Understanding Adaptive Gradient Methods in Training Neural Networks: Risk Bounds and Practical Implications

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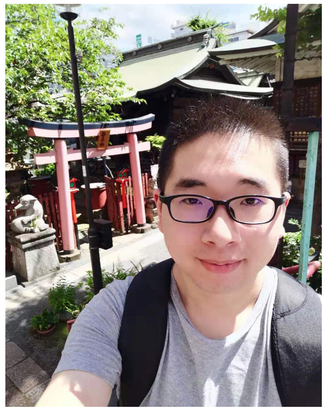
The 9th International Forum on Statistics

Collaborators



Zixiang Chen

Mikhail Belkin

Quanquan Gu

Difan Zou

Yuanzhi Li

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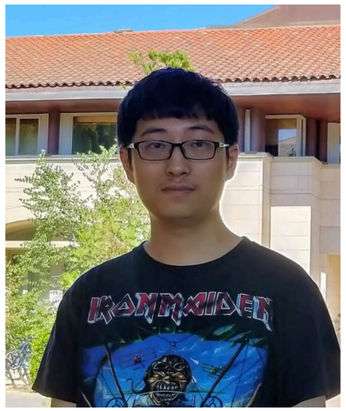
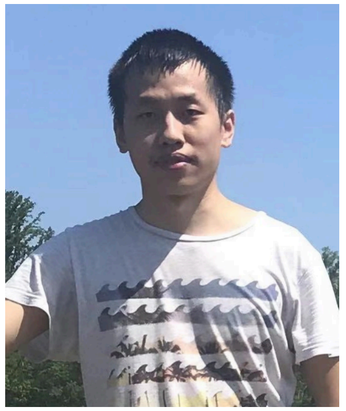


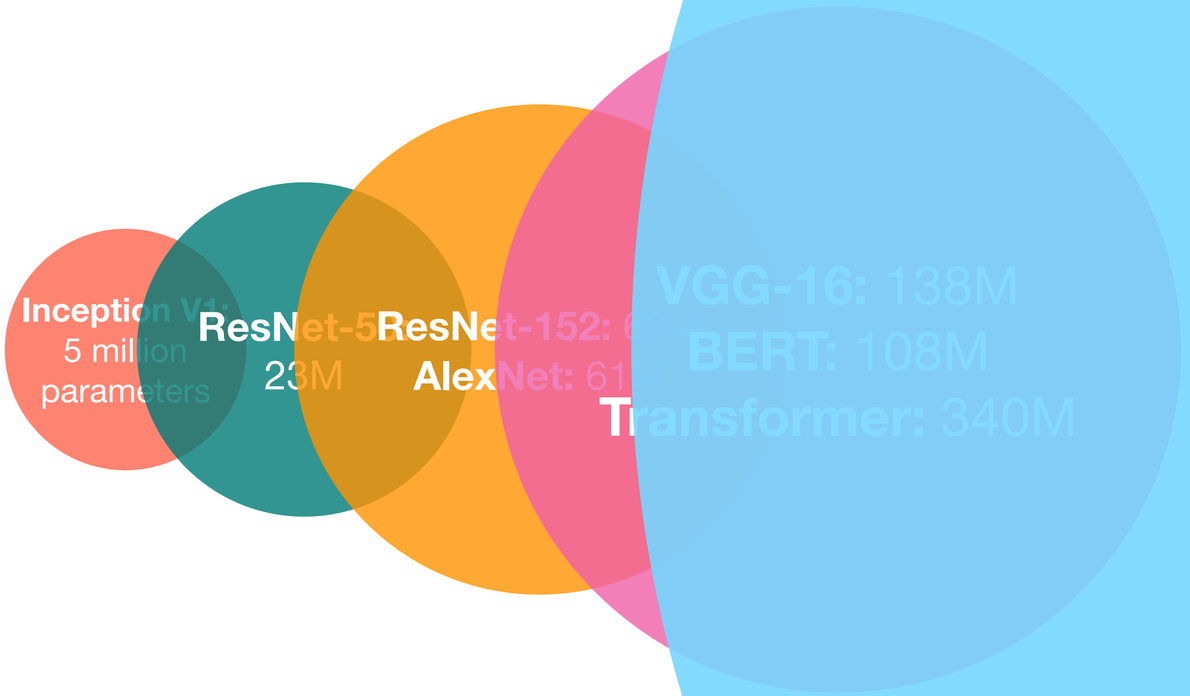
Dongruo Zhou

Ziyan Yang



Yiqi Tang

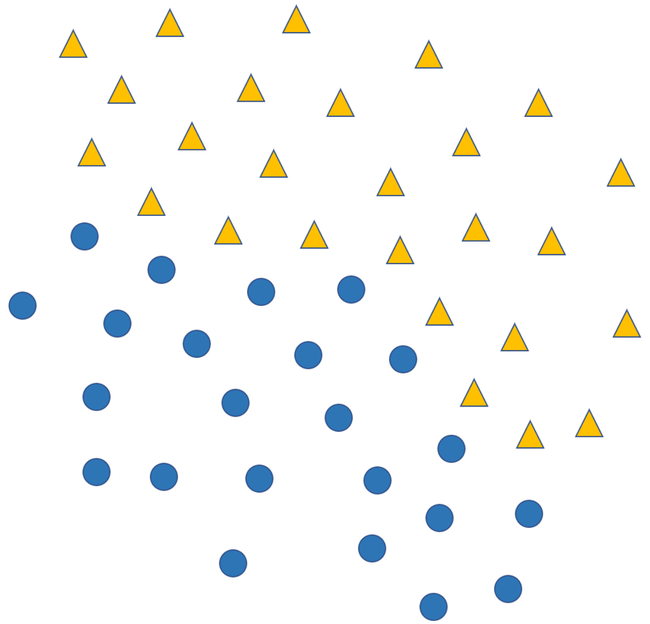
Modern Neural Networks are Over-parameterized



GPT-3:
175 billion parameters

Optimization Matters for Achieving Good Generalization

When learning over-parameterized models, there can be infinitely many predictors that can perfectly fit the limited number of training data.



