Why Adversarial Interaction Creates Non-Homogeneous Patterns: A Pseudo-Reaction Diffusion Model for Turing Instability

Litu Rout

Association for the Advancement of Artificial Intelligence (AAAI-21)

Preprint: https://liturout.github.io/data/aaai21_preprint.pdf

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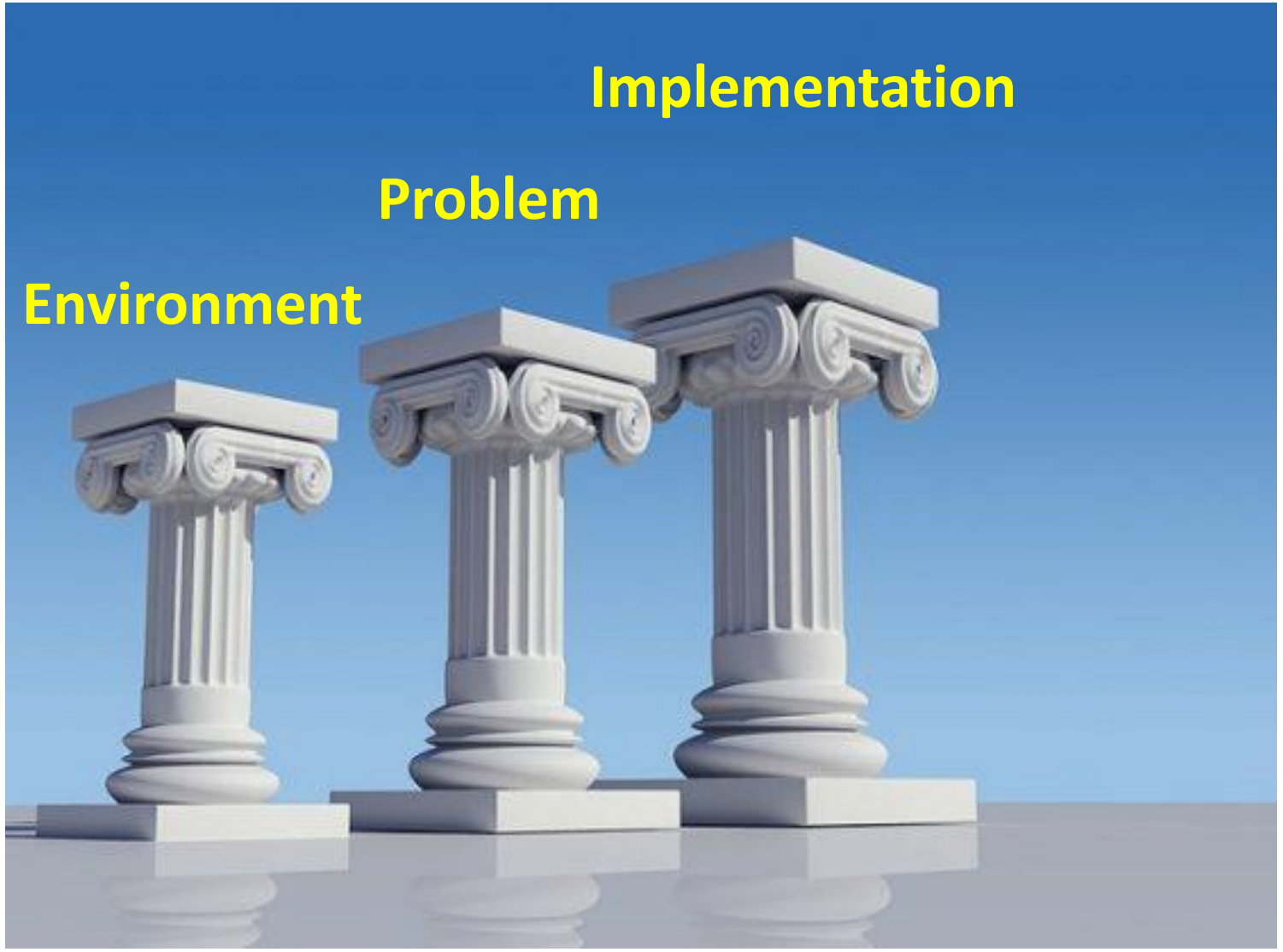
Why Adversarial Interaction Creates Non-Homogeneous Patterns: A Pseudo-Reaction Diffusion Model for Turing Instability

- Adversarial Interaction
  - Generative Adversarial Networks (GANs)
  - Application of conditional GANs
- Non-Homogeneous Patterns
  - Homogeneous patterns
  - Supervised learning
- Reaction-Diffusion
  - Turing's RD model (1952)
  - Gray-Scott RD model (1984)
- Turing Instability
  - Reaction dynamics
  - Diffusion dynamics

Three Pillars of Deep Learning



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Outline

- Maximum Likelihood Estimation
- Reverse KL Divergence
- Introduction to GANs
- GANs in Remote Sensing
  - Problem Formulation

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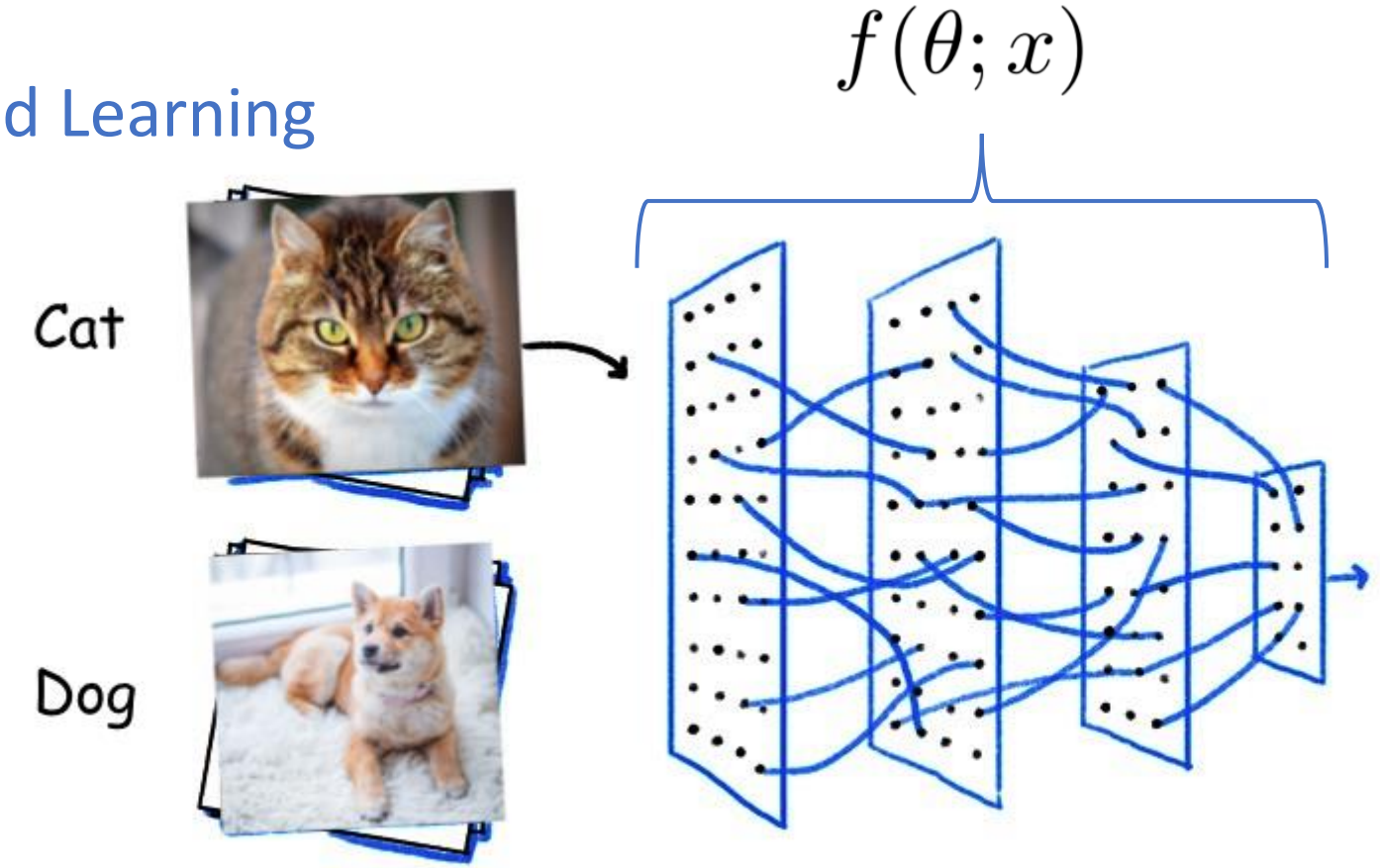
Understanding the Role of Adversarial Regularization in Supervised Learning

- Mitigating Vanishing Gradient
- Asymptotic Iteration Complexity
- Sub-optimality Gap
- Provable Convergence
- Generalization Error (Open Problems)
- Neural Topology Analysis (Open Problems)

L.R., CVPR-AML-CV 2021: https://liturout.github.io/data/cvpr2021_aml_cv.pdf

Problem Setup

- Supervised Learning

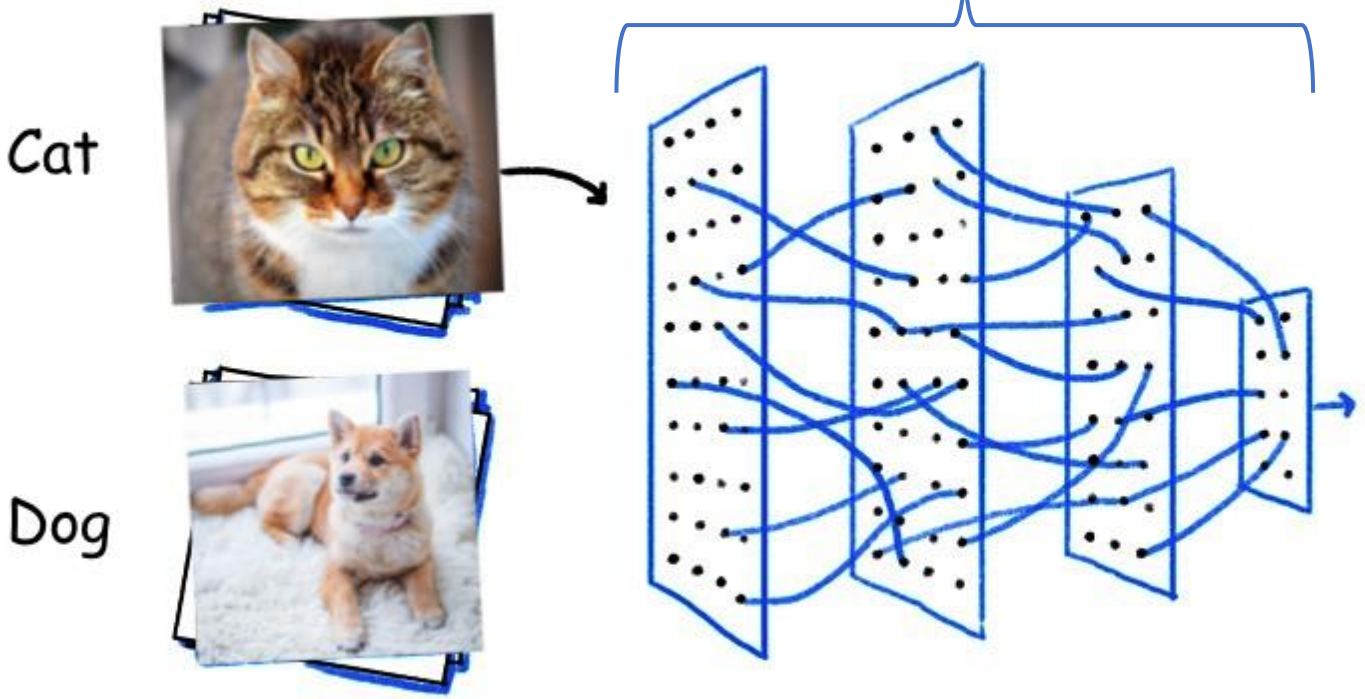


$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} \left[l\left(f(\theta; x); y \right) \right]$$

Problem Setup

- Adversarial Learning

Input: x



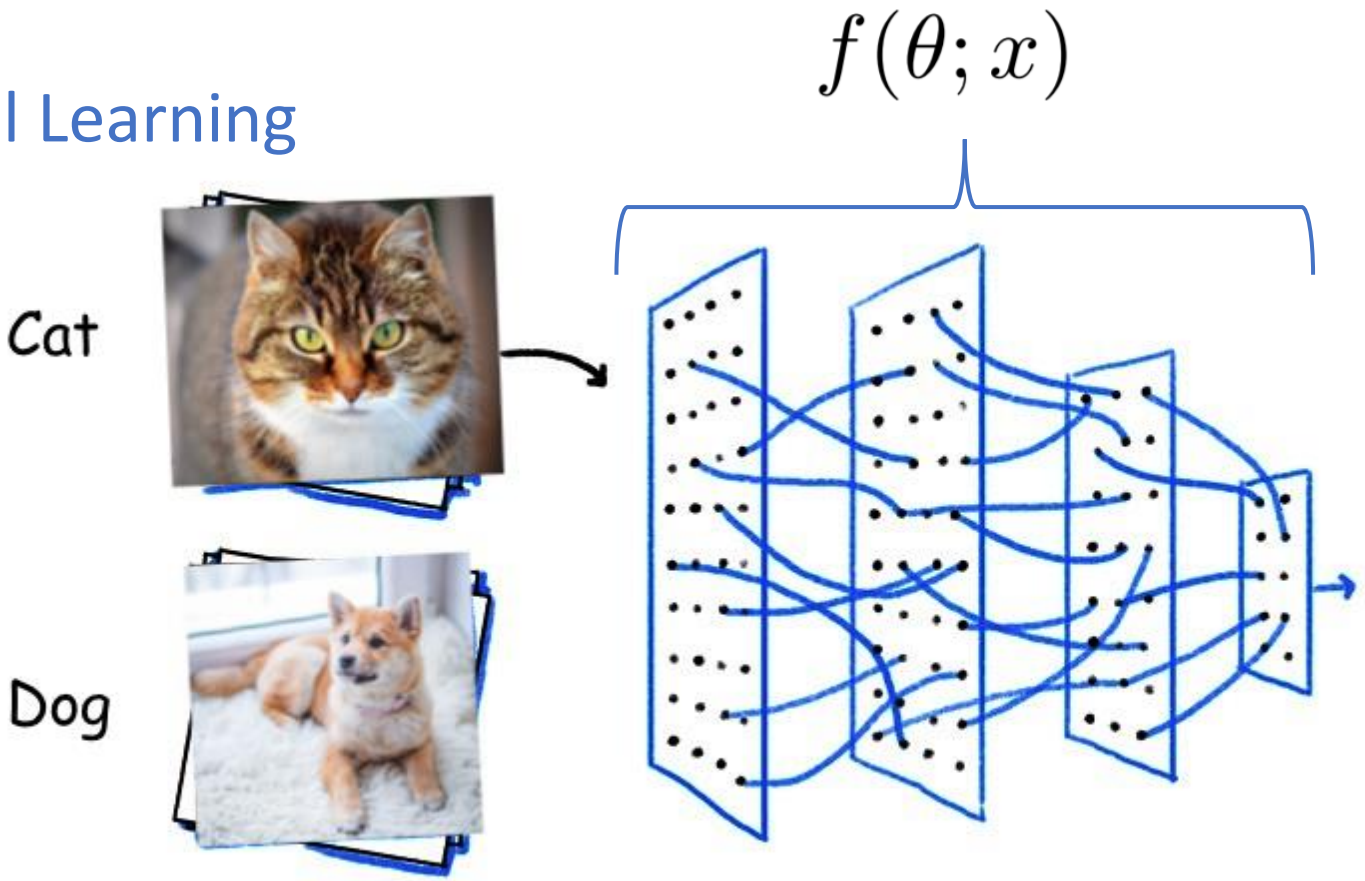
$f(\theta; x)$

Output: y

Problem Setup

Detective
(Discriminator: g(.))

- Adversarial Learning



Input: x

Output: y

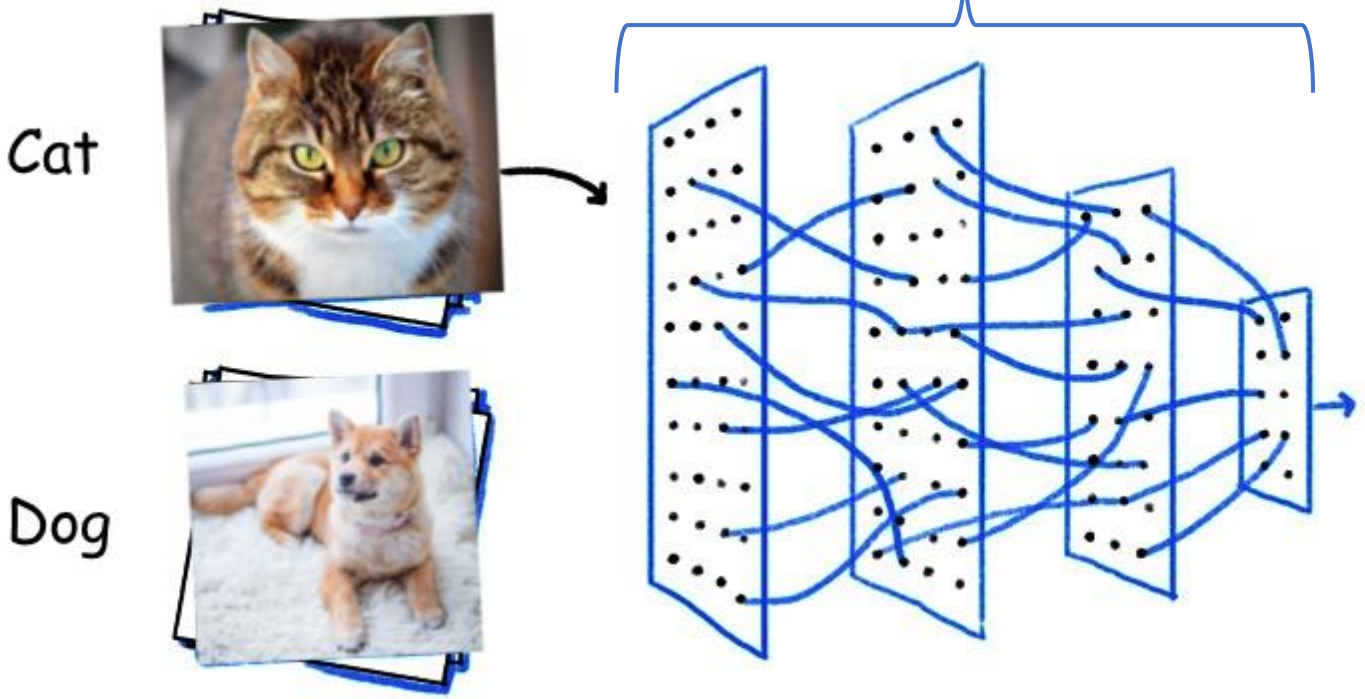
$$\arg\min_{\theta} -\mathbb{E}_{x\sim\mathcal{P}_X}\left[g\left(\psi; f\left(\theta; x\right)\right)\right]$$

Problem Setup

Detective
(Discriminator: g(.))

