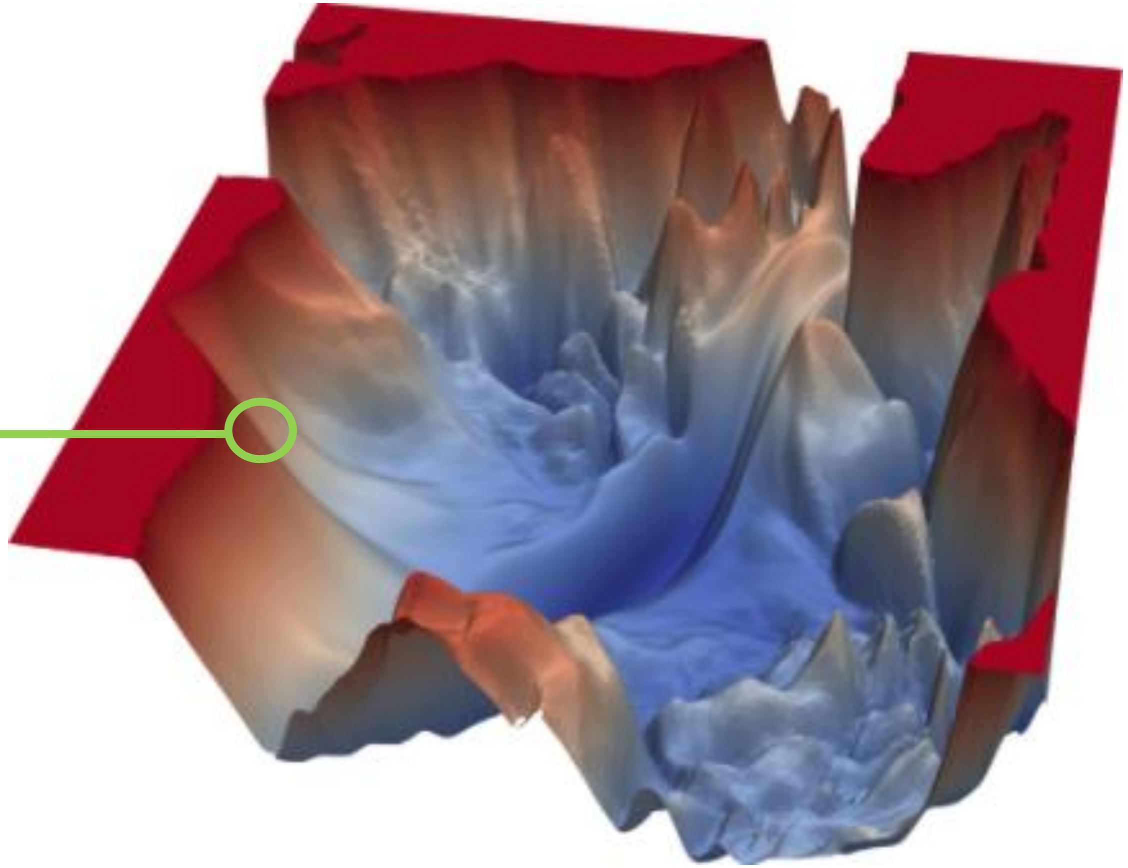
- LSUV (Layer Sequential Unit-Variance initialization)

$$\mathrm{W}_L = \mathrm{W}_L / \sqrt{var(Z_i)}$$

Introduction of Our paper

Motivation

- **What initialization leads to better generalization**
- **How to avoid fluctuation in the training**