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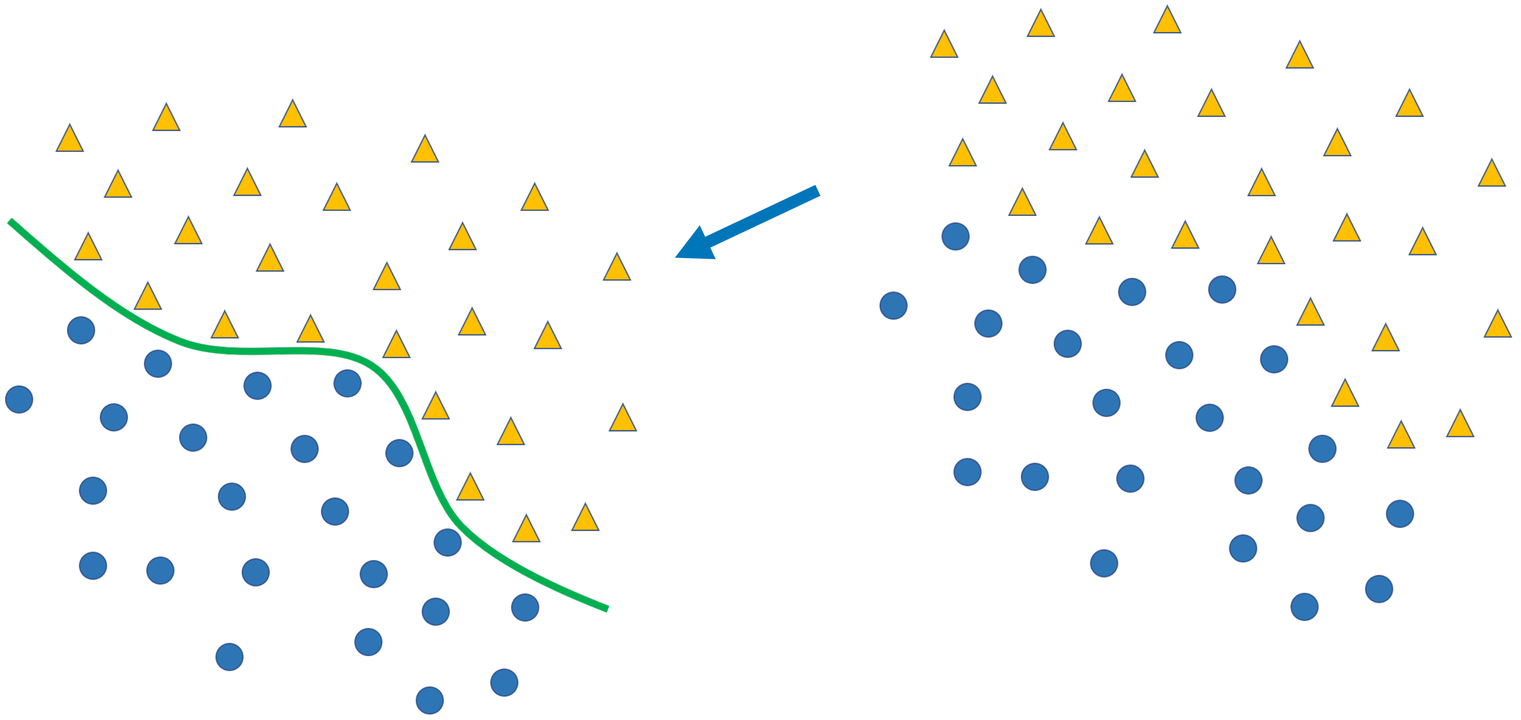

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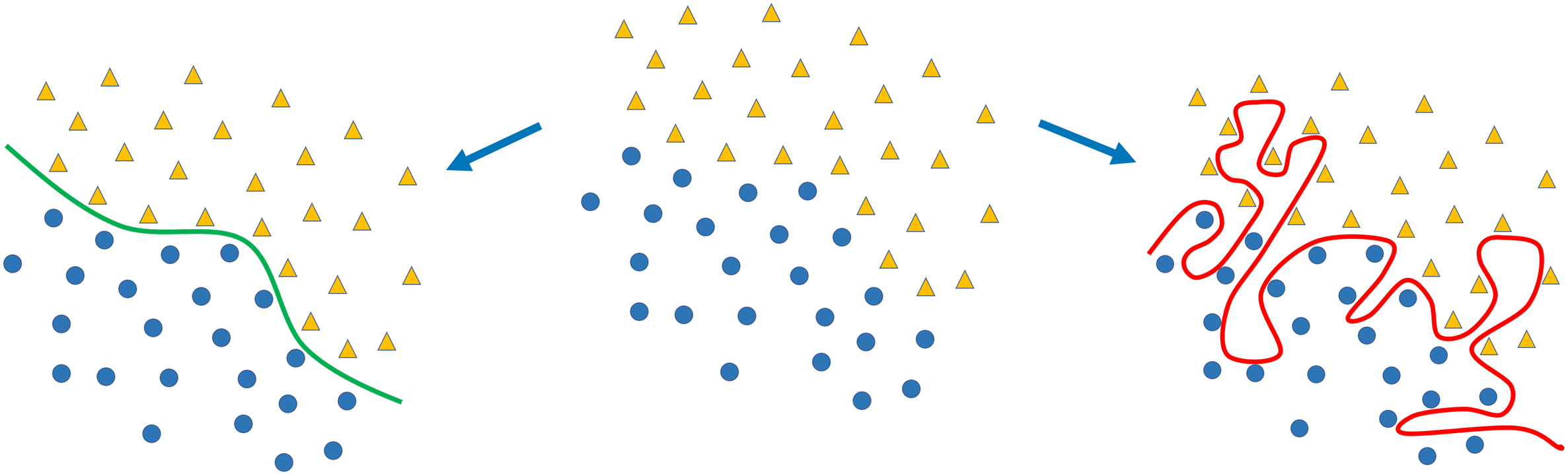

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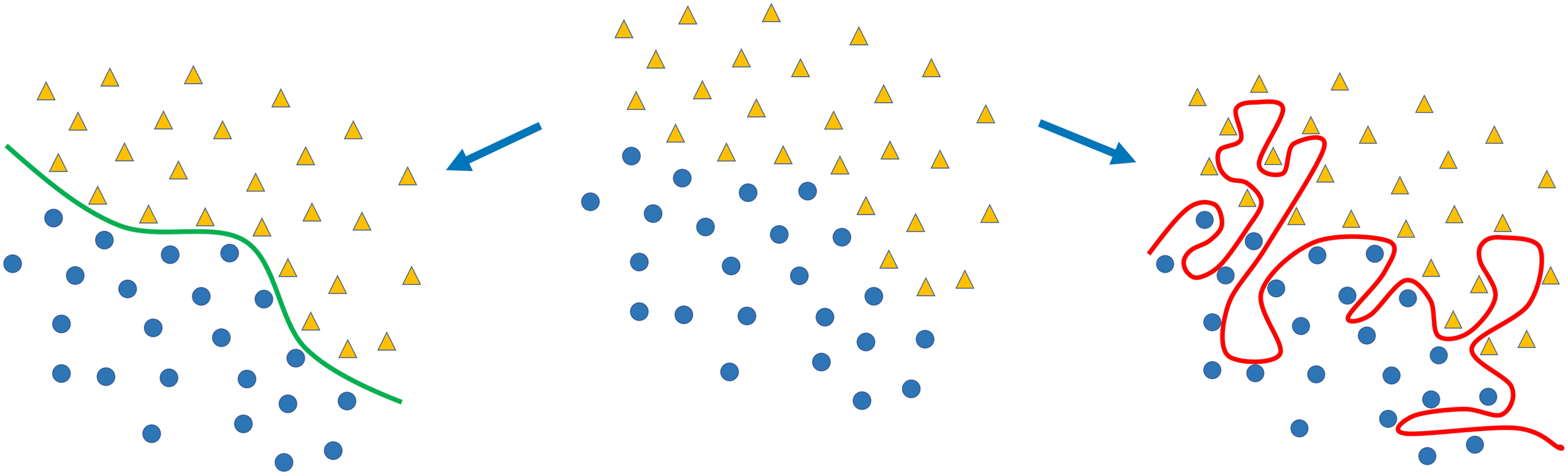
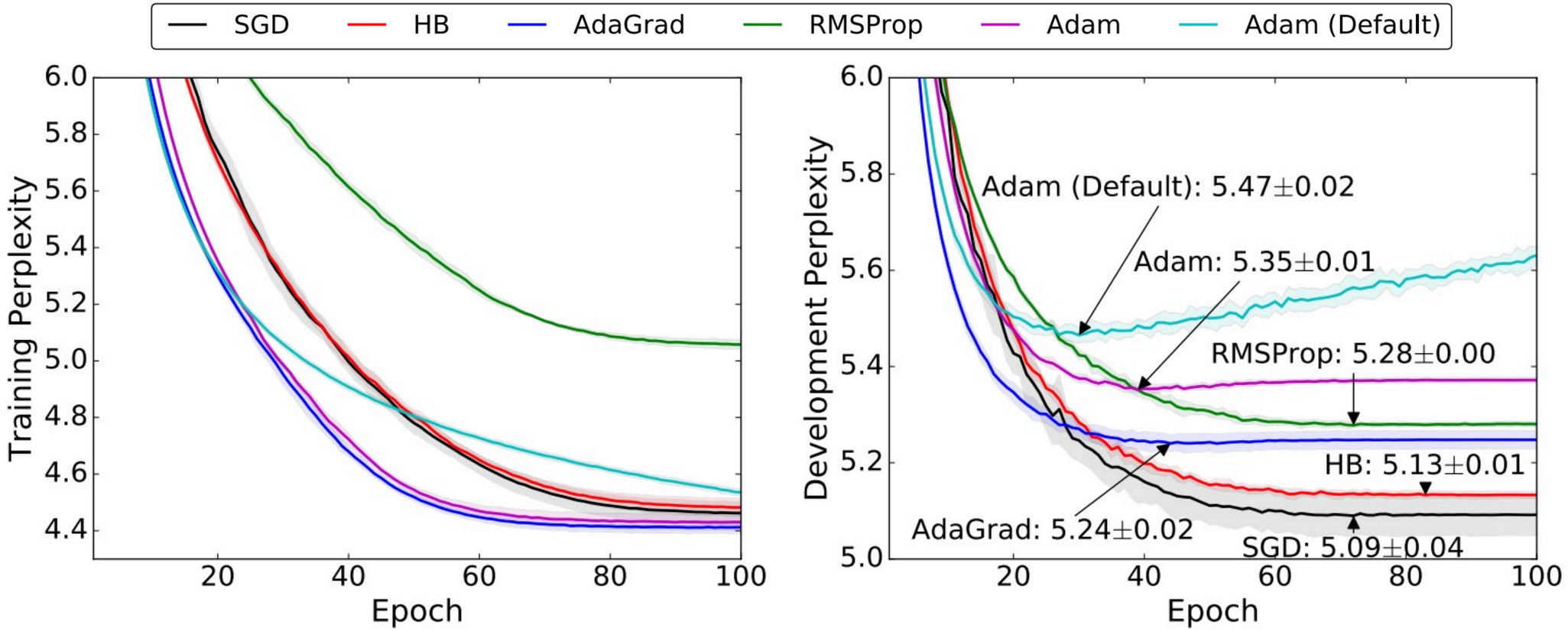