- Adversarial Regularization

Input: x



$f(\theta; x)$

Output: y

$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} \left[l\left(f(\theta; x); y \right) - g\left(\psi; f\left(\theta; x \right) \right) \right]$$

Problem Setup

- Supervised Learning

$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} \left[l\left(f(\theta; x); y \right) \right]$$

Problem Setup

- Supervised Learning

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Problem Setup

- Supervised Learning

$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} [l\left(f(\theta; x); y\right)]$$

- Adversarial Learning

$$\arg\min_{\theta} -\mathbb{E}_{x\sim\mathcal{P}_X} [g\left(\psi; f\left(\theta; x\right)\right)]$$

- Adversarial Regularization

$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} [l\left(f(\theta; x); y\right) - g\left(\psi; f\left(\theta; x\right)\right)]$$

Problem Setup

- Supervised Learning

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$$\arg\min_{\theta} -\mathbb{E}_{x\sim\mathcal{P}_X} [g\left(\psi; f\left(\theta; x\right)\right)]$$

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$$\arg\min_{\theta} \mathbb{E}_{(x,y)\sim\mathcal{P}} [l\left(f(\theta; x); y\right) - g\left(\psi; f\left(\theta; x\right)\right)]$$

Understanding the Role of Adversarial Regularization in Supervised Learning

- Mitigating Vanishing Gradient
- Asymptotic Iteration Complexity
- Sub-optimality Gap
- Provable Convergence
- Generalization Error (Open Problems)
- Neural Topology Analysis (Open Problems)

Mitigating Vanishing Gradient

$$\theta(t+1) = \theta(t) - \eta \frac{\partial L(\theta)}{\partial \theta(t)}$$

Supervised Objective

Assumption 1. *The function $f(\theta; x)$ is L-Lipschitz in θ.*

Assumption 2. *The loss function $l(p; y)$, where $p = f(\theta; x)$, is β-smooth in p.*

Lemma 1. *Let **Assumption 1** and **Assumption 2** hold. If $\|\theta - \theta^*\| \leq \epsilon$, then $\left\|\nabla_\theta \mathbb{E}_{(x,y)\sim\mathcal{P}} \left[l\left(f(\theta; x); y\right)\right]\right\| \leq L^2\beta\epsilon$.*

Mitigating Vanishing Gradient

$$\theta(t+1) = \theta(t) - \eta \frac{\partial L(\theta)}{\partial \theta(t)}$$

Augmented Objective

Theorem 1 (Informal).

Under valid assumptions, the adversarial regularization mitigates vanishing gradient in the near optimal region.

Theorem 1. *Let us suppose* ***Assumption 1*** *and* ***Assumption 2*** *hold. If* $\|\theta - \theta^*\| \leq \epsilon$ *and* $\|g - g^*\| \leq \delta$, *then* $\left\|\nabla_\theta \mathbb{E}_{(x,y)\sim\mathcal{P}} \left[l\left(f(\theta; x); y\right) - g\left(\psi; f\left(\theta; x\right)\right)\right]\right\| \leq \left(L^2\beta\epsilon + L\delta\right)$.

Mitigating Vanishing Gradient

Experimental Result

- Gradient norm in hidden layer
- Gradient norm in top layer
- Application of adversarial regularization

Mitigating Vanishing Gradient

Experimental Result

- Gradient norm in hidden layer
- Gradient norm in top layer
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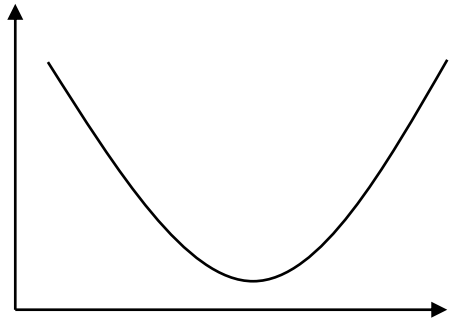
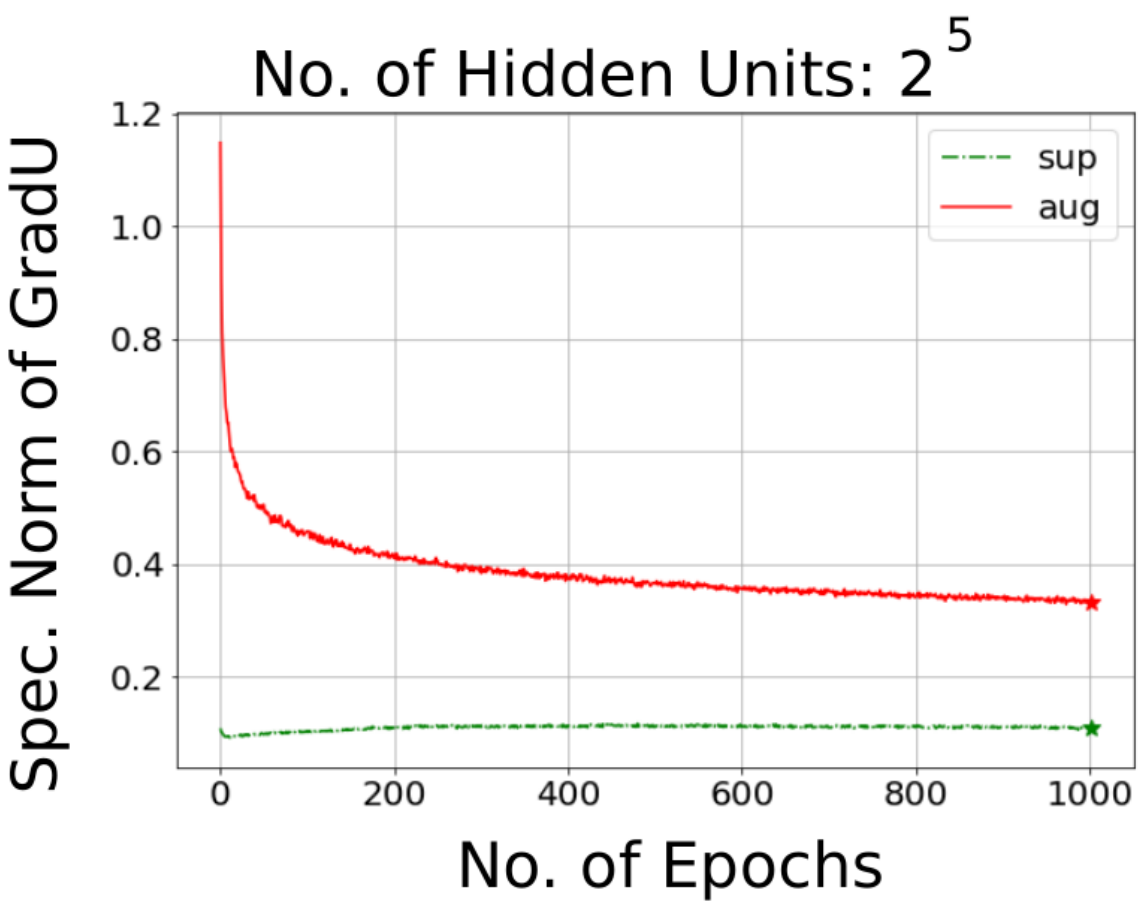
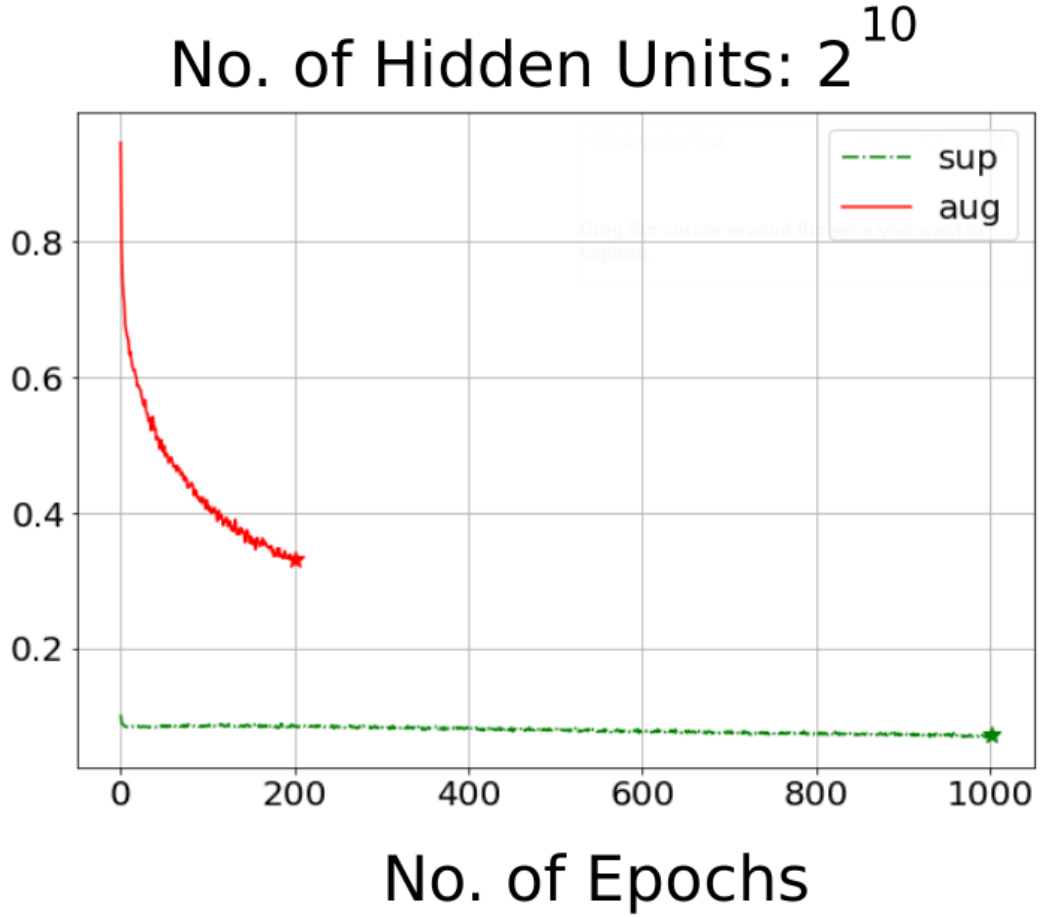
Mitigating Vanishing Gradient







Mitigating Vanishing Gradient

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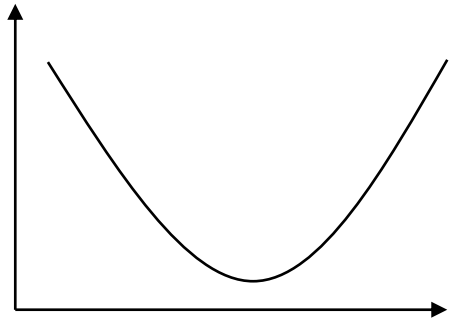
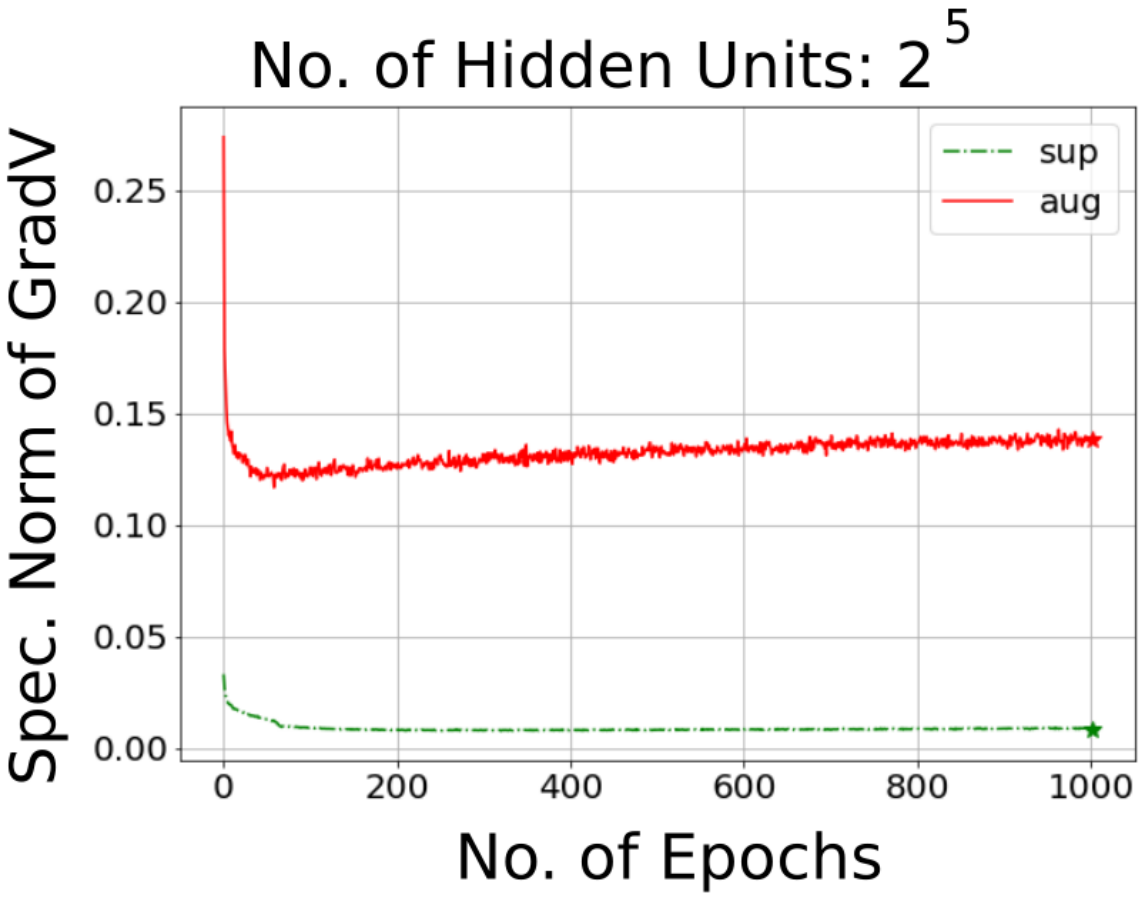
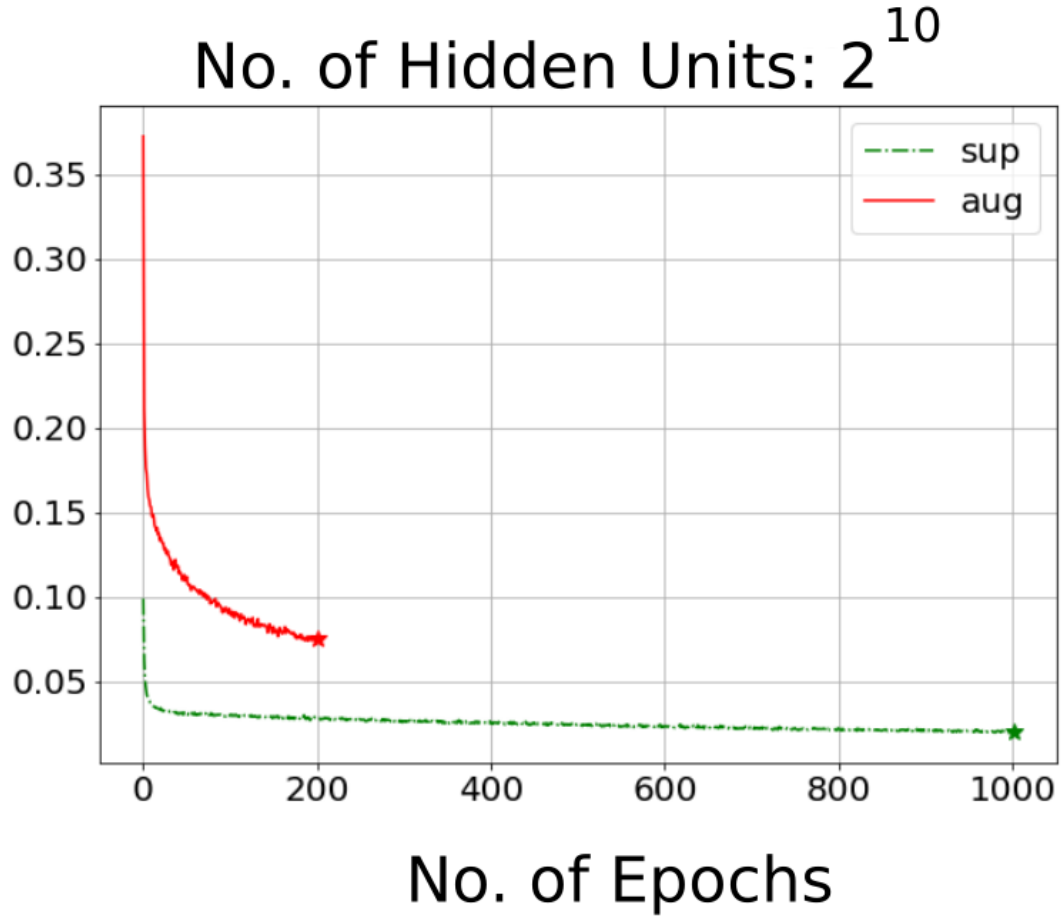
Mitigating Vanishing Gradient







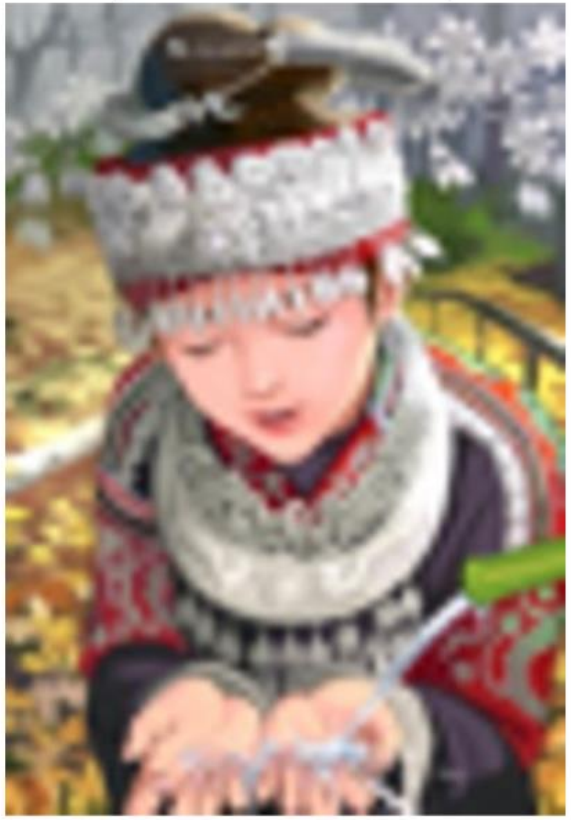
Mitigating Vanishing Gradient

Experimental Result

- Gradient norm in hidden layer
- Gradient norm in top layer
- Application of adversarial regularization

Mitigating Vanishing Gradient

bicubic
(21.59dB/0.6423)