Good point we want

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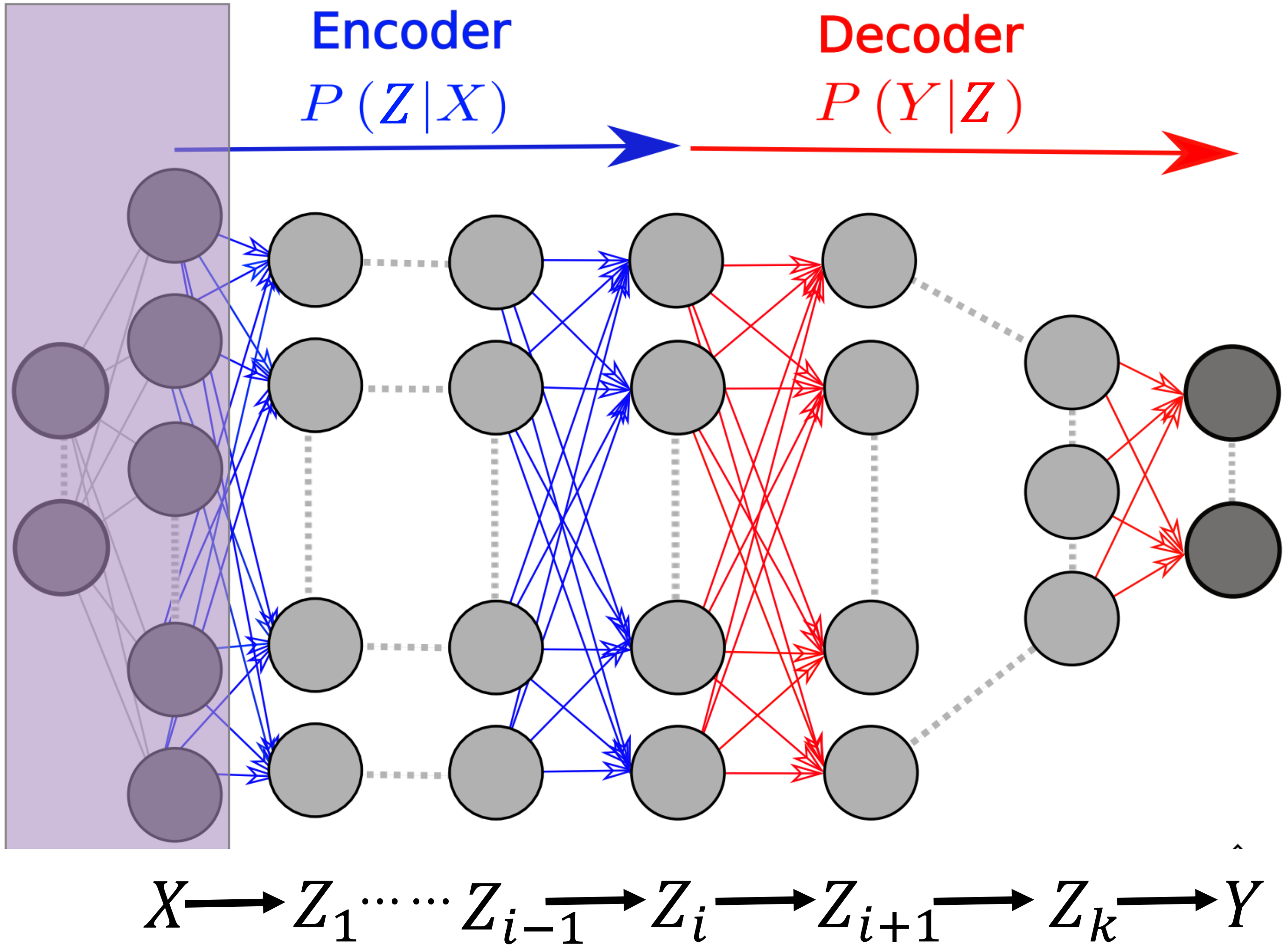
Approach

- **What is the good initialization point leads to better generalization**
  Two criteria guided by the Information Bottleneck Theory

- **How to find the local minima?**
  Neuron Campaign Initialization algorithm

Information Bottleneck Theory and measurement



- Input information maintenance:
  $$I(X;Z_i)$$
- Target-related information enhancement
  $$I(Z_i;Y)$$
- Criterion:
  $$\alpha I(X;Z_i) + (1-\alpha) I(Z_i;Y)$$
- The front layer should focus more on input information maintenance