We need to study the impact of the learning algorithm: Which predictor will the training algorithm actually converge to, among the infinitely many minimizers of the training loss?

Adam vs. Gradient Descent

Adaptive gradient methods can converge faster than SGD, but sometimes generalize worse for largely over-parameterized problems [Wilson et al.,2017]



Wilson, Ashia C., Rebecca Roelofs, Mitchell Stern, Nati Srebro, and Benjamin Recht. "The marginal value of adaptive gradient methods in machine learning." In *Advances in neural information processing systems*, pp. 4148-4158. 2017.

Outline

- A simple statistical learning task and theoretical guarantees for learning two-layer CNNs with GD

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- Practical implications: Padam and beyond

Jinghui Chen, Dongruo Zhou, Yiqi Tang, Ziyan Yang, Yuan Cao and Quanquan Gu, "Closing the Generalization Gap of Adaptive Gradient Methods in Training Deep Neural Networks." in International Joint Conference on Artificial Intelligence 2020

A simple statistical learning task and theoretical guarantees for learning two-layer CNNs with GD

A Simple Statistical Learning Task

In image-based prediction tasks, it is common to assume that only a small patch of the image is relavant to the labels. [Wu & Feng, 2022]

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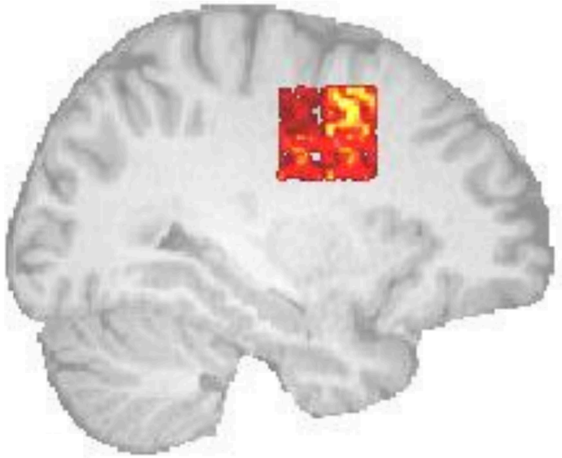

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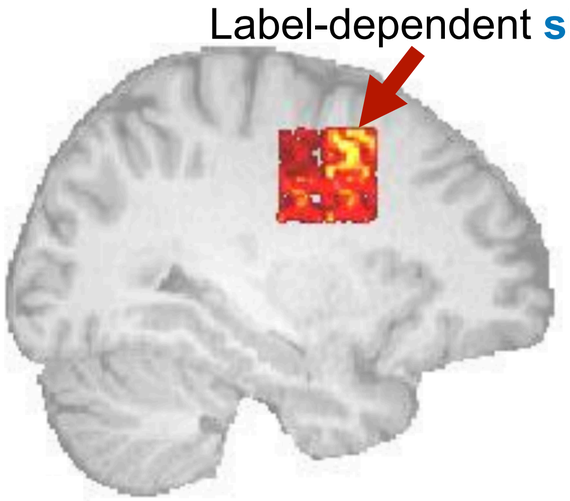

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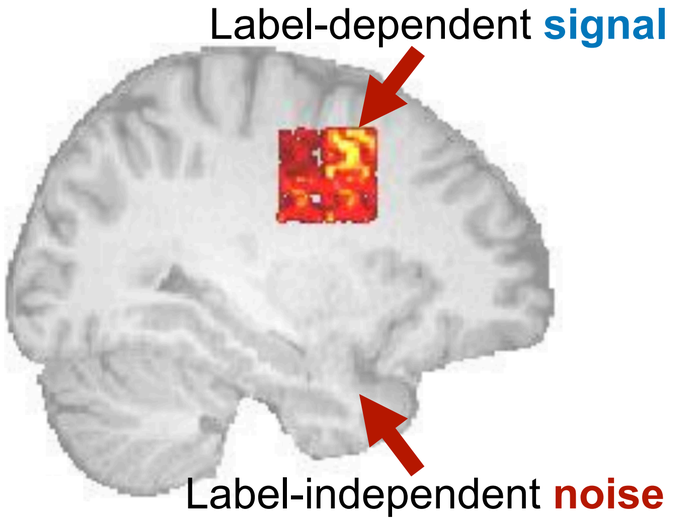

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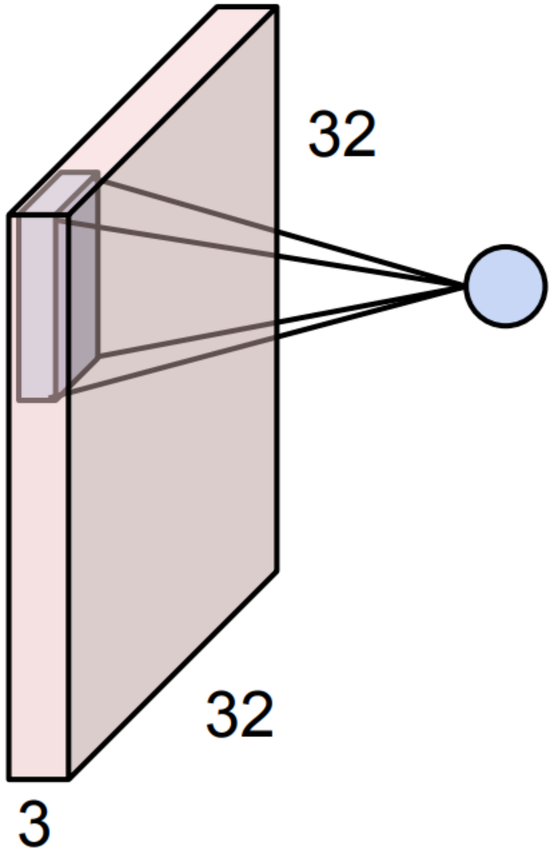