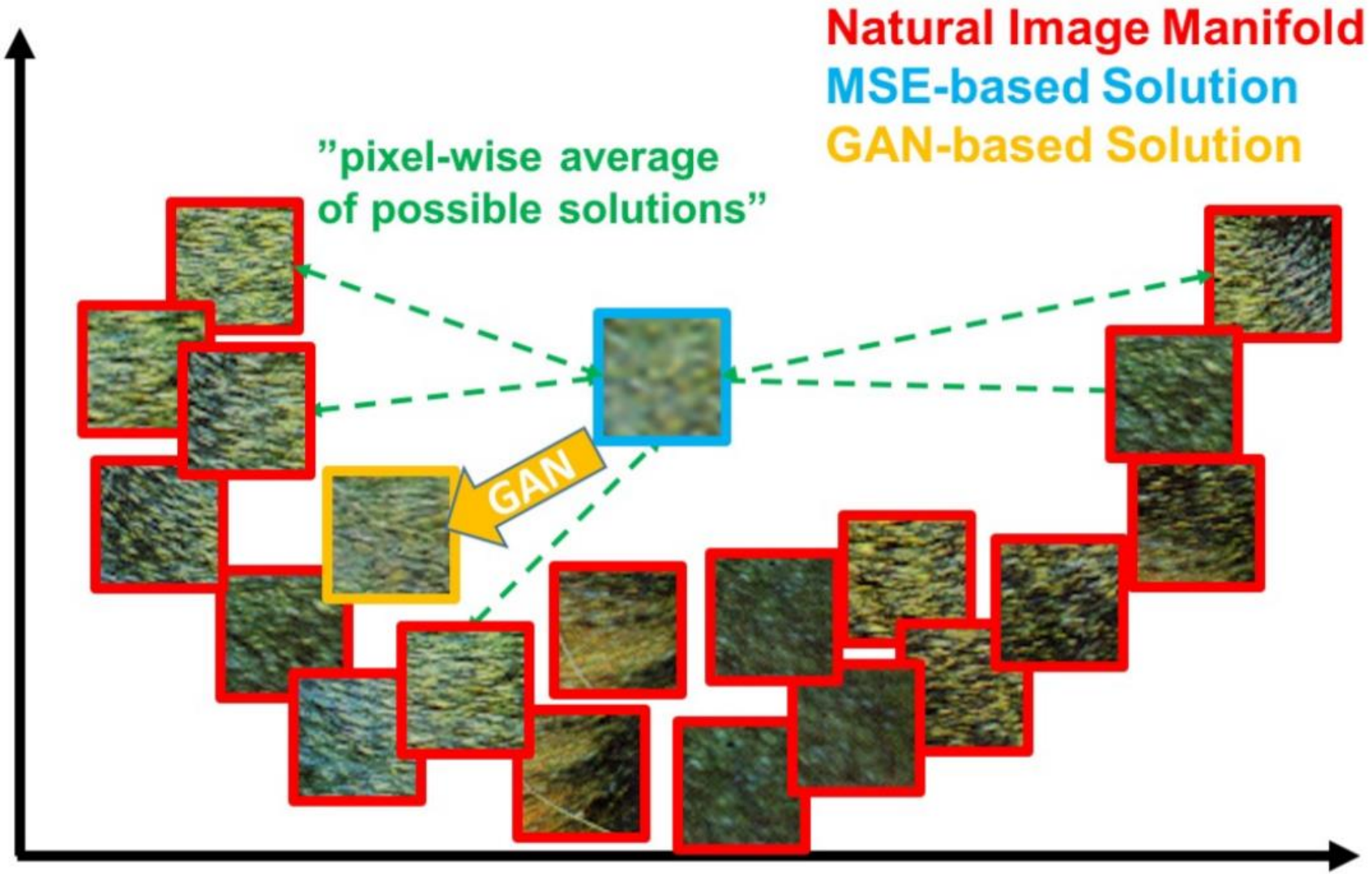
SRResNet
(23.53dB/0.7832)

SRGAN
(21.15dB/0.6868)

original

Ledig et al. CVPR, 2017

Mitigating Vanishing Gradient



Ledig et al. CVPR, 2017

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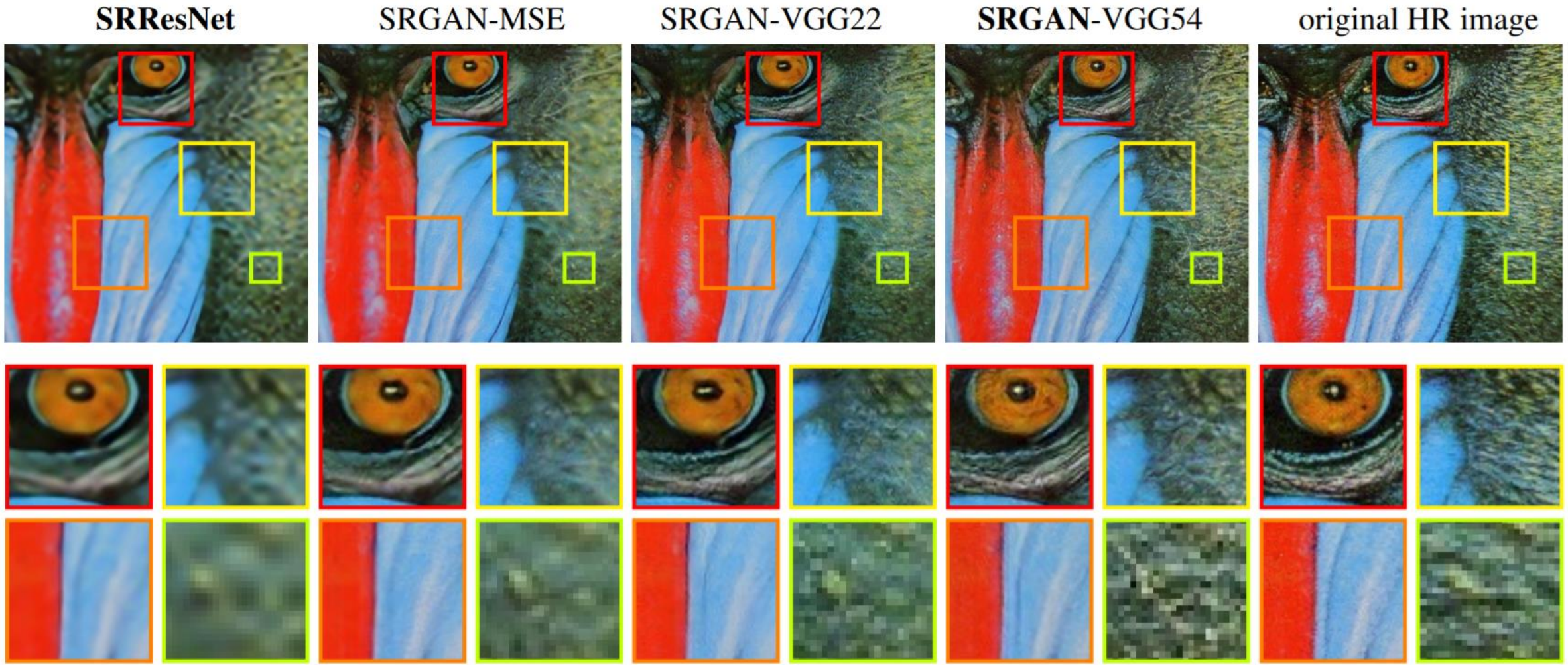

Ledig et al. CVPR, 2017

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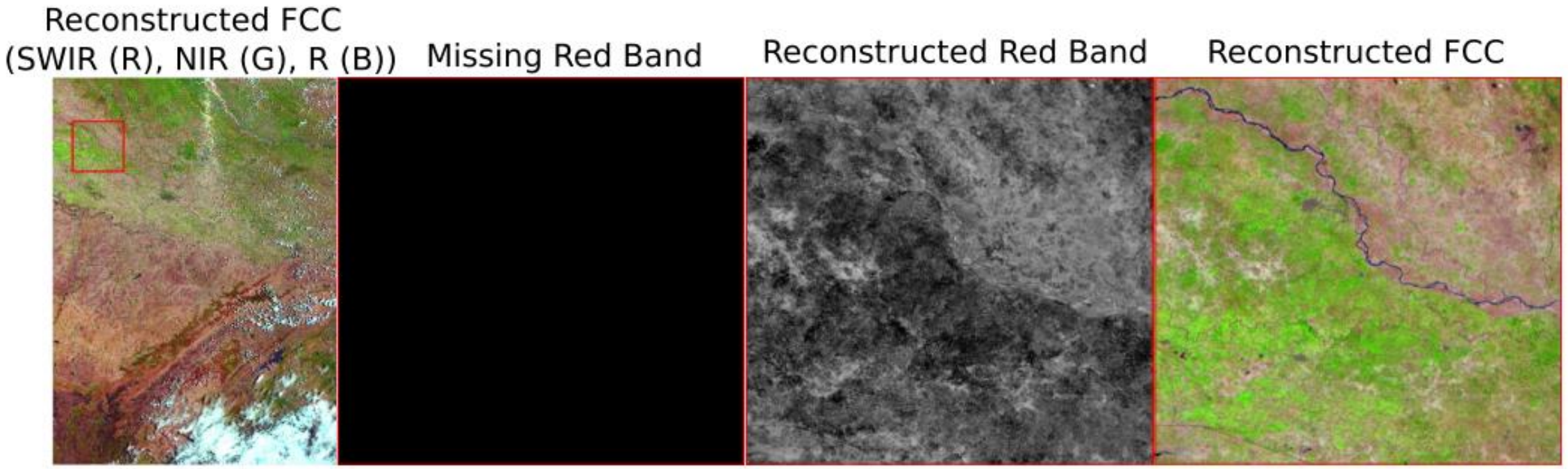

Metrics	Parameters	Training epochs	Training RMSE	Inference Time
AeroGAN	2 M	100	41.57	64 s
DeepAWiFS	4.7 M	1000	18.2	495 s
DSen2	4.7 M	1000	21.2	456 s
ALERT	2.8 M	50	10.3	70 s
% gain	40.42	95.00	51.41	84.64

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Asymptotic Iteration Complexity

Supervised Objective

Assumption 5 ((L_0, L_1)-Smoothness). *The function is (L_0, L_1)-smooth, i.e., there exist positive constants L_0 and L_1 such that* $\left\|\nabla^2 l(\theta)\right\| \leq L_0 + L_1 \left\|\nabla l(\theta)\right\|$.

Theorem 2. *Suppose the functions in $\mathscr{L}$ satisfy* ***Assumption 3, 4*** *and* ***5****. Given $\epsilon > 0$, the iteration complexity in sole supervision is upper bounded by*

$$\mathcal{O}\left(\frac{(l(\theta_0)-l^*)\left(L_0+L_1L^2\beta\epsilon\right)}{\epsilon^2}\right).$$

Asymptotic Iteration Complexity

Augmented Objective

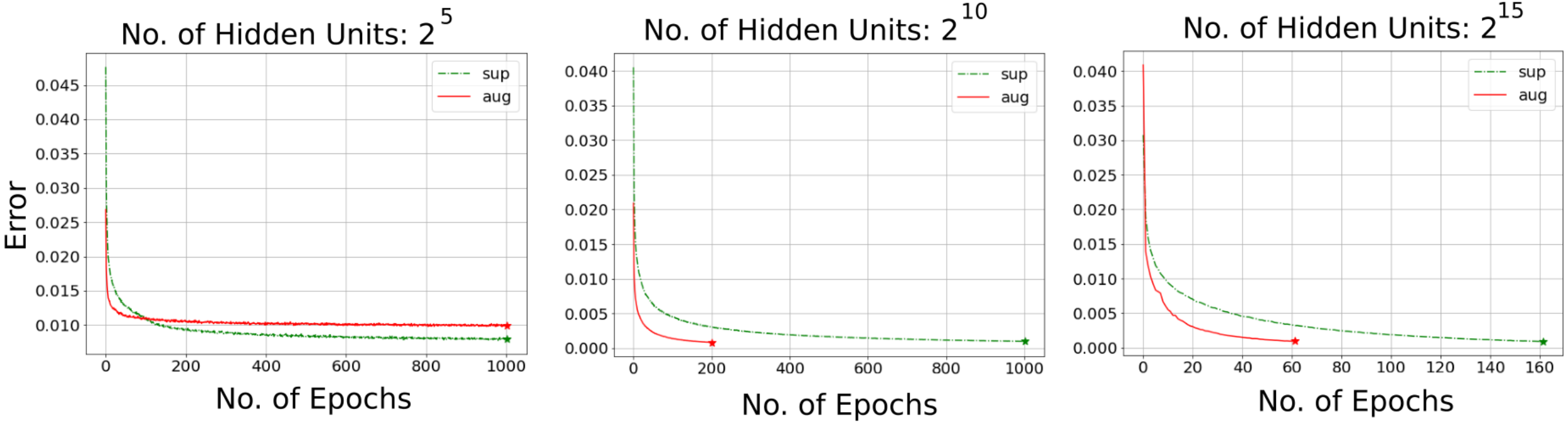
Theorem 2 and 3 (Informal).

Under valid assumptions, the number of iterations required to find a good solution in the augmented objective is equal to or less than supervised objective.

Theorem 3. *Suppose the functions in* $\mathscr{L}$ *satisfy* ***Assumption 3, 4*** *and* ***5****. Given* ***Assumption 6*** *holds,* $\epsilon > 0$ *and* $\delta \leq \frac{\sqrt{2\epsilon\zeta}}{L}$*, the iteration complexity in adversarial regularization is upper bounded by* $\mathcal{O}\left(\frac{(l(\theta_0)-l^*)\left(L_0+L_1L^2\beta\epsilon\right)}{\epsilon^2+2\epsilon\zeta-L^2\delta^2}\right)$.

Asymptotic Iteration Complexity

Experimental Result



Asymptotic Iteration Complexity

Experimental Result: Generator Network Configurations

Architecture	No. Layer	Activation	No. ResBlock	No. DenseBlock	No. Epoch Sup	No. Epoch Aug	Hypothesis
MLP-Deep	6	ELU	2	0	391	55	✓
CNN-ResNet	6	ReLU	2	0	215	41	✓
CNN-DenseNet	6	ReLU	2	1	163	39	✓
CNN-DenseNet-L1	6	ReLU	2	1	1000	39	✓
CNN-DenseNet-L2	6	ReLU	2	1	155	39	✓
CNN-ResNet-AvgPool	6	ReLU	2	0	109	29	✓

Adversarial regularization is at least as good as sole supervision.

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Sub-optimality Gap

Supervised Objective

Theorem 4. *In purely supervised learning, the sub-optimality gap at the average over all iterates in a trajectory of T time steps is upper bounded by* $\mathcal{O}\left(\frac{\|\theta(0)-\theta^*\|^2}{2T}\right)$.

Generator: $\kappa(t) = \kappa(\theta(t)) := l(\theta(t)) - l(\theta^*)$

Sub-optimality Gap

Augmented Objective

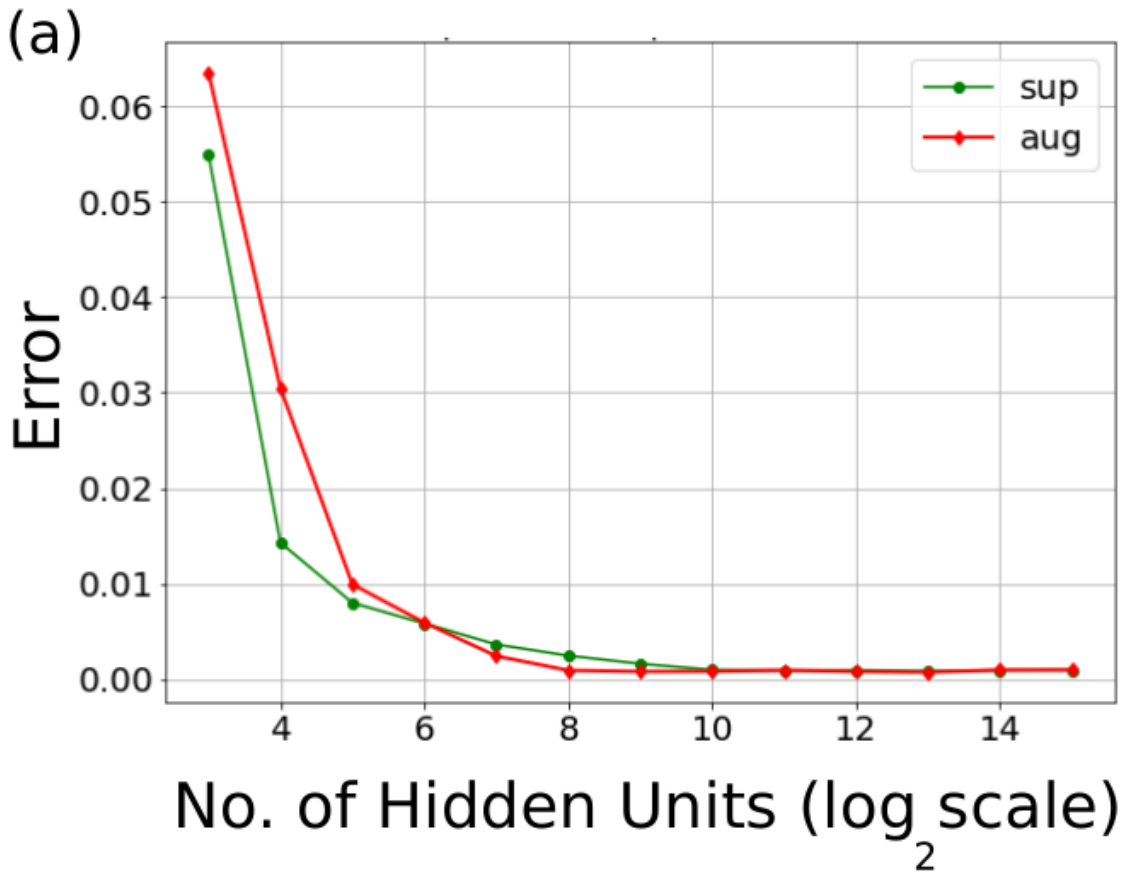
Theorem 5. *In supervised learning with adversarial regularization, the sub-optimality gap at the average over all iterates in a trajectory of T time steps is upper bounded by*

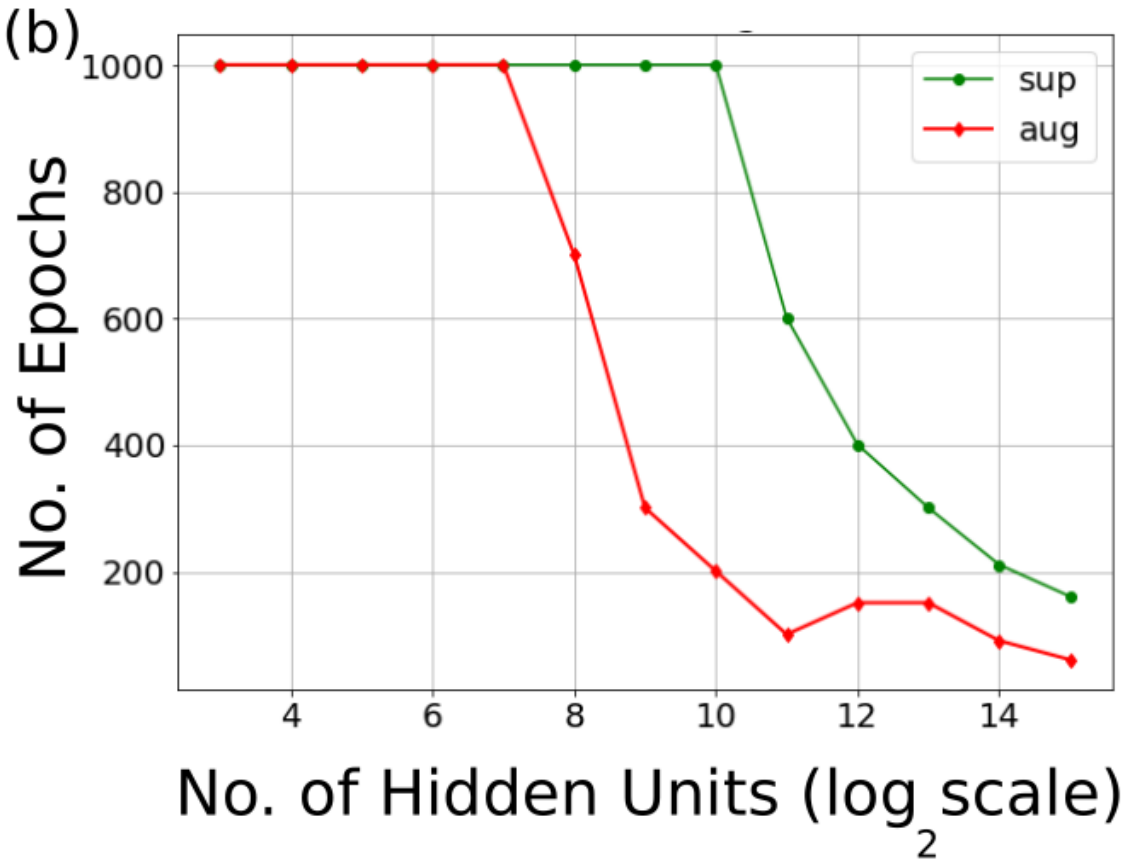
$$\mathcal{O}\left(\frac{\|\theta(0)-\theta^*\|^2}{2T}-\pi\left(\frac{1}{T}\int_0^T\theta(t)dt\right)\right).$$