Criteria Simplification with High Efficiency

- $I(X;Z_i)$ input information maintenance criterion

  $I(X;Z_i)$= H(Z) – H(Z|X) = H(Z)

$$tr(\Sigma_i)$$

  where Σ_i is the covariance matrix of Z_i

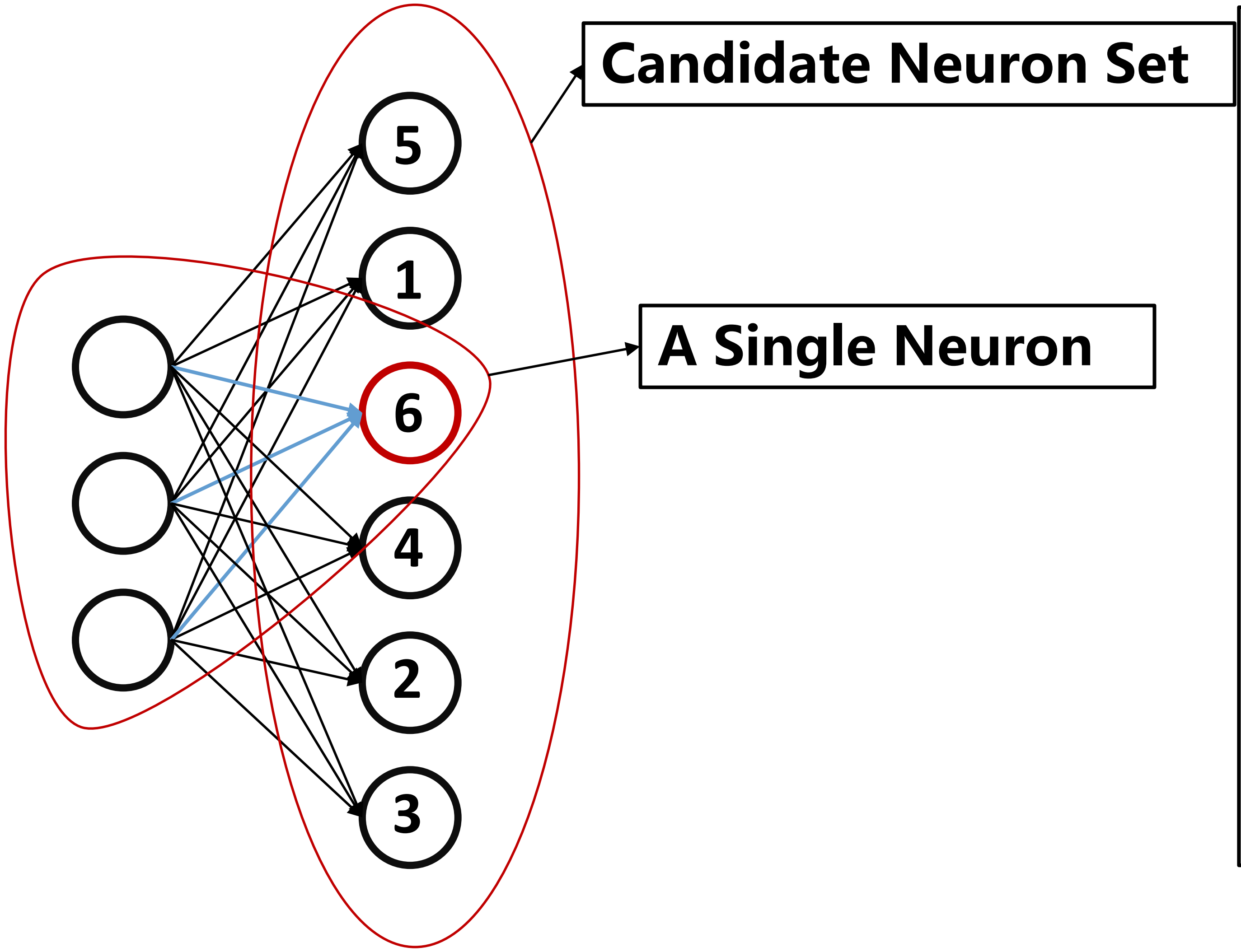
- $I(Z_i;Y)$ target-related maintenance criterion

$$tr\left(\widehat{H}\widehat{H}^T\right) - \frac{1}{N}\sum_{j=0}^{N} tr\left(\hat{Z}_i^T \Pi^j \hat{Z}_i\right)$$