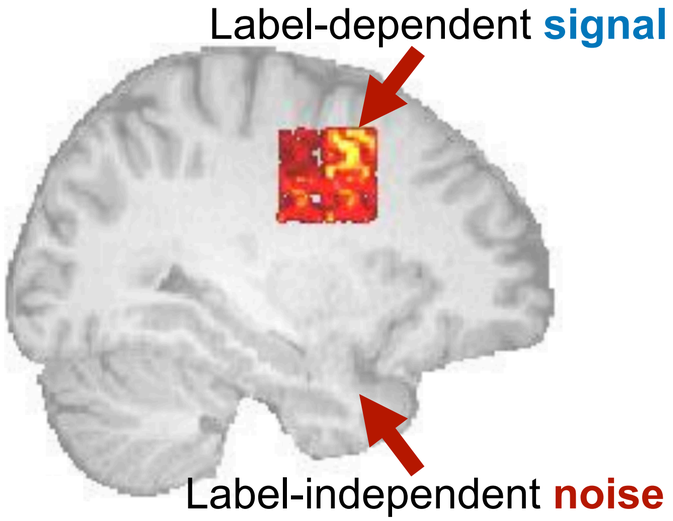

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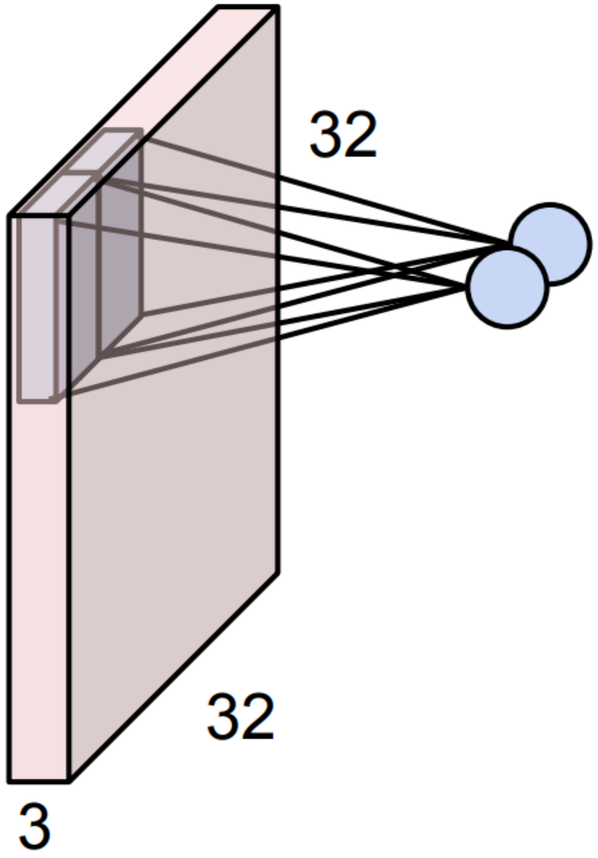

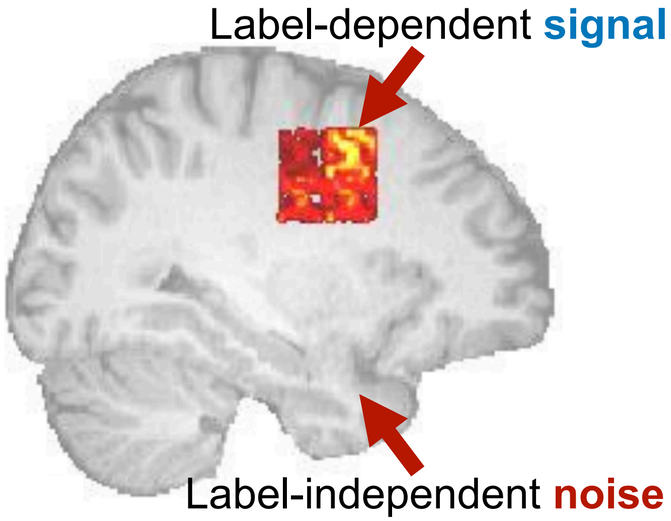

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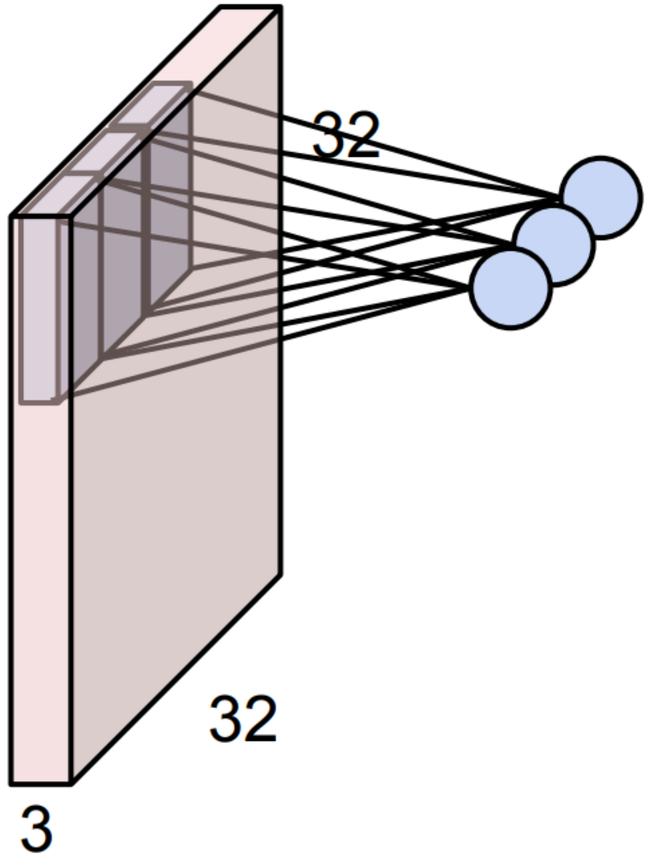