Discriminator: $\pi(t) = \pi(\theta(t)) := g(\theta^*) - g(\theta(t))$

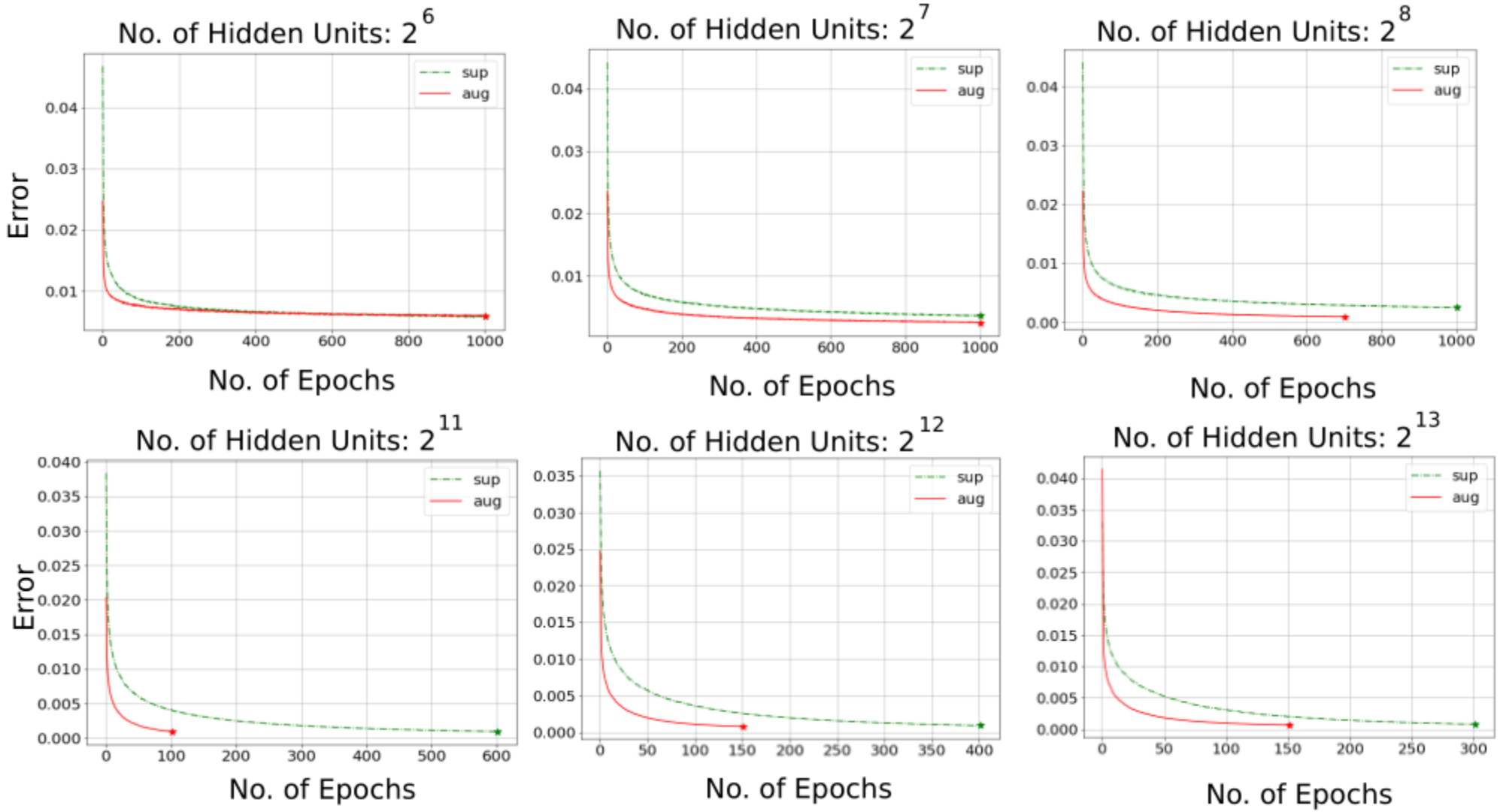
Sub-optimality Gap

Experimental Result

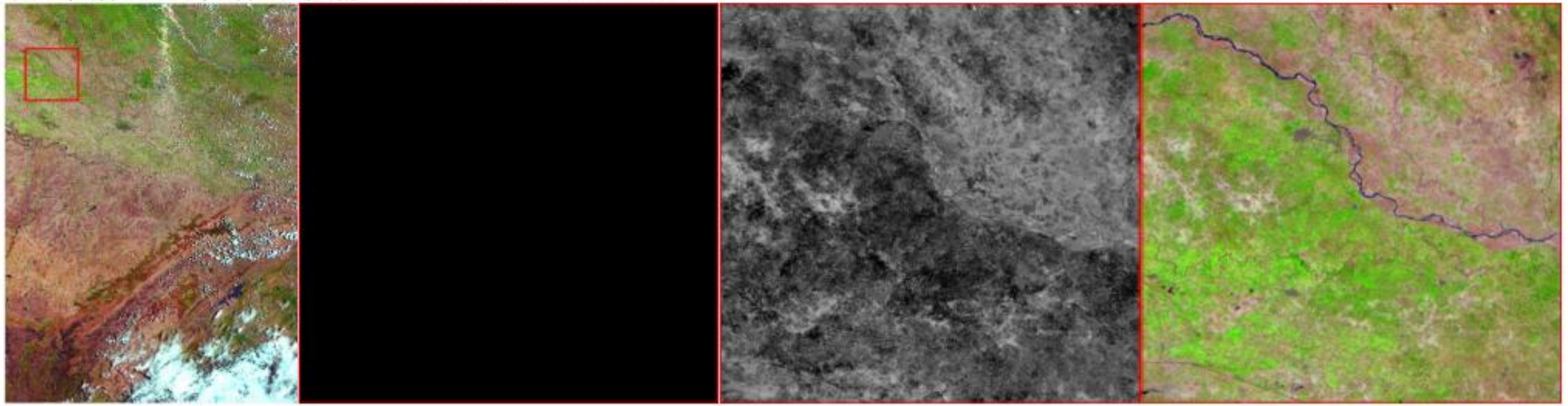




Sub-optimality Gap



Sub-optimality Gap



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Provable Convergence

Augmented Objective

Theorem 6 (Strongly-convex-strongly-concave convergence). *Suppose* ***Assumption 7*** *holds. Let* $l(\theta_k) \triangleq l(\theta_k) - g(\theta_k)$ *is a* μ*-strongly convex function. Let* $\{\theta_k\}$ *be the sequence of iterates obtained using global clipping on SGD with zero momentum. Define the output to be* k*-weighted combination of iterates:* $\bar{\theta} = \frac{\sum_{k=1}^{T} k\theta_{k-1}}{\sum_{k=1}^{T} k}$. *If adaptive clipping* $\tau_k = Gk^{\frac{1}{\alpha}}\mu^{\frac{1}{\alpha}}$ *and step size* $\eta_k = \frac{5}{2\mu(k+1)}$, *then the output iterate* $\bar{\theta}$ *satisfies*

$$\mathbb{E}\left[l\left(\bar{\theta}\right)\right] - l\left(\theta^*\right) \leq \mathcal{O}\left(G^2\left(\mu\left(T+1\right)\right)^{\frac{2-2\alpha}{\alpha}} - \left(g\left(\theta^*\right) - \mathbb{E}\left[g\left(\bar{\theta}\right)\right]\right)\right).$$

Provable Convergence

Augmented Objective

Theorem 7 (Nonconvex-nonconcave convergence). *Suppose* ***Assumption 7*** *holds. Let* $l(\theta_k) \triangleq l(\theta_k) - g(\theta_k)$ *is a possible L-smooth function and* $\{\theta_k\}$ *be the sequence of iterates obtained using global clipping on SGD with zero momentum. Given constant clipping* $\tau_k = G(\eta_k L)^{\frac{-1}{\alpha}}$ *and constant step size* $\eta_k = \left(\frac{R_0^\alpha L^{2-2\alpha}}{G^2 T^\alpha}\right)^{\frac{1}{3\alpha-2}}$, *where* $R_0 = l(\theta_0) - l(\theta^*)$, *the sequence* $\{\theta_k\}$ *satisfies*

$$\frac{1}{T}\sum_{k=1}^{T}\mathbb{E}\left[\|\nabla l(\theta_{k-1})\|^2\right] \leq \mathcal{O}\left(G^{\frac{2\alpha}{3\alpha-2}}\left(\frac{R_0 L}{T}\right)^{\frac{2\alpha-2}{3\alpha-2}} - \frac{1}{T}\sum_{k=1}^{T}\mathbb{E}\left[\|\nabla g(\theta_{k-1})\|^2\right]\right).$$

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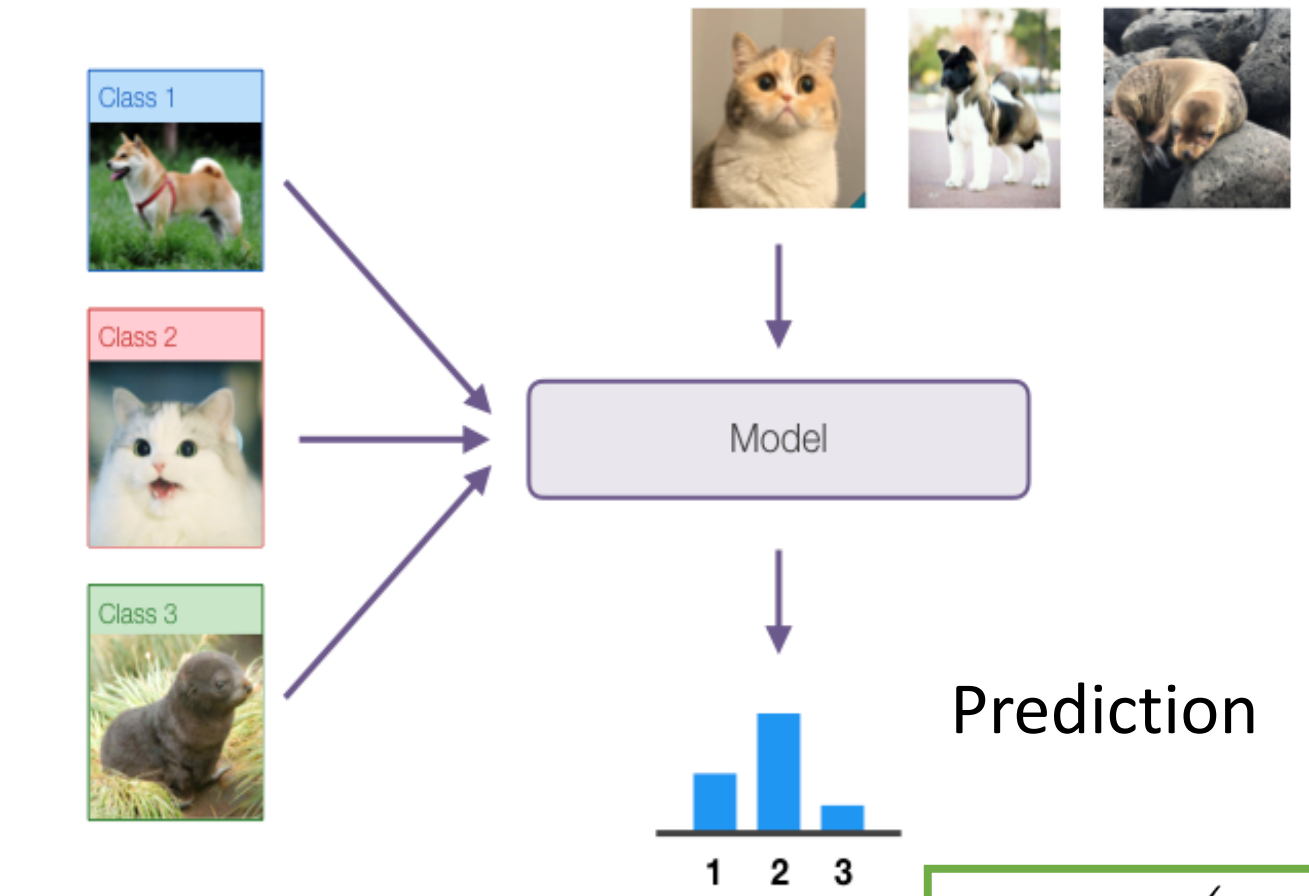
Generalization Error



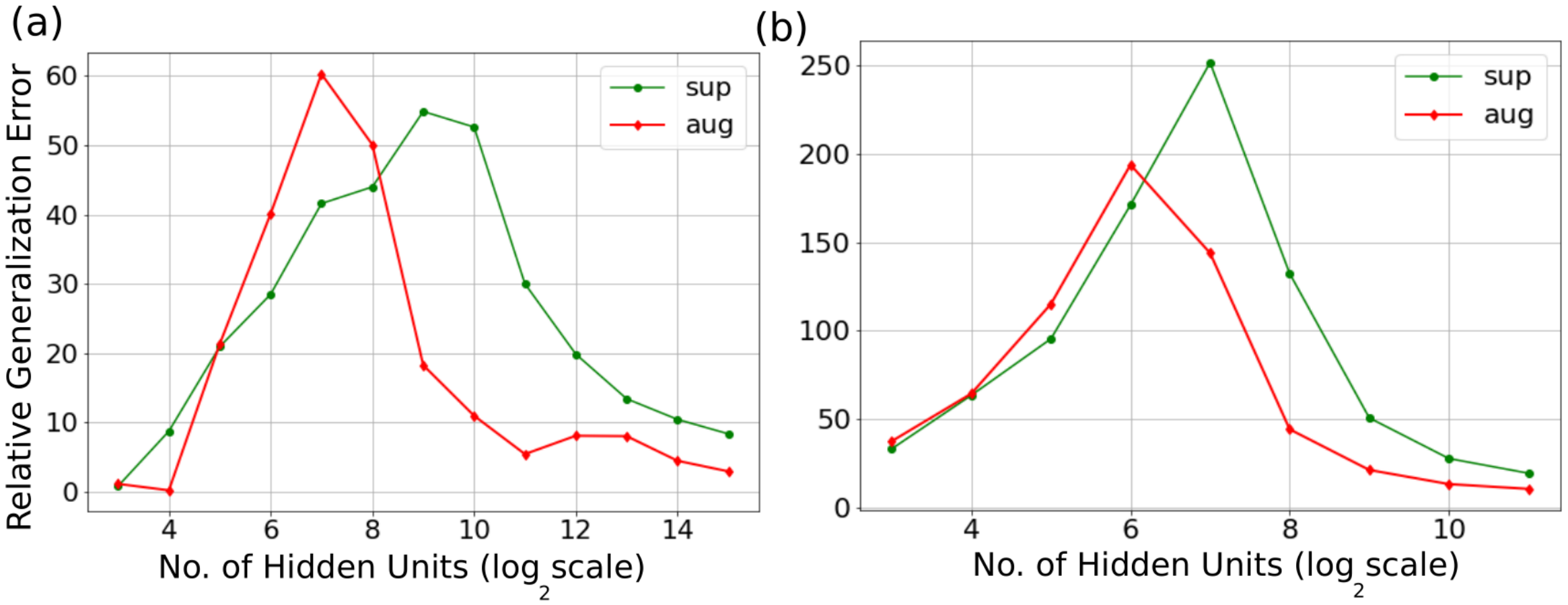
Testing Data

Prediction

Training Data

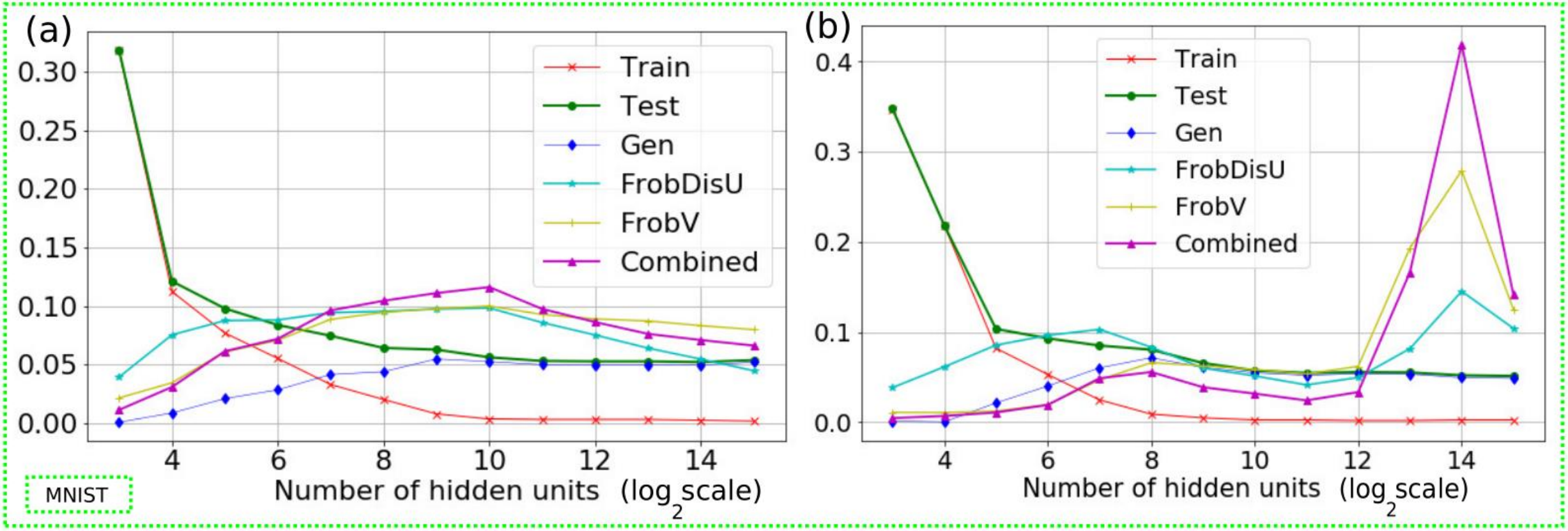
$$e_{gen} = \left(\mathbb{E}_{(x,y)\sim\mathcal{D}} [l \; o \; f] - \frac{1}{m} \sum_{i=1}^{m} l\left(f(x); y\right) \right)$$