Inter-class variance

Intra-class variance

Neuron Campaign Initialization algorithm



Output: weight with size [3, 3]

- Pre-Initialize a large neuron set with size [3, 6]
- Select neuron with well-designed criteria (based on IB) and **orthogonal** score
- Combine neurons as initial weight

Algorithm details

$X{:}[60000, 784] \xrightarrow{W} Z{:}[60000, 1000] \longrightarrow s{:}[1000]$

$X{:}[60000, 100] \xrightarrow{W} Z{:}[60000, 200] \longrightarrow s{:}[200]$

Algorithm 1 Neuron Campaign initialization algorithm

Input: Candidate weight matrix $\mathbf{W}$ [784, 1000]

1: **for** t=1 to T **do** T = 100

2: Update generalized orthnormalization matrix at t steps: $\mathbf{A}_t = (\mathbf{A}_{t-1}, \mathbf{a}_t^T)^T$ [784, t]

3: Calculate the null space projection by $\mathbf{P}_t = \mathbf{P}_{t-1} - \mathbf{a}_t\mathbf{a}_t^T\mathbf{W}$

4: Select optimal neuron whose index is chosen by $i = \max_i s_i \frac{||\mathbf{p}_t^i||}{||\mathbf{W}_i||}$

5: Update $\mathbf{w}^* = \mathbf{W}_{\cdot,i}$

6: Normalize basis of the generalized orthnormalization matrix as $\mathbf{a}_{\mathbf{t+1}} = \mathbf{p}_t^i/||\mathbf{p}_t^i||$

7: **end for**

Output: Winning neurons formed weight matrix $\mathbf{W}'$ [784, 100]

Ensure orthogonality of the selected neurons

Select the neuron with largest score

Evaluation

Experimental details

Table 1: minimal error rate and corresponding epoch comparison of IBCI with baseline methods on MNIST.

Strategy	Layers	Vanilla	LSUV	**IBCI**
Xavier	2	2.04 ± 0.03 (75)	2.05 ± 0.06 (51)	$\mathbf{1.93 \pm 0.06}$ **(60)**
	3	1.82 ± 0.05 (52)	1.80 ± 0.07 (63)	$\mathbf{1.71 \pm 0.09}$ **(36)**
	5	2.83 ± 0.16 (98)	3.13 ± 0.17 (69)	$\mathbf{2.53 \pm 0.09}$ **(78)**
He	2	2.03 ± 0.03 (65)	2.00 ± 0.04 (70)	$\mathbf{1.93 \pm 0.07}$ **(57)**
	3	1.83 ± 0.05 (54)	1.86 ± 0.07 (71)	$\mathbf{1.73 \pm 0.04}$ **(35)**
	5	2.76 ± 0.07 (80)	2.90 ± 0.12 (77)	$\mathbf{2.62 \pm 0.08}$ **(73)**

Hidden layer dimension setting

layers	Hidden Layer Dimension
2	784, 100, 10
3	784, 256, 100, 10
5	784, 32, 32, 32, 32, 10

Ablation Study

Table 2: minimal error rate and corresponding epoch comparison of IBCI with methods with only one criterion.

Strategy	Layers	IBCI	TIE	IIM
Xavier	2	**1.93 ± 0.06 (60)**	2.04 ± 0.07 (58)	2.07 ± 0.09 (84)
	3	**1.71 ± 0.09 (36)**	1.82 ± 0.03 (43)	1.82 ± 0.05 (52)
	5	**2.53 ± 0.09 (78)**	2.68 ± 0.05 (82)	2.57 ± 0.09 (84)
He	2	**1.93 ± 0.07 (57)**	2.07 ± 0.06 (59)	2.034 ± 0.09 (62)
	3	**1.73 ± 0.04 (35)**	1.83 ± 0.07 (42)	1.856 ± 0.05 (55)
	5	**2.62± 0.08 (73)**	2.89 ± 0.11 (74)	2.67 ± 0.12 (86)

Target Information Enhancement, i.e., IBCI without IIM

Input Information Maximization , i.e., IBCI without TIE

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Conclusion & Future work

Conclusion & Future Work

Conclusion

- Introduce the Information Bottleneck Theory into practice use.
- Propose a novel and interesting neuron campaign initialization algorithm.