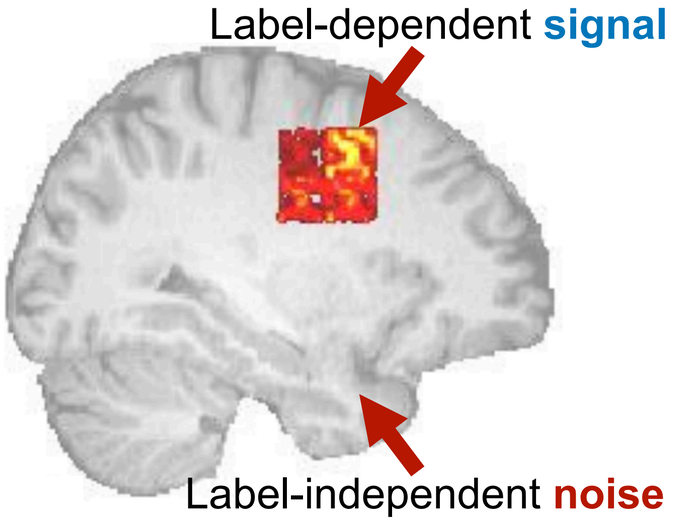

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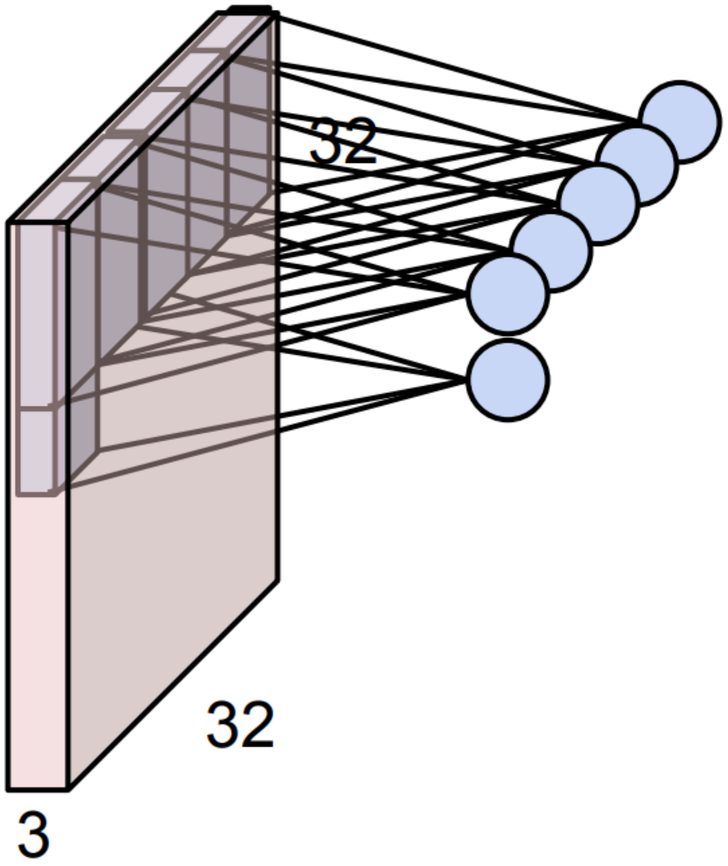

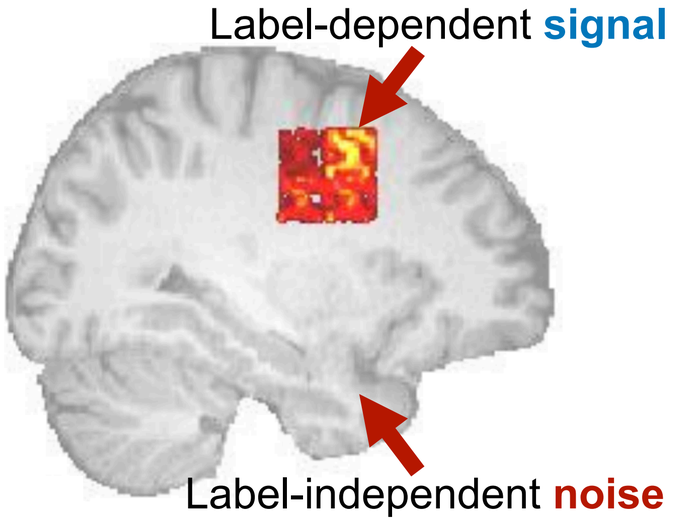

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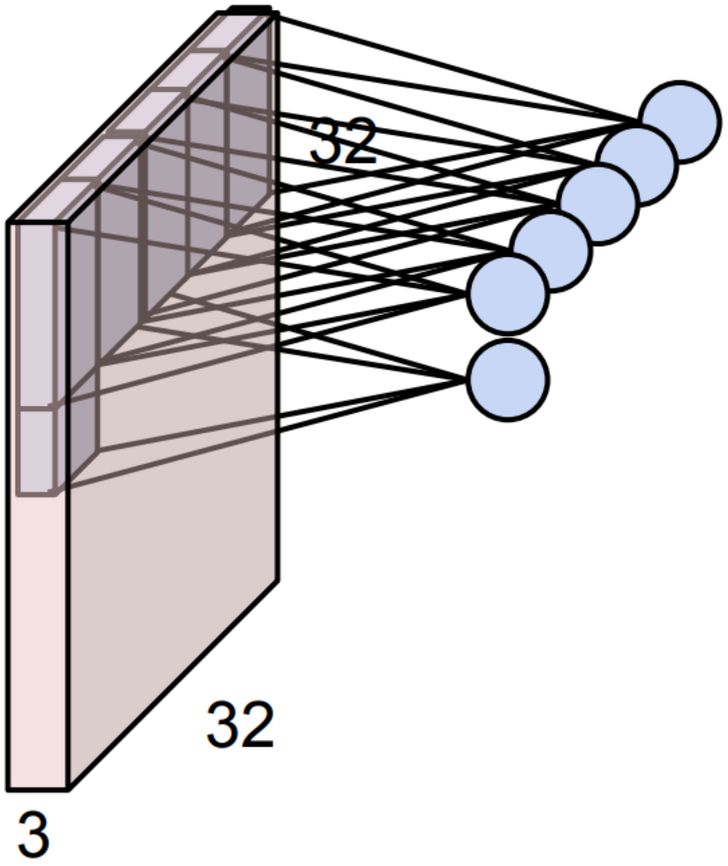

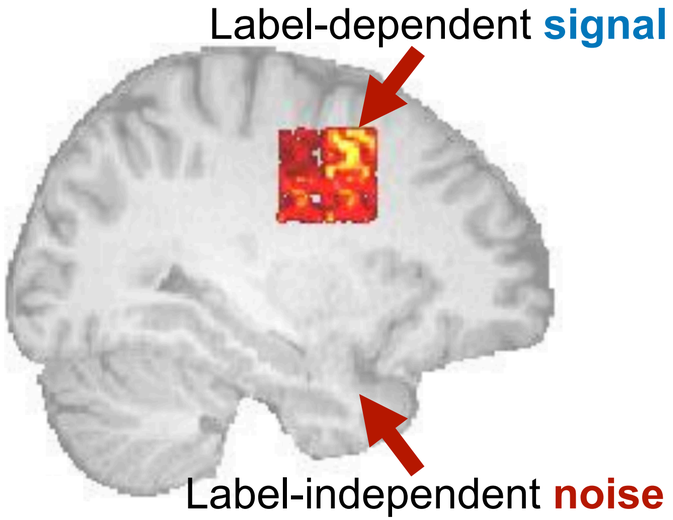

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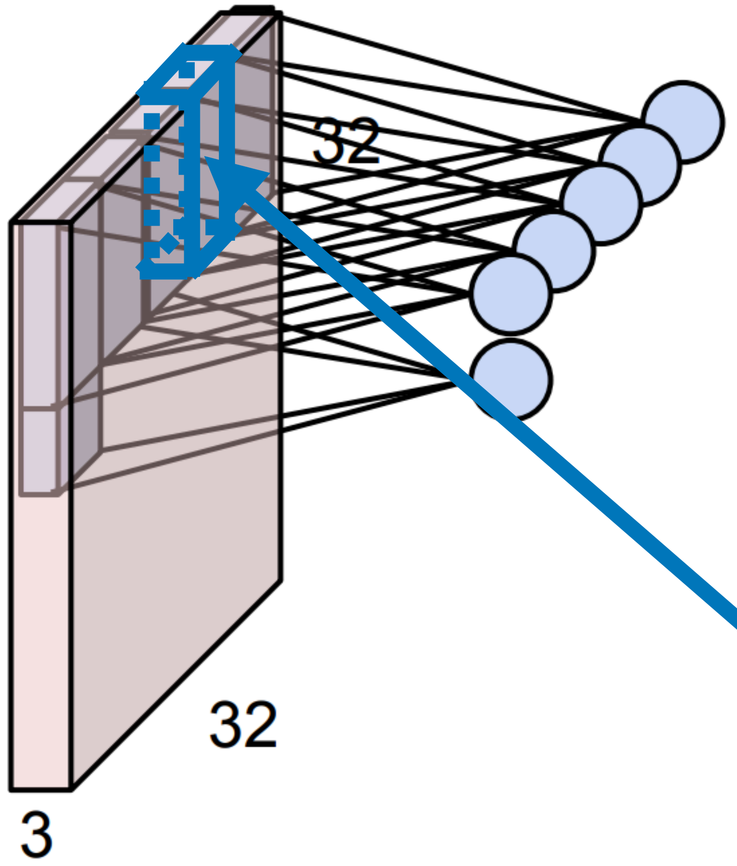