Generalization Error



$$e_{gen,r} = \left(\mathbb{E}_{(x,y)\sim\mathcal{D}} \left[l \; o \; f \right] - \frac{1}{m} \sum_{i=1}^{m} l\left(f(x); y \right) \right) \times \mathcal{N}$$

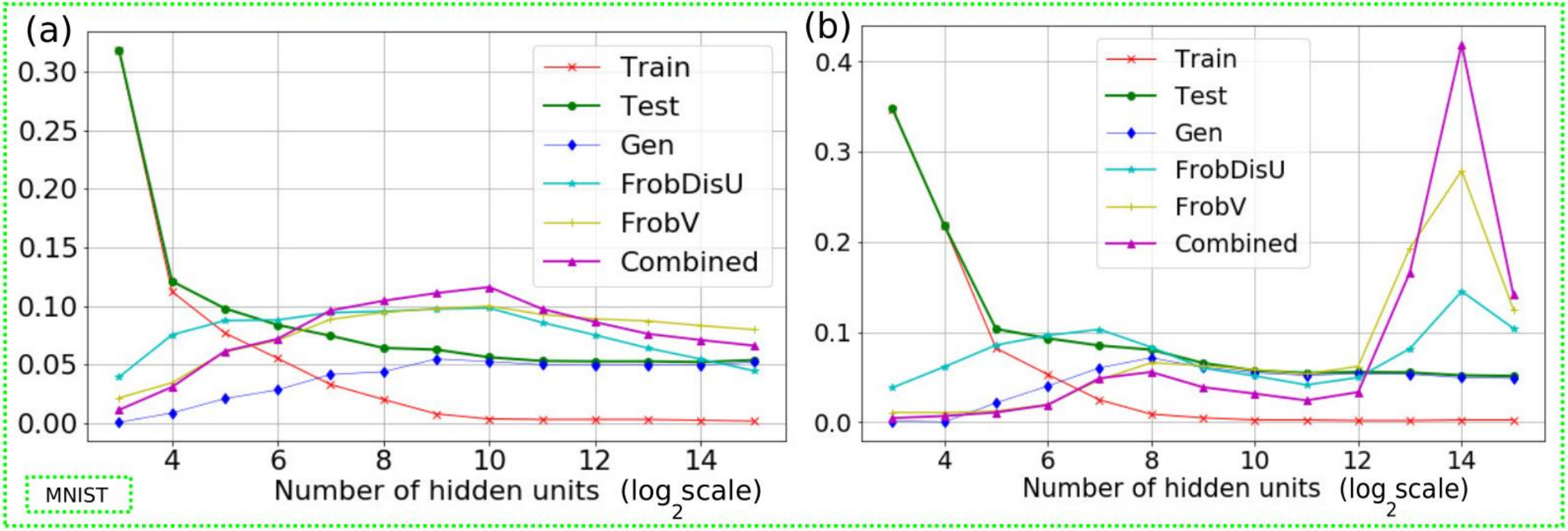
Generalization Error



Combined Metric: $\mathcal{O}\left(\left\|U^0\right\|_2 \|V\|_F + \left\|U - U^0\right\|_F \|V\|_F + \sqrt{h}\right)$

Neyshabur et al. ICLR ,2019

Generalization Error



Open Problem: How to explain the generalization behaviour of the augmented objective?

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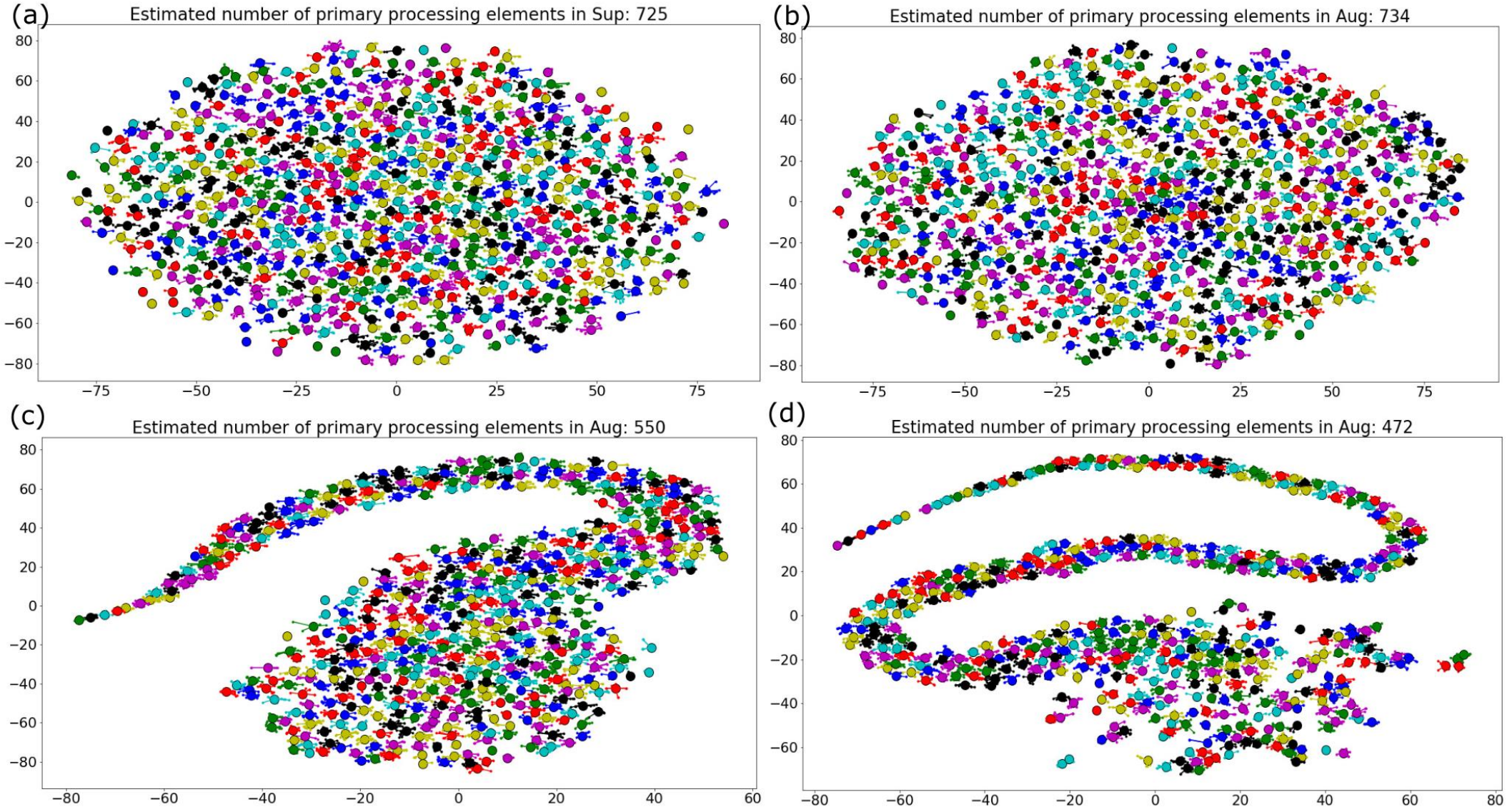
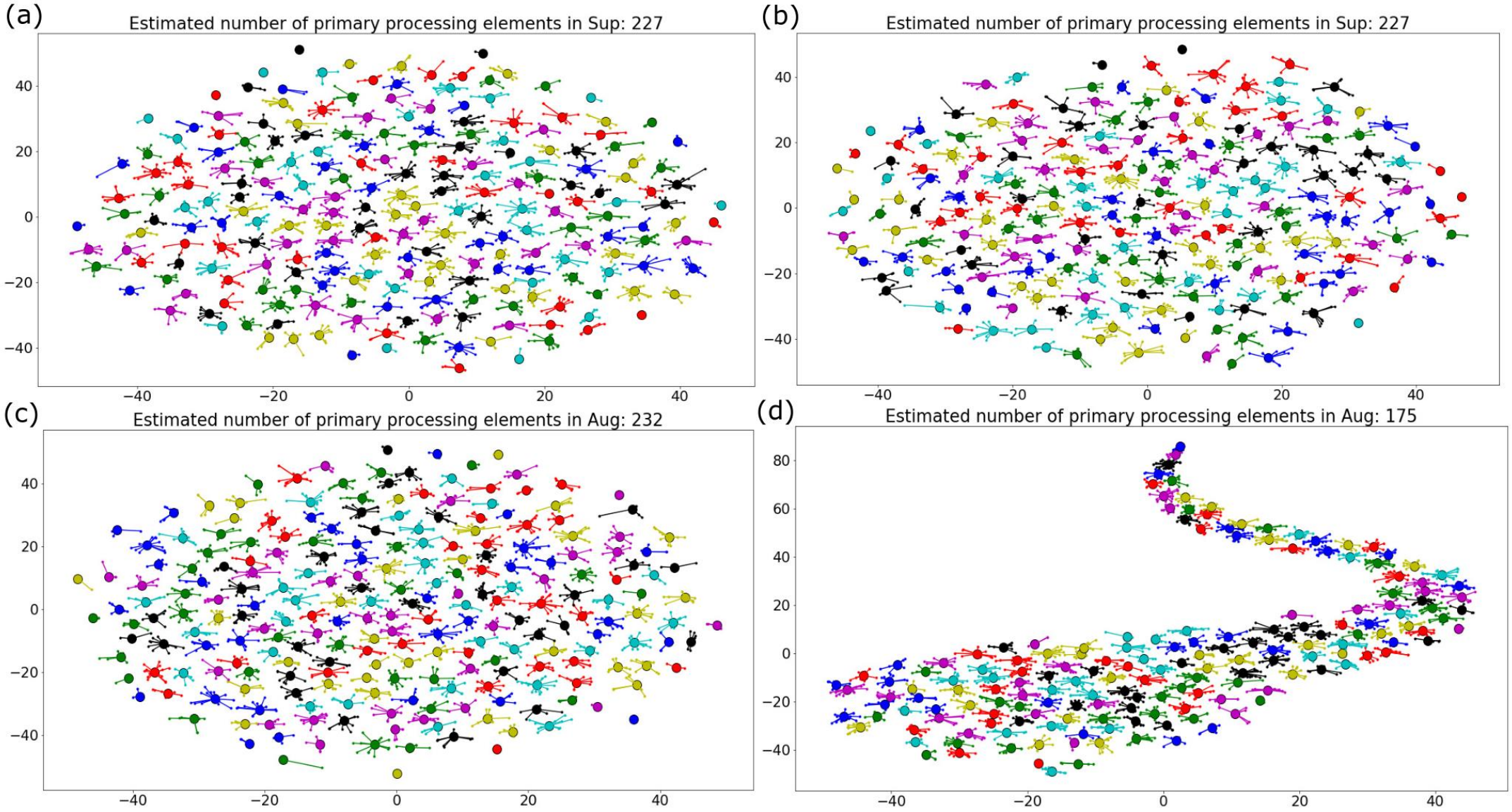
- Neural Topology Analysis (Open Problems)