Future work

- Introduce to broader neural network architectures.
- Can we help to understand the recent popular initialization with pretrain?

Further Exploration

Neuron with Steady Response Leads to Better Generalization

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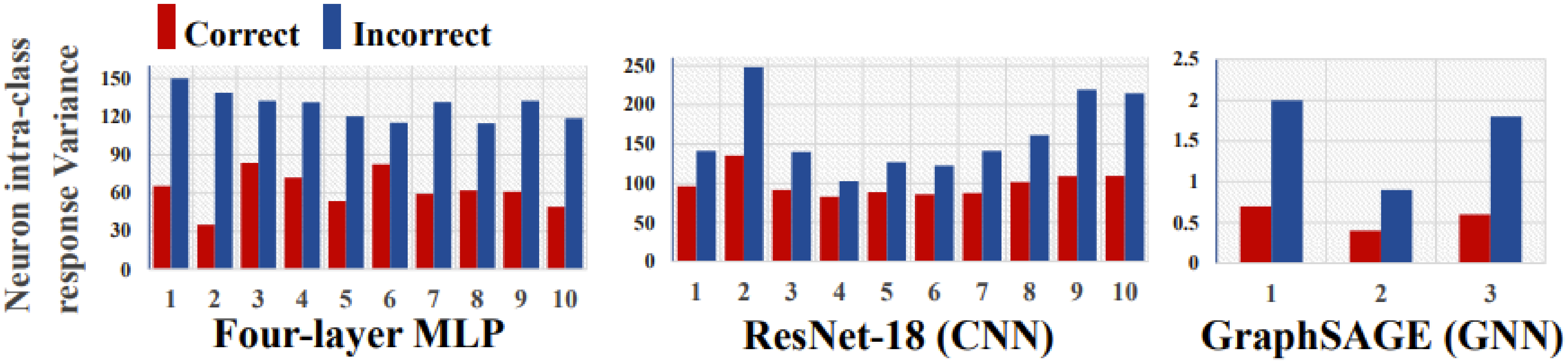
Observation 1

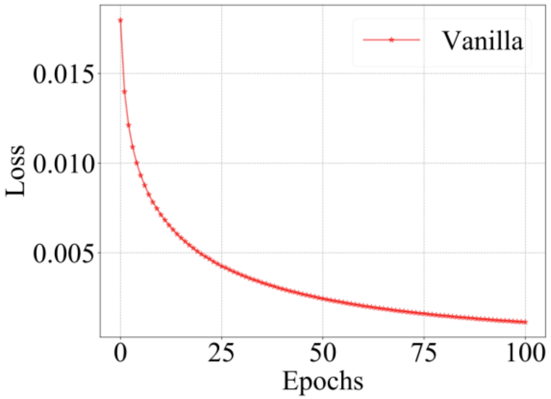
- Intra-class response variance of correctly classified samples is smaller than that of misclassified ones on arbitrary class
- Smaller intra-class response variance leads to better generalization



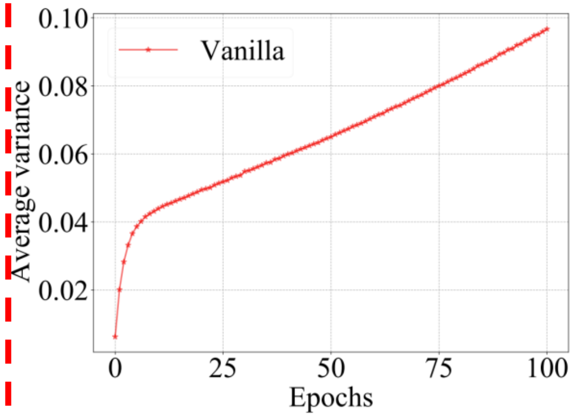
The horizontal axis and the vertical axis represent class indexes and the value of intra-class response variance, respectively.
Each bar represents the intra-class response variance aggregated from all neurons in the penultimate layer.