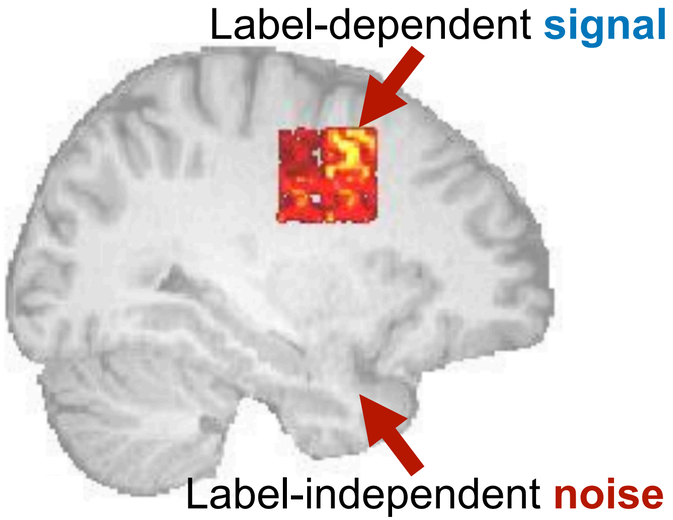

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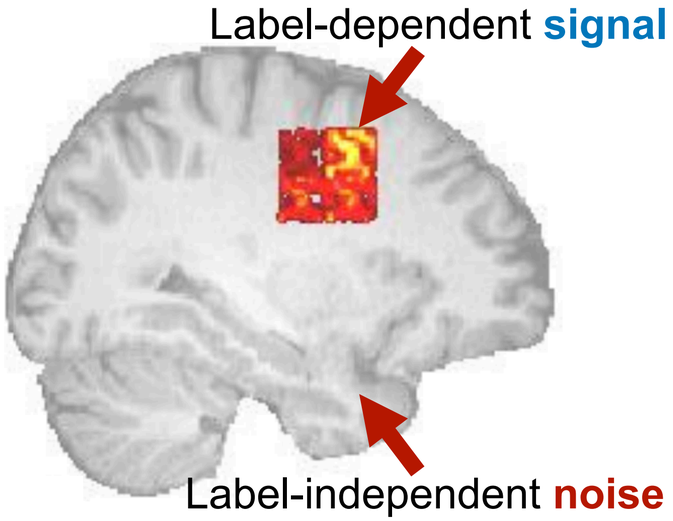

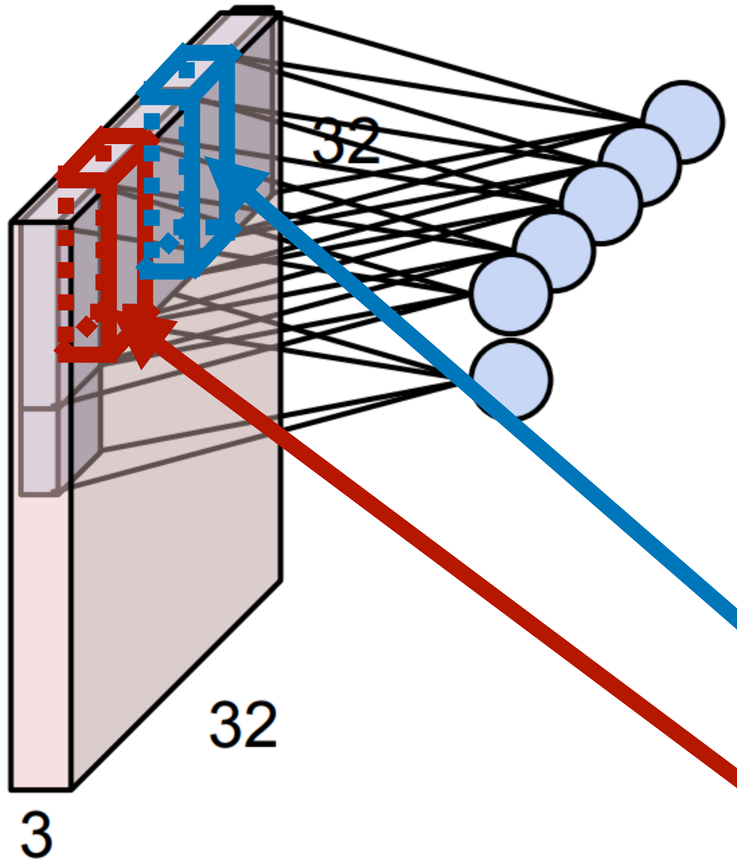

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Noise patch : $\boldsymbol{\xi} \sim N(0, \sigma_p^2 \mathbf{I})$

CNN models

The corresponding two-layer CNN:

$$f_{\mathbf{W}}(\mathbf{x}) = F_{+1}(\mathbf{W}_{+1}, \mathbf{x}) - F_{-1}(\mathbf{W}_{-1}, \mathbf{x})$$

$$F_j(\mathbf{W}_j, \mathbf{x}) = \frac{1}{m} \sum_{r=1}^{m} \left[\sigma(\langle \mathbf{w}_{j,r}, \mathbf{x}^{(1)} \rangle) + \sigma(\langle \mathbf{w}_{j,r}, \mathbf{x}^{(2)} \rangle)\right], \; j \in \{\pm 1\}$$

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- We consider the case $\sigma(x) = \mathrm{ReLU}^q(x)$ for $q > 2$. The power q here ensures smoothness. The results can also be applied to the "Huberized ReLU":

$$\sigma(z) = \begin{cases} 0, & z < 0 \\ z^q/(qh^{q-1}), & z \in [0, h] \\ z - (q-1)h/q, & \text{otherwise.} \end{cases}$$

Risk Bounds of Two-Layer CNNs Trained by GD

Definition. Signal-to-noise ratio $SNR = \dfrac{\|\boldsymbol{\mu}\|_2}{\sigma_p \sqrt{d}} \approx \dfrac{\|\boldsymbol{\mu}\|_2}{\|\boldsymbol{\xi}\|_2}$.

Training/test losses $L_S(\mathbf{W}) := \dfrac{1}{n} \sum_{i=1}^{n} \ell[y_i \cdot f_{\mathbf{W}}(\mathbf{x_i})], \;\; L_{\mathscr{D}}(\mathbf{W}) := \mathbb{E}_{(\mathbf{x},y)\sim\mathscr{D}} \ell[y \cdot f_{\mathbf{W}}(\mathbf{x})]$.

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Sharp phase transition!

Proof Sketch - Signal-Noise Decomposition

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Discrete dynamical system of coefficients

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$$\gamma_{j,r}^{(t+1)} = \gamma_{j,r}^{(t)} - \frac{\eta}{nm} \cdot \sum_{i=1}^{n} \ell_i'^{(t)} \cdot \sigma'(\langle \mathbf{w}_{j,r}^{(0)}, y_i \cdot \boldsymbol{\mu} \rangle + jy\gamma_{j,r}^{(t)}) \cdot \|\boldsymbol{\mu}\|_2^2$$

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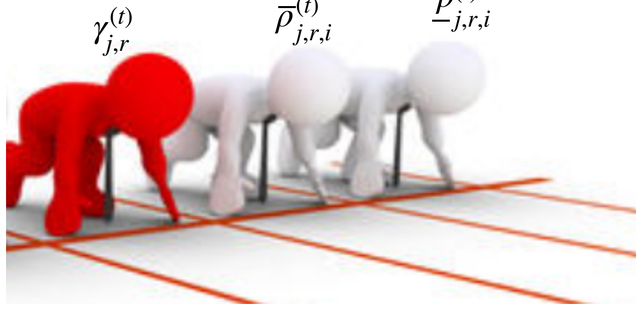

The Generalization Gap Between Adam and GD

The Adam Algorithm

$$\mathbf{M}^{(t+1)} = \beta_1 \cdot \mathbf{M}^{(t)} + (1 - \beta_1) \cdot \nabla_{\mathbf{W}} L_S(\mathbf{W}^{(t)})$$

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Such entry-wise operation can **increase the speed of noise memorization**!