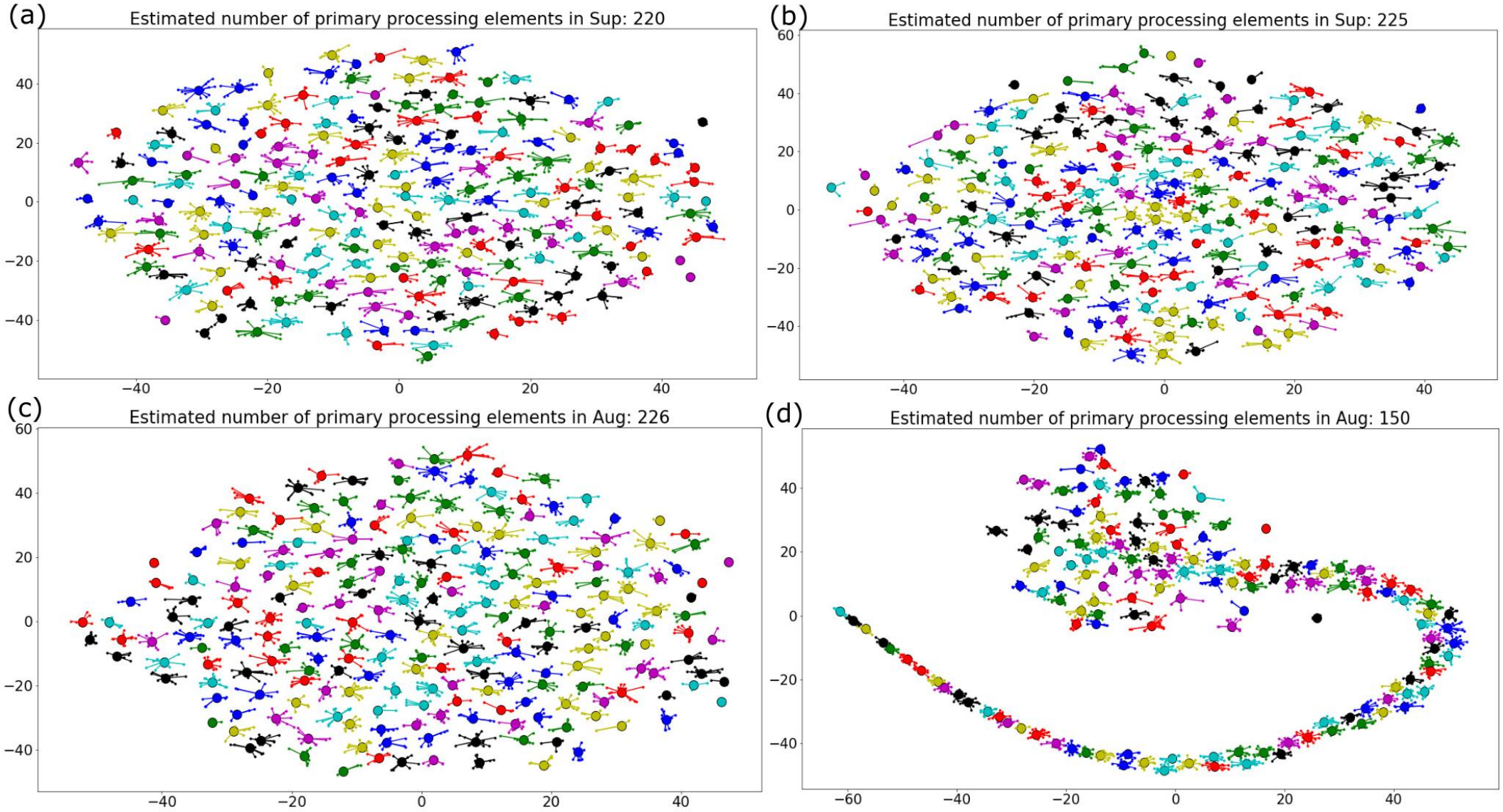
Neural Topology Analysis



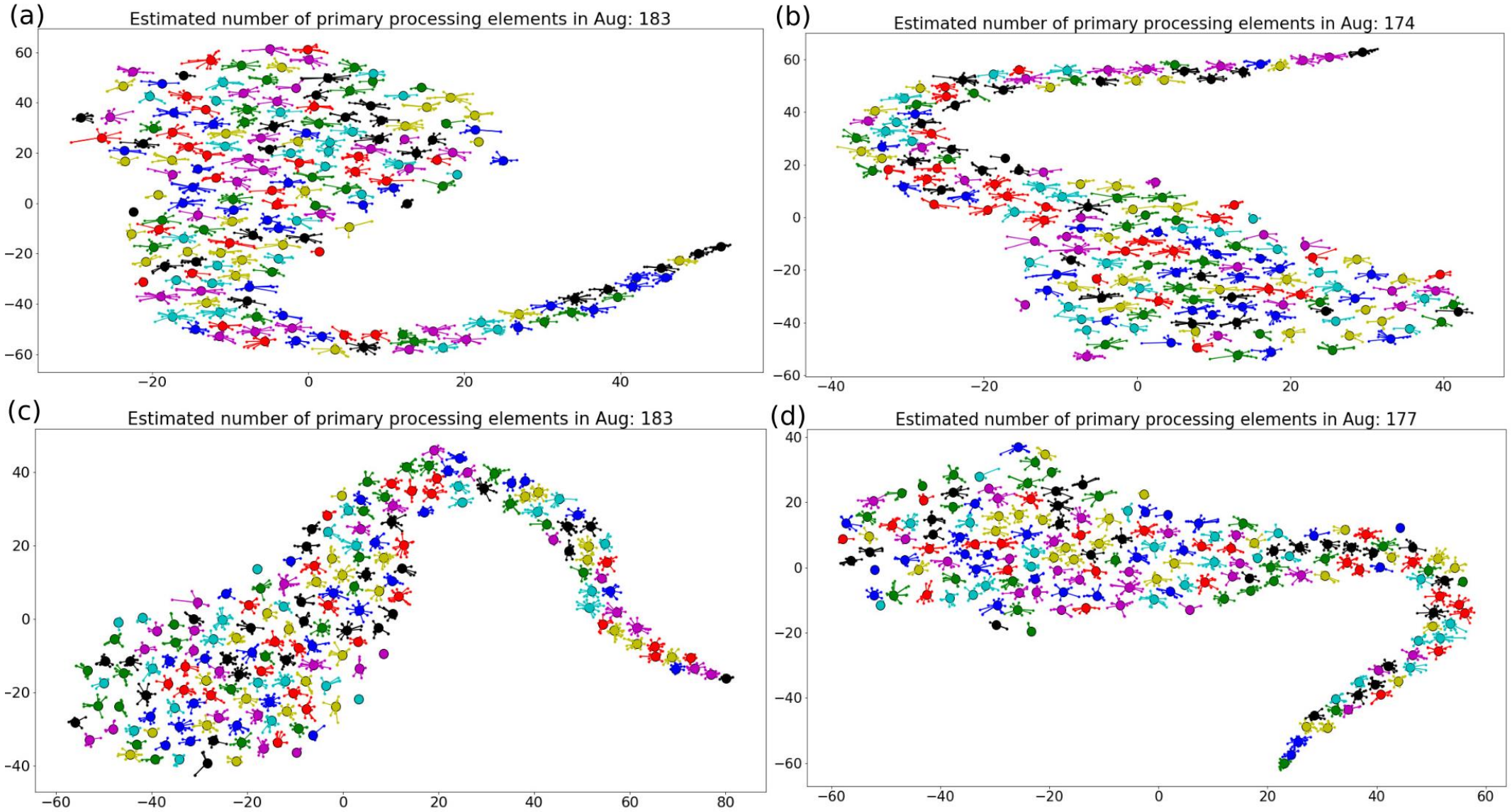
Neural Topology Analysis: Hidden Layer



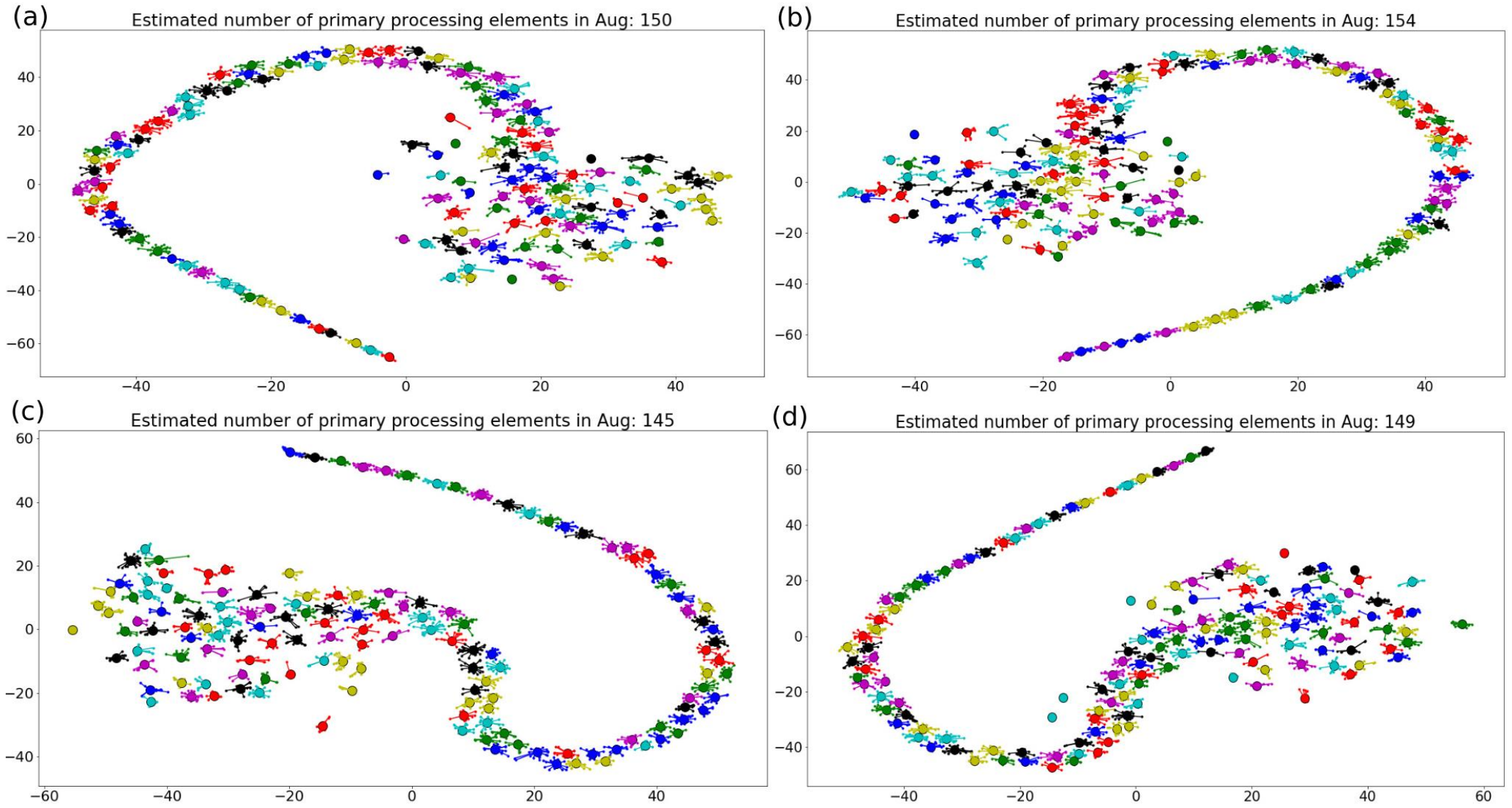
Neural Topology Analysis: Top Layer



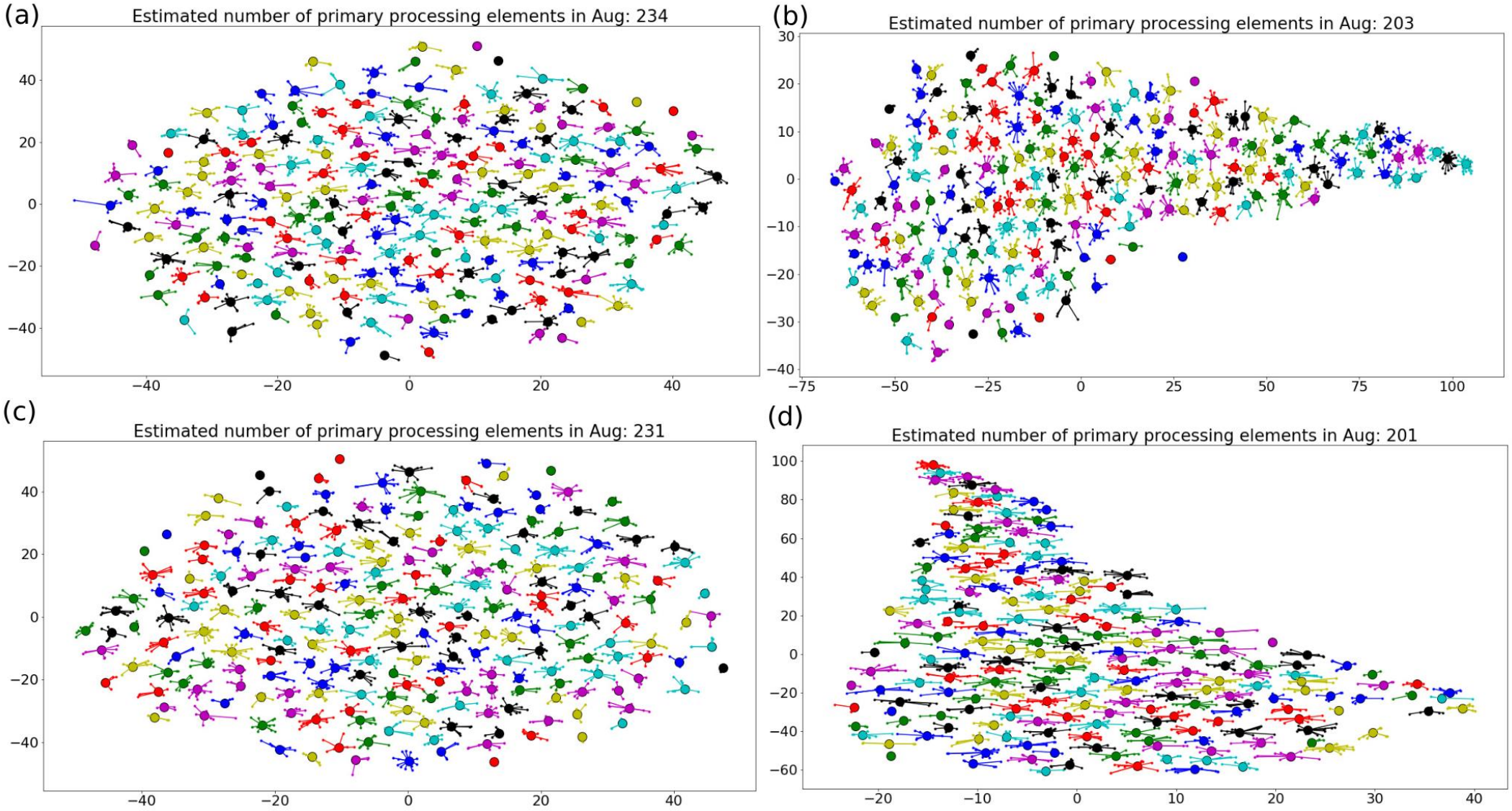
Neural Topology Analysis: Hidden Layer Subsets



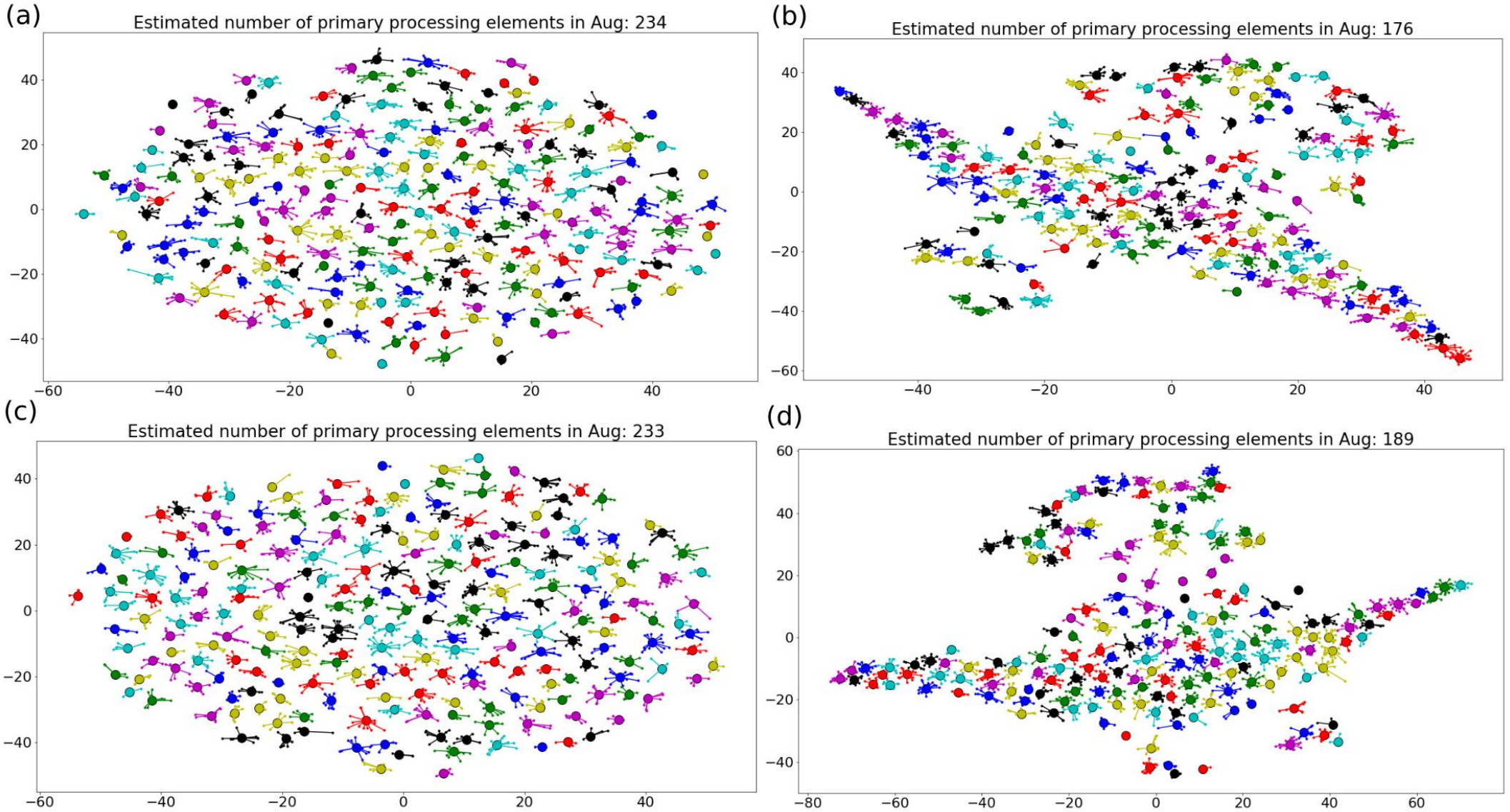
Neural Topology Analysis: Top Layer Subsets



Neural Topology Analysis: Hidden Layer FMNIST



Neural Topology Analysis: Top Layer FMNIST



Interesting Problems

- Why does adversarial interaction create non-homogeneous patterns?
- How do we predict the shape of the non-homogeneous patterns?
- What happens to the parameters if the supervised cost is augmented in the discriminator objective?
- Is gradient descent or backpropagation the optimal learning algorithm?

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Why Adversarial Interaction Creates Non-Homogeneous Patterns: A Pseudo-Reaction Diffusion Model for Turing Instability

- Adversarial Interaction
  - Generative Adversarial Networks (GANs)
  - Application of conditional GANs
- Non-Homogeneous Patterns
  - Homogeneous patterns
  - Supervised learning
- Reaction-Diffusion
  - Turing's RD model (1952)
  - Gray-Scott RD model (1984)
- Turing Instability
  - Reaction dynamics
  - Diffusion dynamics

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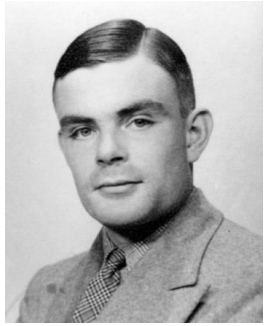
Turing's Reaction-Diffusion Model



$$\frac{d\boldsymbol{u}_j}{dt} = \mathfrak{R}_j^{\boldsymbol{u}}\left(\boldsymbol{u}_j, \boldsymbol{v}_j\right) + \mathfrak{D}_j^{\boldsymbol{u}}\left(\nabla^2 \boldsymbol{u}_j\right)$$

$$\frac{d\boldsymbol{v}_j}{dt} = \mathfrak{R}_j^{\boldsymbol{v}}\left(\boldsymbol{u}_j, \boldsymbol{v}_j\right) + \mathfrak{D}_j^{\boldsymbol{v}}\left(\nabla^2 \boldsymbol{v}_j\right)$$

A. M. Turing, 1952

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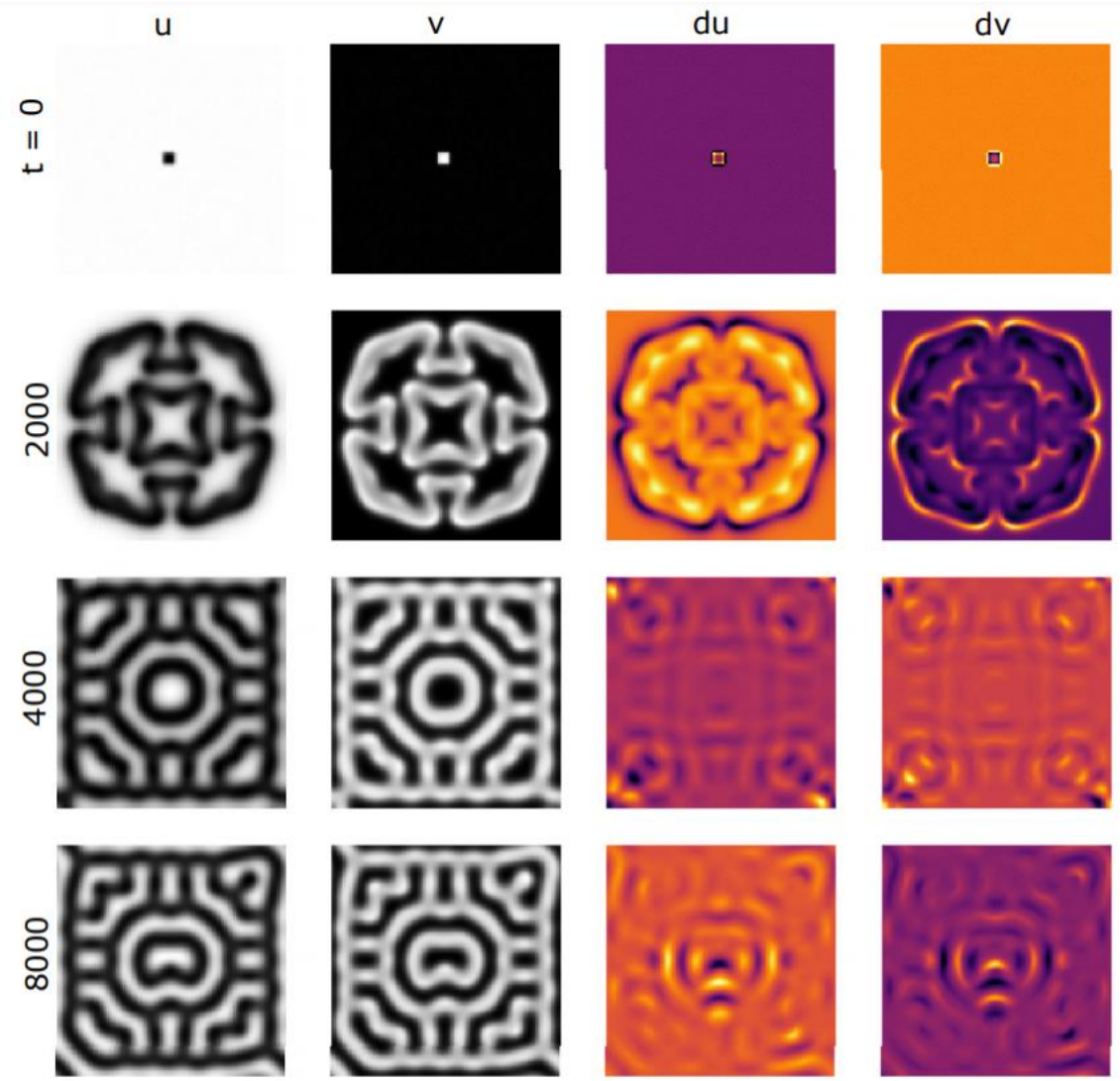
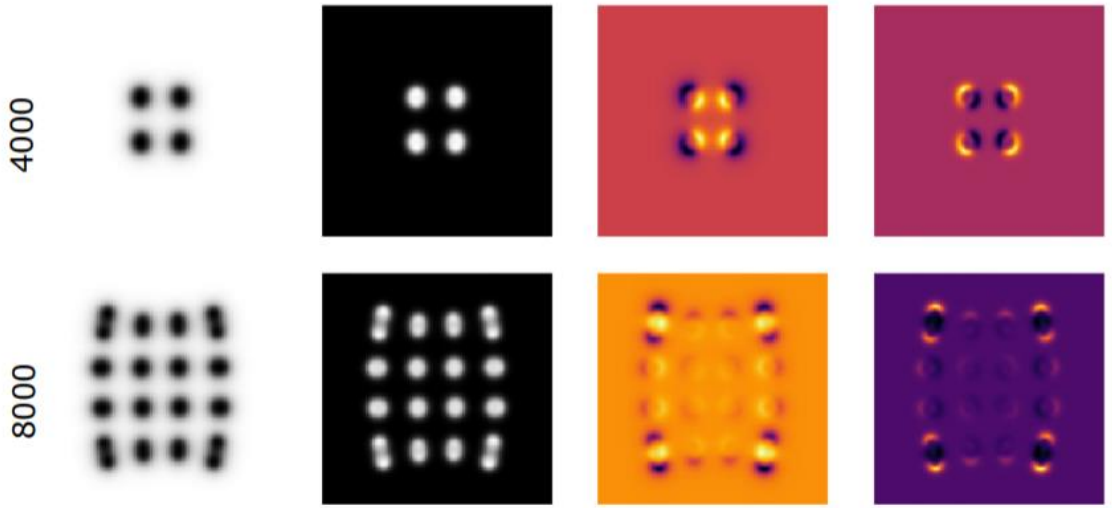
Gray-Scott Reaction-Diffusion Model