Observation 2

- Does cross entropy control intra-class response variance well? No!
- The ascending intra-class response variance shows the potential improvement space for the regularization



(a) Training cross-entropy loss



(b) Training intra-class variance

Ascending Variance!

Training procedure of vanilla four-layer MLP on MNIST

Key Insight

- Neuron with small intra-class responses variance can lead to better generalization
- Cross entropy can NOT control intra-class response variance well

Regularization on intra-class response variance is needed!

Neuron Steadiness Regularization (NSR)

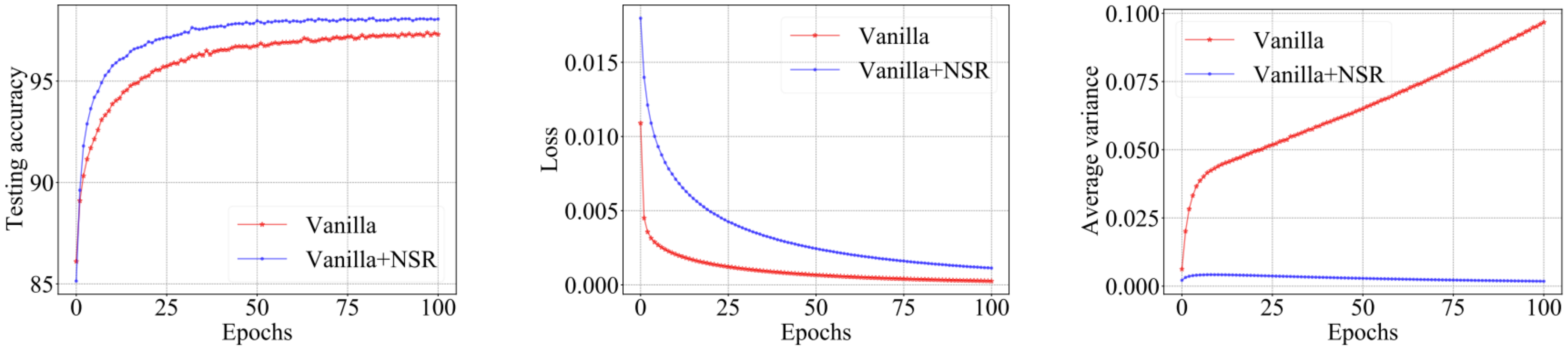
- We propose a new regularization method called NSR
  - NSR is the first work to encode inductive bias from the perspective of **class-dependent response distribution** of individual neurons
- NSR improves generalization by controlling neuron intra-class response variance
  - Significant improvement on MLP, CNN, and GNN
  - Bigger improvement than typical regularizations like L1/L2/Jacobian
  - Further gain when combining with Batch Normalization and Dropout
- NSR has low overhead on both memory and computation

Evaluation Setting

Network Architecture	Vanilla model	Dataset	Optimization
Multiplayer Perceptron	MLP-3,4,6,8,10	MNIST	SGD
Convolutional Neural Network	ResNet-18	CIFAR-10	Momentum
	VGG-19		
	ResNet-50	ImageNet	Adam
Graph Neural Network	GraphSAGE	WikiCS, PubMed, Amazon-Photo, Computers	Adam
	GCN		

Dynamics of Training & Testing

- Neuron intra-class response variance is growing larger in vanilla model
- NSR could control neuron intra-class response variance well
- NSR has higher testing accuracy although its cross-entropy loss is even larger



(a) Testing accuracy (b) Training cross-entropy loss (c) Training intra-class variance

Training procedure of vanilla four-layer MLP and four-layer MLP with our Neuron Steadiness Regularization on MNIST

Some advice for undergraduate Research

- 培养感恩和善良的心
- 失败是常态, 学会去面对
- 打好机器学习基础&写一写博客，对社区有一些贡献
- shoot low, aim high
- 关注心理健康, 学会自我调节
  - 书籍：活出心花怒放的人生
  - Up主： 是慢慢丫

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Thanks & QA

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