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Now suppose that we just have ONE sample from the noisy MNIST data set:

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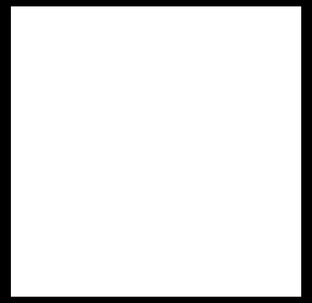
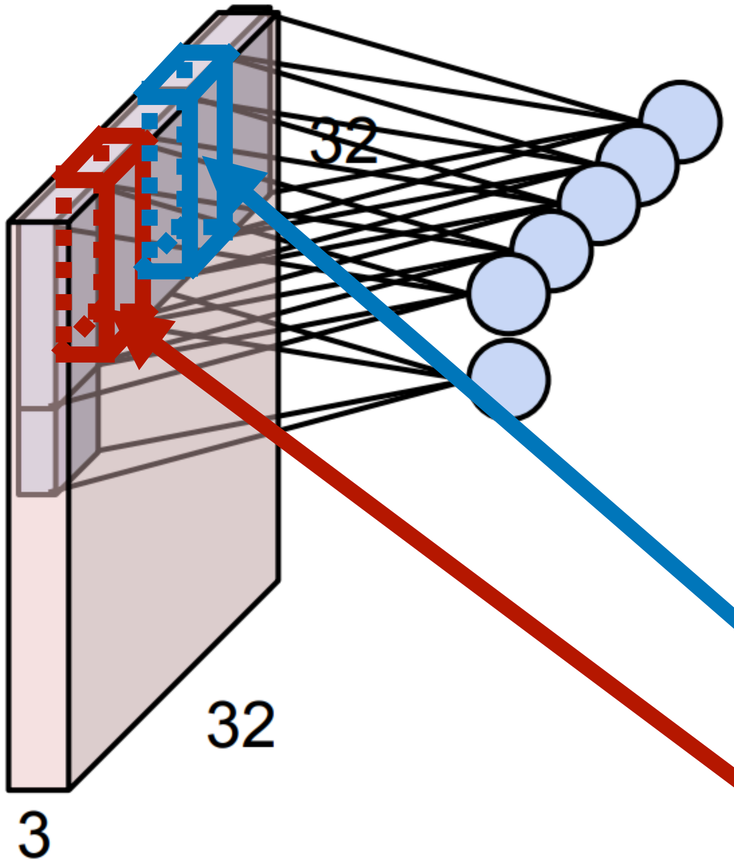


Data Model for the CNN Case

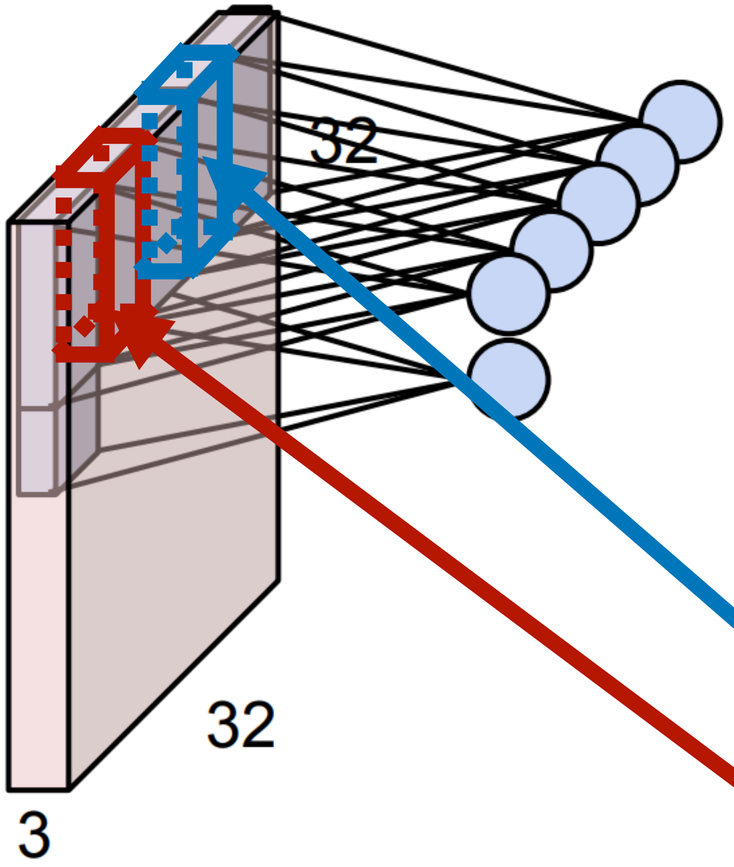


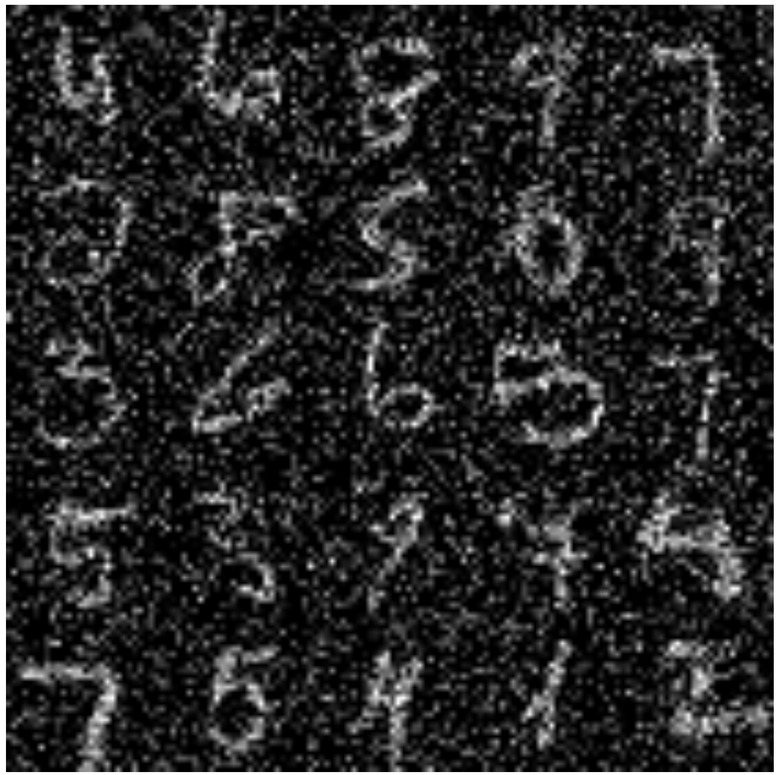
Our data model $\mathscr{D}$:

1. $y \sim \text{Rademacher}$
2. Signal patch: sparse, but non-zero entries are relatively large

Noise patch: dense, but entry-wisely small

Data Model for the CNN Case





Our data model $\mathscr{D}$:

1. $y \sim \text{Rademacher}$
2. Signal patch: sparse, but non-zero entries are relatively large

Noise patch: dense, but entry-wisely small

Main Results

Theorem

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Under certain conditions, there exists $\lambda_0 > 0$ such that for all weight decay regularization parameter $\lambda < \lambda_0$, the following hold with high probability:

- Adam gives a CNN model $\hat{\mathbf{W}}_{\text{Adam}}$ with approximately 0 training loss, and approximately 0.5 test error.
- GD gives a CNN model $\hat{\mathbf{W}}_{\text{GD}}$ with approximately 0 training loss, and approximately 0 test error.