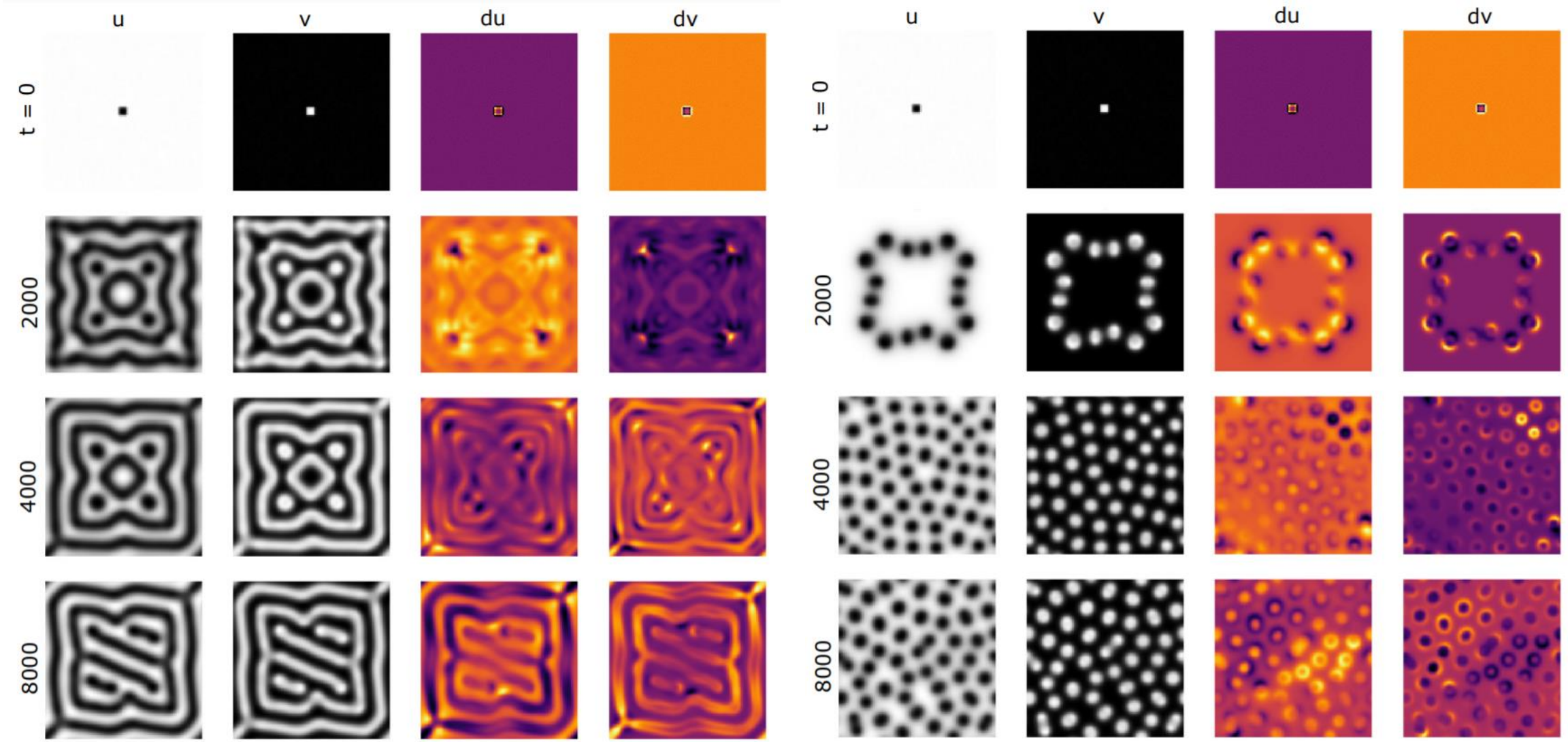
$$\frac{\partial u}{\partial t} = F(1-u) - uv^2 + \mu'\nabla^2 u$$

$$\frac{\partial v}{\partial t} = -(F+k)v + uv^2 + \nu'\nabla^2 v$$



Gray and Scott, 1984

Gray-Scott Reaction-Diffusion Model



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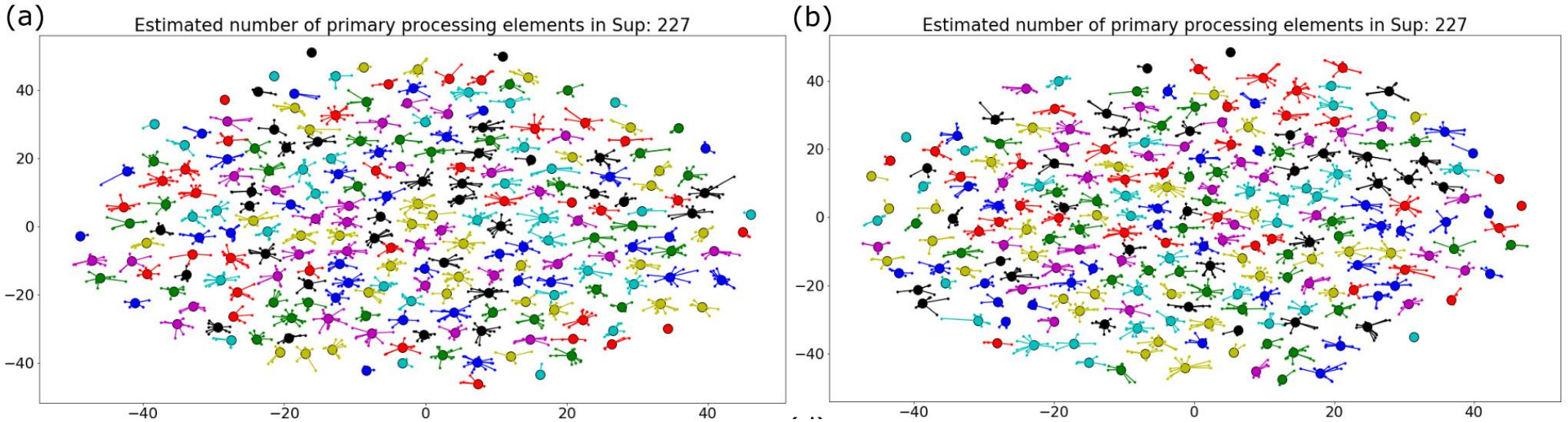
Symmetry and Homogeneity

Supervised Learning

$$\mathcal{L}_{sup}(\boldsymbol{U}, \boldsymbol{V}) = \frac{1}{2} \sum_{p=1}^{n} \left\| \frac{1}{\sqrt{d_{out} m}} \boldsymbol{V} \sigma(\boldsymbol{U} \boldsymbol{x}_p) - \boldsymbol{y}_p \right\|_2^2$$



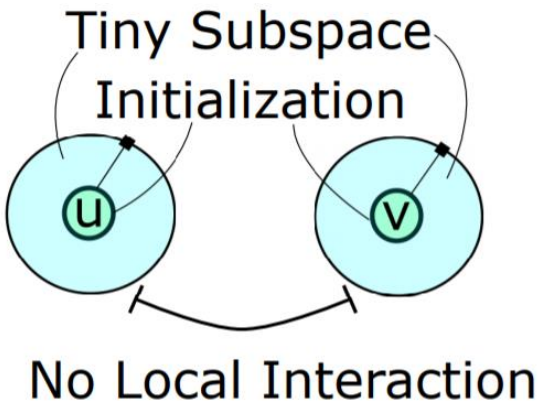
Symmetry and Homogeneity

Theorem (Symmetry and Homogeneity)

Suppose **Assumption 1** *holds. Let us i.i.d. initialize* $u_j \sim \mathcal{N}(0, I)$ *and sample* v_j *uniformly from* $\{+1, -1\}$ *for all* $j \in [m]$. *If we choose* $\|x_p\|_2 = 1$ *for* $p \in [n]$, *then we obtain the following with probability at least* $1 - \delta$:

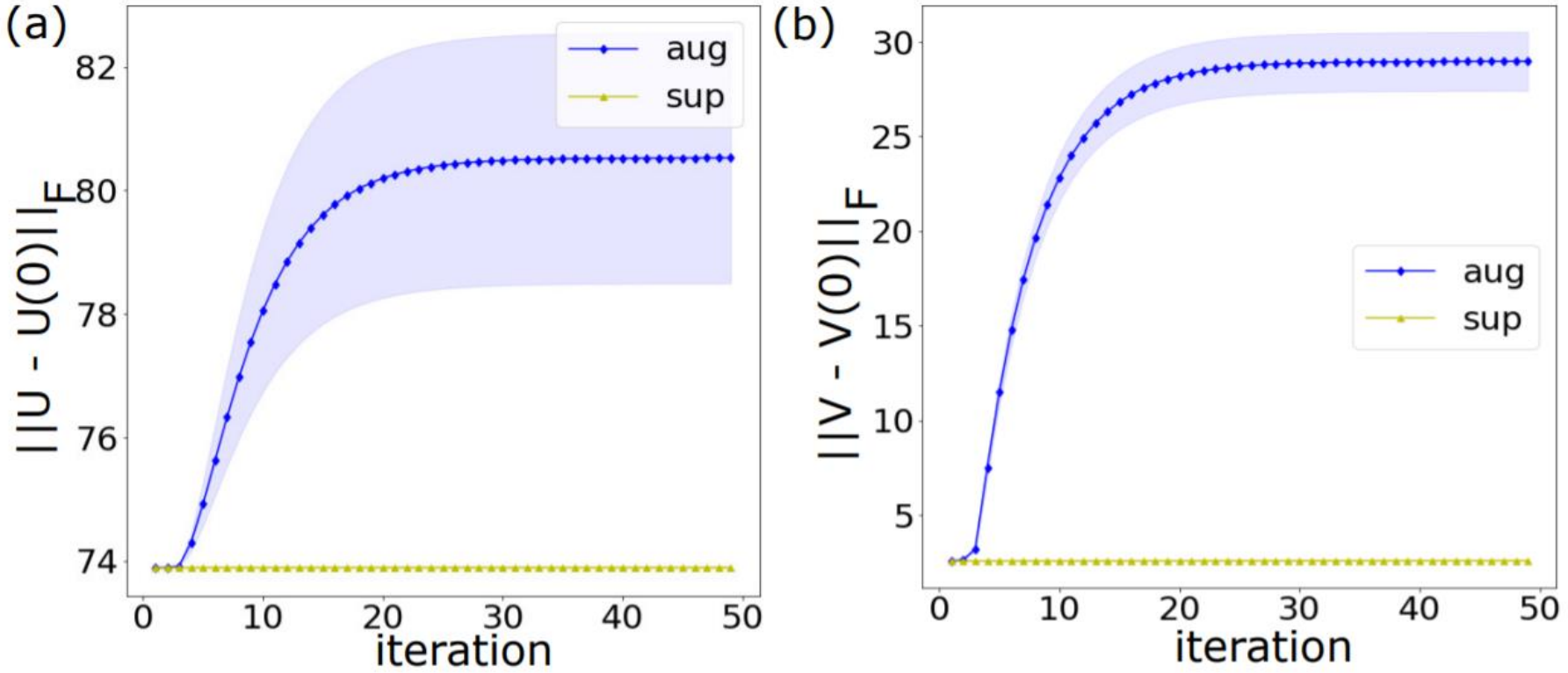
$$\|\boldsymbol{u}_j(t) - \boldsymbol{u}_j(0)\|_2 \leq \mathcal{O}\left(\frac{n^{3/2}}{\sqrt{m}\lambda_0\delta}\right),$$

$$\|\boldsymbol{U}(t) - \boldsymbol{U}(0)\|_F \leq \mathcal{O}\left(\frac{n^{3/2}}{\lambda_0\delta}\right).$$



Symmetry and Homogeneity

Supervised Learning



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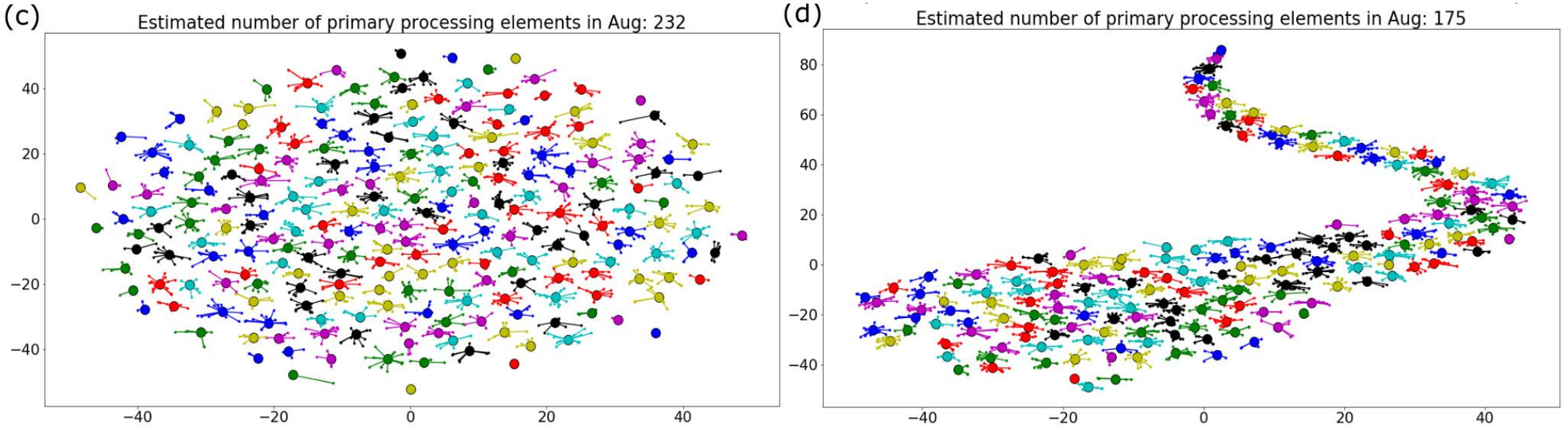
Breakdown of Symmetry and Homogeneity

Adversarial Regularization

$$\mathcal{L}_{aug}(\boldsymbol{U},\boldsymbol{V},\boldsymbol{W},\boldsymbol{a}) = \underbrace{\frac{1}{2}\left\|\frac{1}{\sqrt{d_{out}m}}\boldsymbol{V}\sigma(\boldsymbol{U}\boldsymbol{X})-\boldsymbol{Y}\right\|_F^2}_{\mathcal{L}_{sup}}$$

$$-\frac{1}{m\sqrt{d_{out}}}\sum_{p=1}^{n}\boldsymbol{a}^T\sigma(\boldsymbol{W}\boldsymbol{V}\sigma(\boldsymbol{U}\boldsymbol{x}_p))$$



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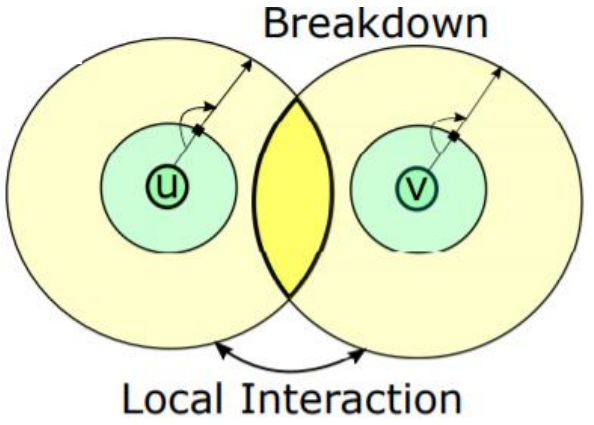
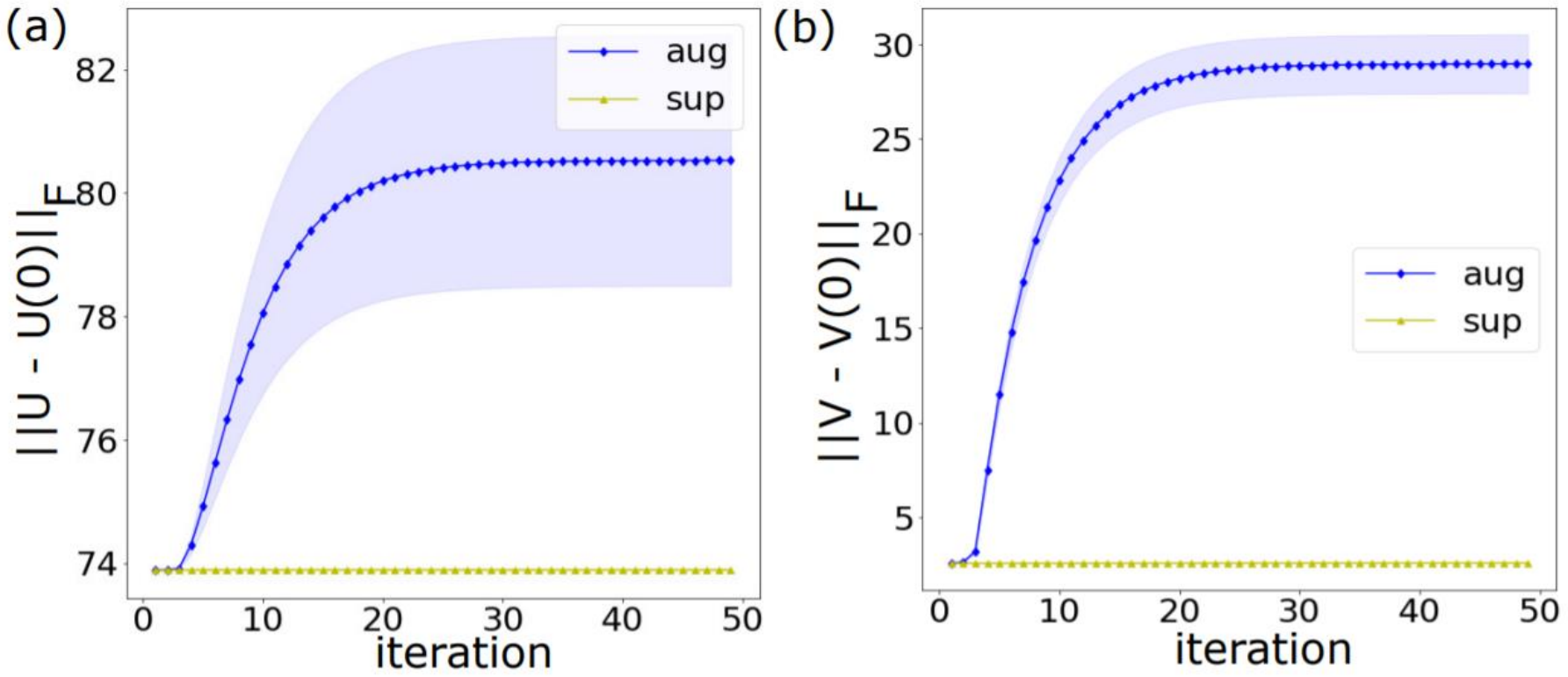
$$\|\boldsymbol{u}_j(t) - \boldsymbol{u}_j(0)\|_2 \leq \mathcal{O}\left(\frac{n^{3/2}}{\sqrt{m}\lambda_0\delta} + \left(\frac{\mu\left(1+\kappa\sqrt{n}\right)}{\sqrt{m}}\right)t\right),$$

$$\|\boldsymbol{U}(t) - \boldsymbol{U}(0)\|_F \leq \mathcal{O}\left(\frac{n^{3/2}}{\lambda_0\delta} + \mu\left(1+\kappa\sqrt{n}\right)t\right).$$

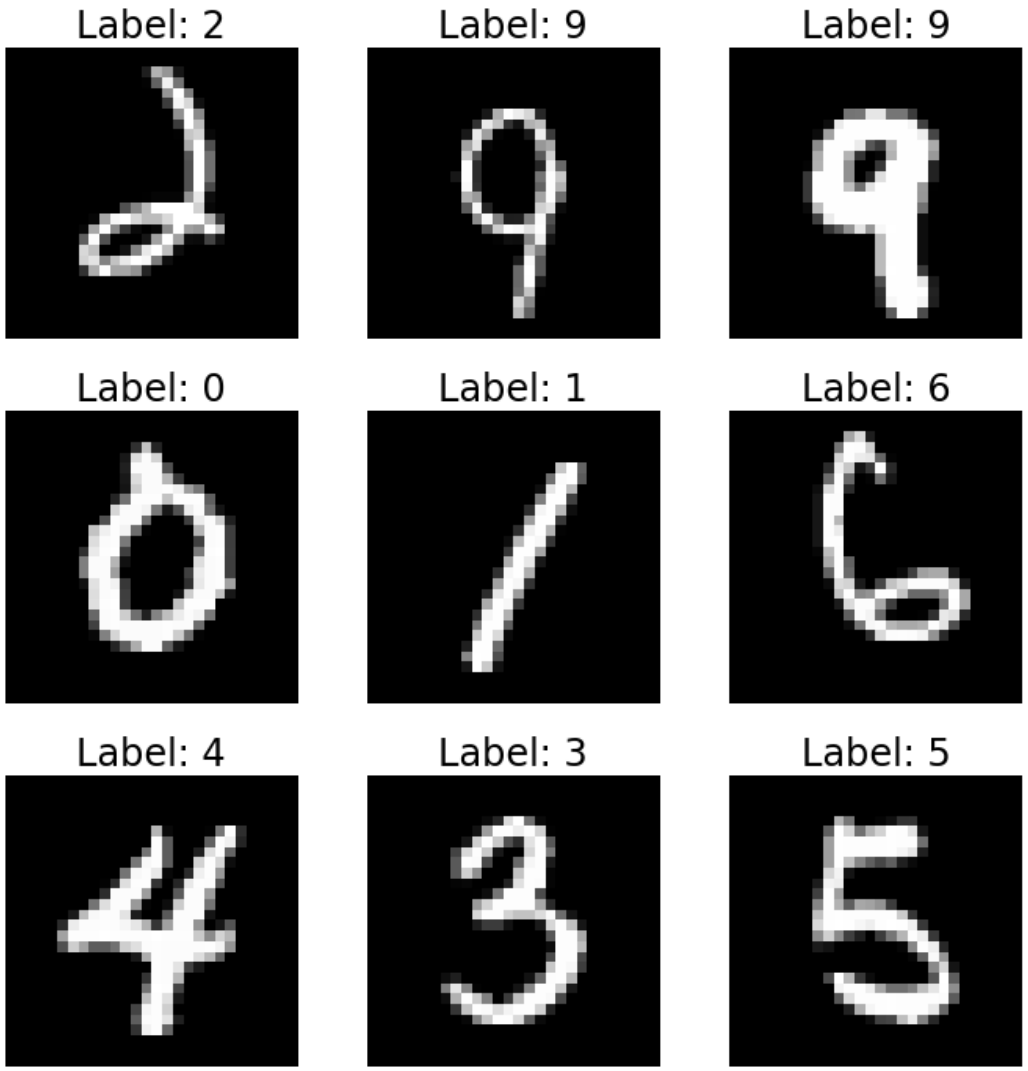


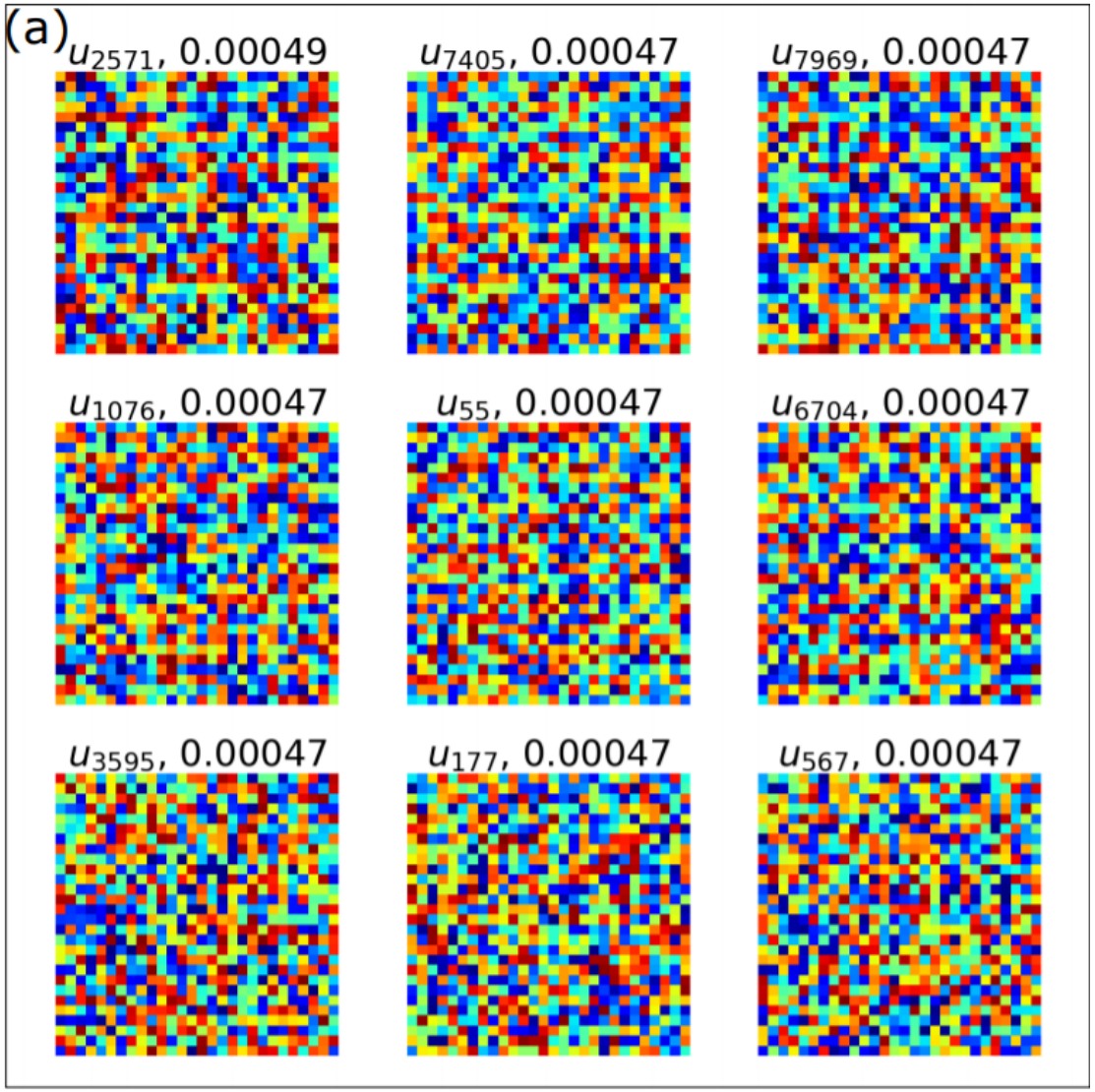
Breakdown of Symmetry and Homogeneity

Adversarial Regularization

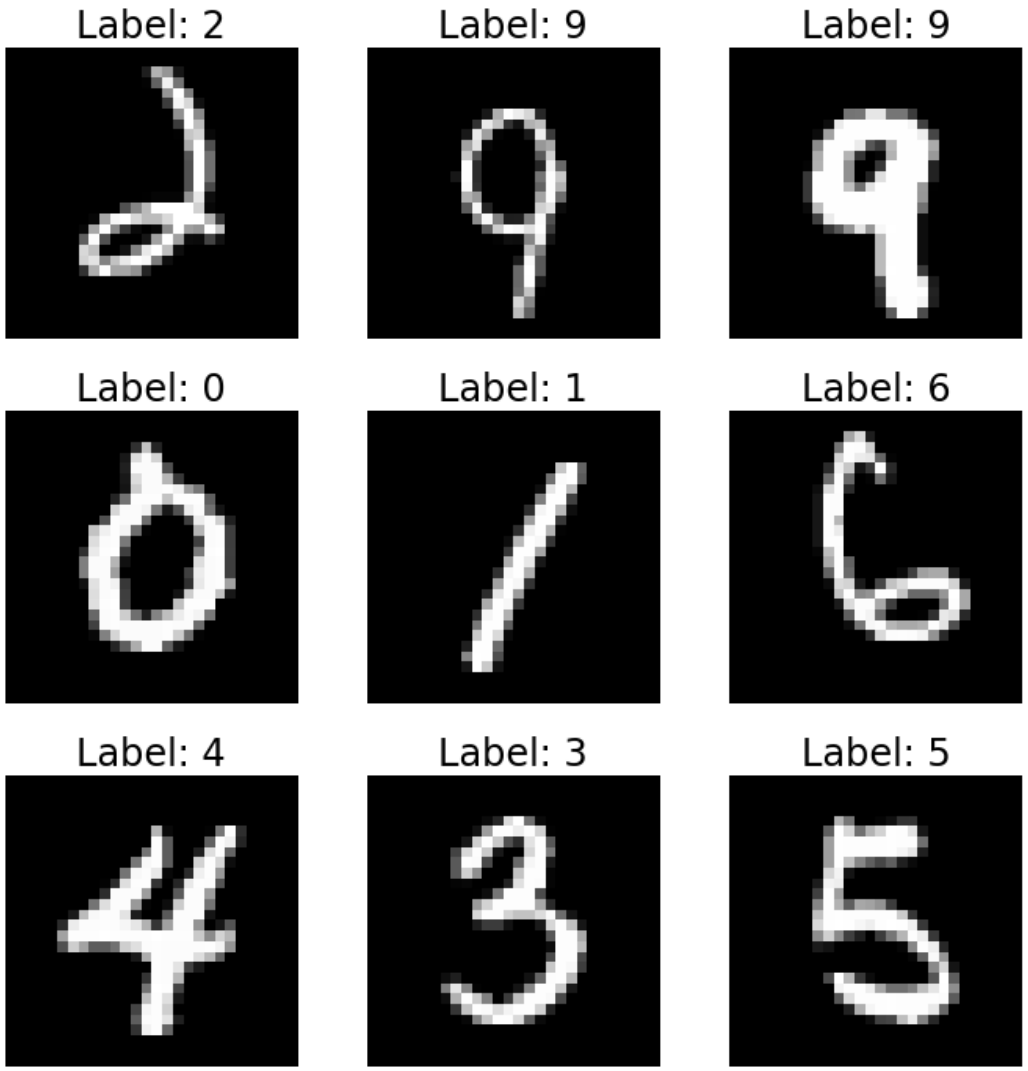


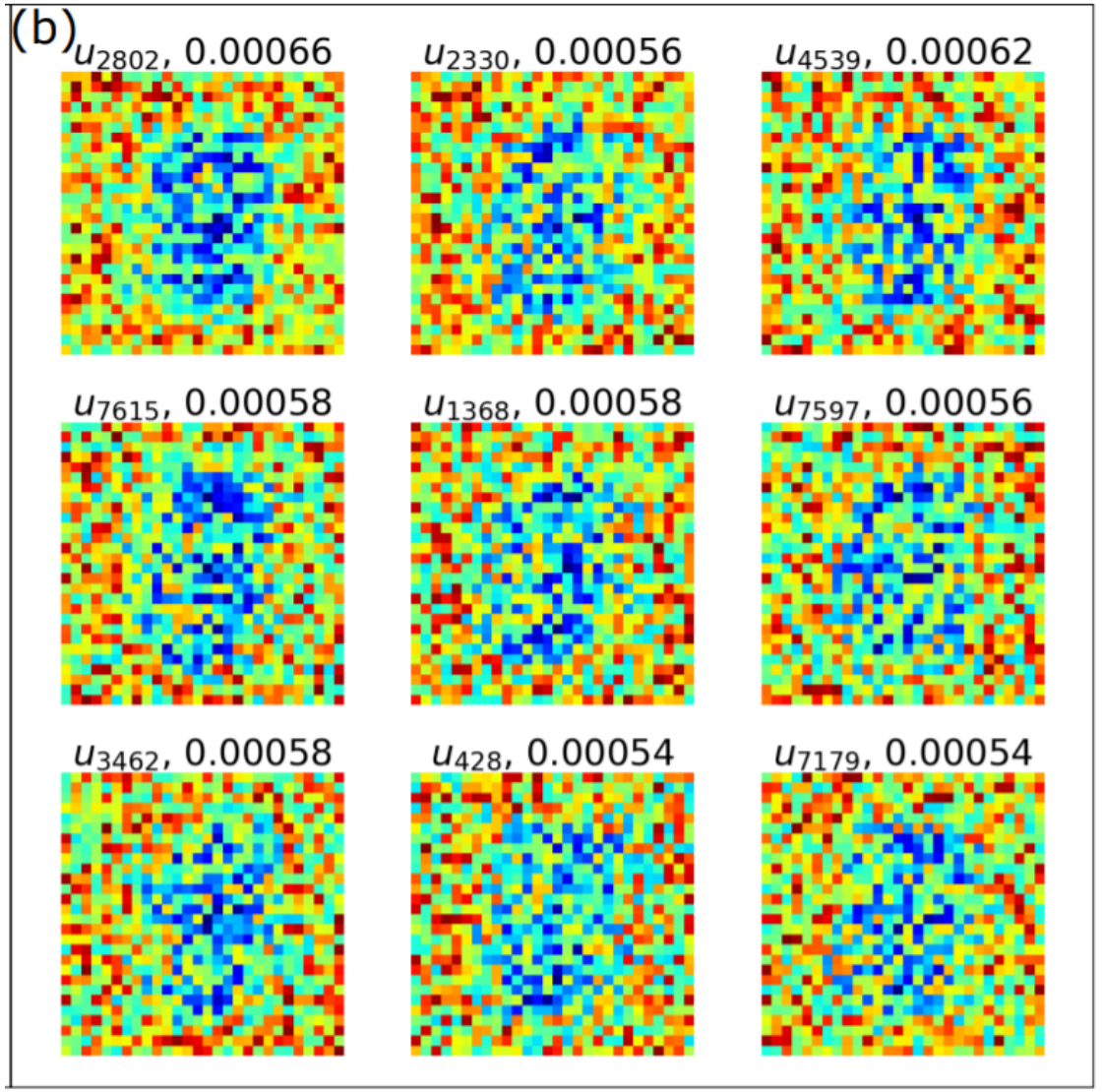
Interpretability of Supervised Learning





Interpretability of Adversarial Regularization





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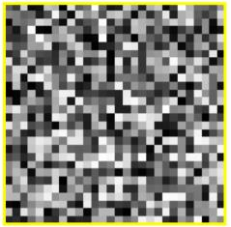

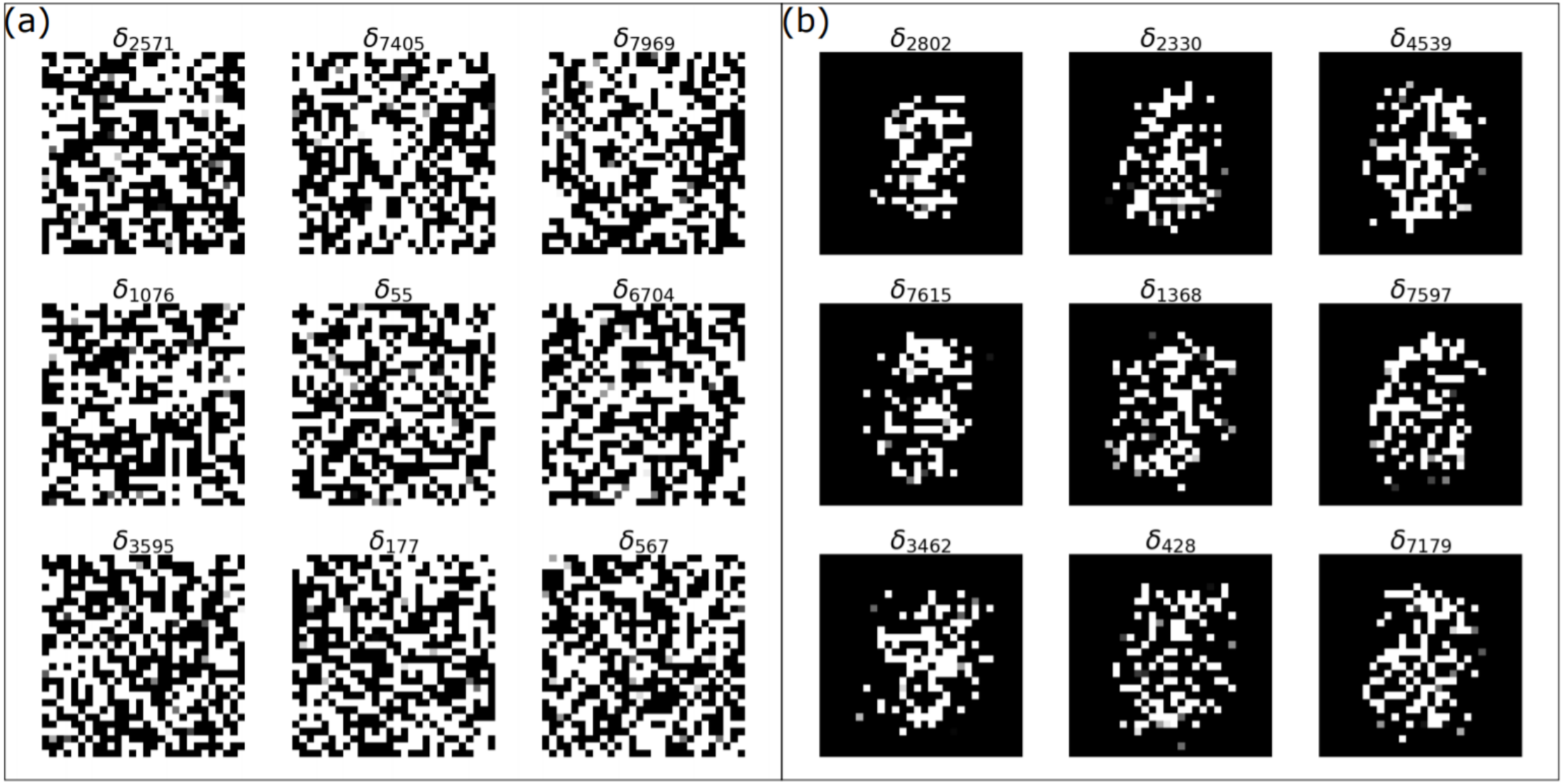

Jointly Training Both Layers

$$\mathfrak{R}_j^{\boldsymbol{u}}\left(\boldsymbol{u}_j, \boldsymbol{v}_j\right) = \mathcal{O}\left(nd_{in}\sqrt{\frac{d_{out}}{m}}\right)$$

$$\mathfrak{D}_j^{\boldsymbol{u}}\left(\nabla^2 \boldsymbol{u}_j\right) = \mathcal{O}\left(nm^2 d_{in} d_{out}^{3/2}\right)$$

$$\mathfrak{R}_j^{\boldsymbol{v}}\left(\boldsymbol{u}_j, \boldsymbol{v}_j\right) = \mathcal{O}\left(nd_{in}\sqrt{\frac{d_{out}}{m}}\right)$$

$$\mathfrak{D}_j^{\boldsymbol{v}}\left(\nabla^2 \boldsymbol{v}_j\right) = \mathcal{O}\left(nm^2 d_{in} d_{out}^{1/2}\right)$$

Bernoulli Differential Equation

$$\frac{dx(t)}{dt} + P(t)x(t) = Q(t)x^n(t) \text{ for } n \in \mathbb{R}\setminus\{0,1\}$$

Natural Phenomena

- Population Growth
- Tumour Growth
- Fermi-Dirac Statistics
- Diffusion of Innovation

$$\frac{dP}{dt} = rP\left(1 - \frac{P}{K}\right)$$

J. Bernoulli, 1695

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Adversarial Regularization

$$\frac{d\psi}{dt} \leq r\psi^{1/2}\left(1 - \frac{\psi^{1/2}}{K}\right)$$

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