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- When the training loss function is convex, then weight decay will ensure that Adam and GD converge to the same unique global optimum!
- Our result shows that when training neural networks, weight decay regularization cannot resolve the issue of Adam!

Practical implications: Padam and beyond

The Padam Algorithm - “Interpolation” between Adam & SGD

Adam:

$$\mathbf{M}^{(t+1)} = \beta_1 \cdot \mathbf{M}^{(t)} + (1-\beta_1) \cdot \nabla_{\mathbf{W}} L_S(\mathbf{W}^{(t)})$$

$$\mathbf{V}^{(t+1)} = \beta_2 \cdot \mathbf{V}^{(t)} + (1-\beta_2) \cdot [\nabla_{\mathbf{W}} L_S(\mathbf{W}^{(t)})]^2$$

$$\mathbf{W}^{(t+1)} = \mathbf{W}^{(t)} - \eta \cdot \mathbf{M}^{(t)} / \sqrt{\mathbf{V}^{(t)}}$$

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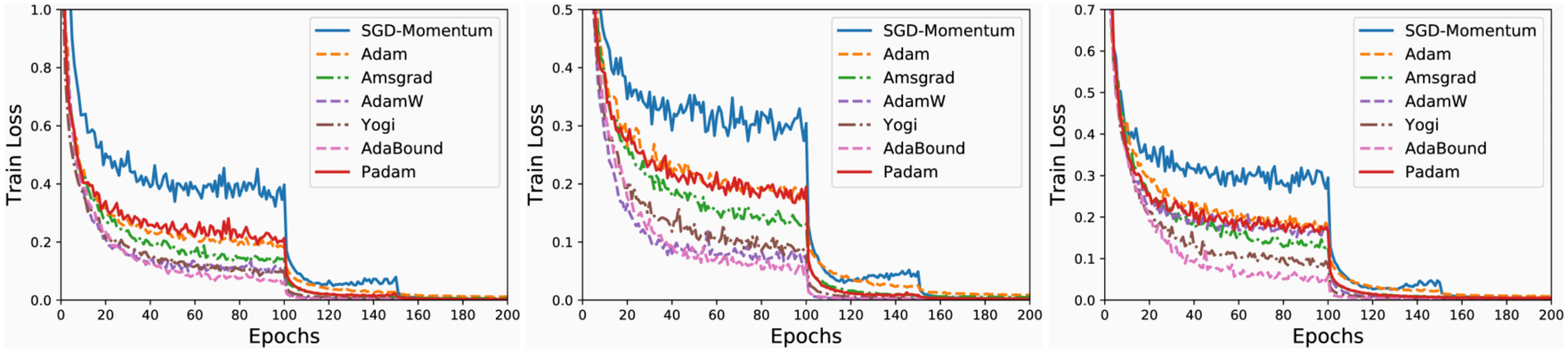
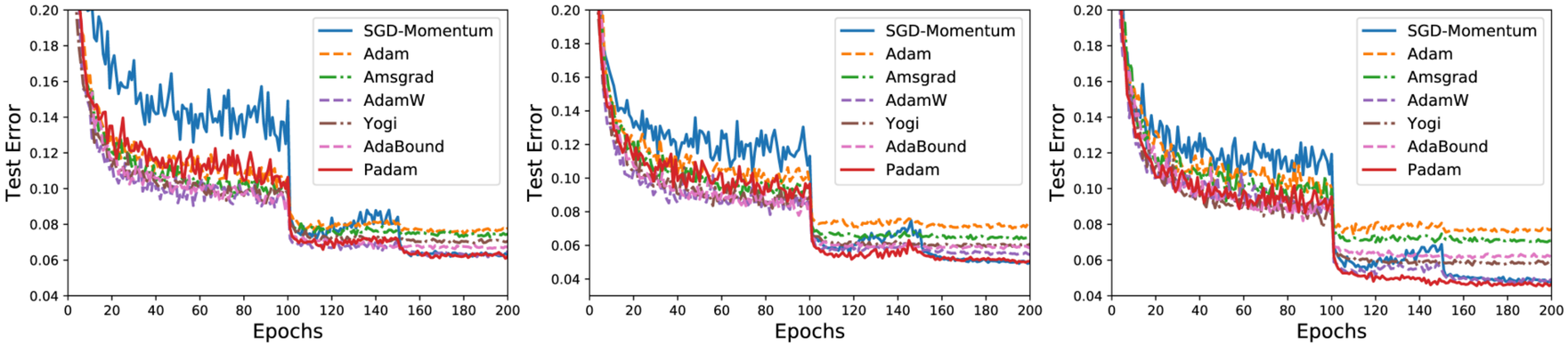
- p controls the level of **adaptivity** in the optimization algorithm
- If we set $p = 1/2$, it recovers the Adam; and if $p = 0$, it recovers SGD with momentum

Experimental Results

Training loss and test error (top-1 error) on CIFAR-10.



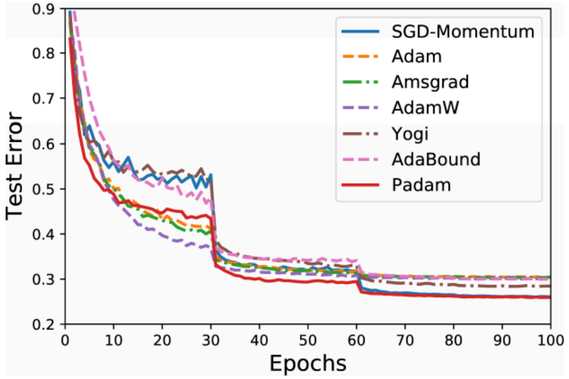
(a) Train Loss for VGGNet (b) Train Loss for ResNet (c) Train Loss for WideResNet



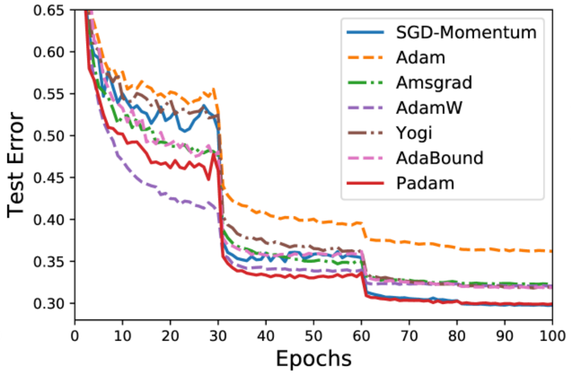
(d) Test Error for VGGNet (e) Test Error for ResNet (f) Test Error for WideResNet

Experimental Results

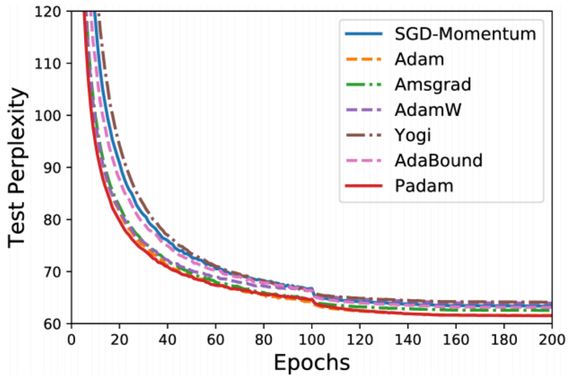
Test error on the ImageNet dataset (left and middle columns), and test perplexity on the Penn Treebank dataset (right column)



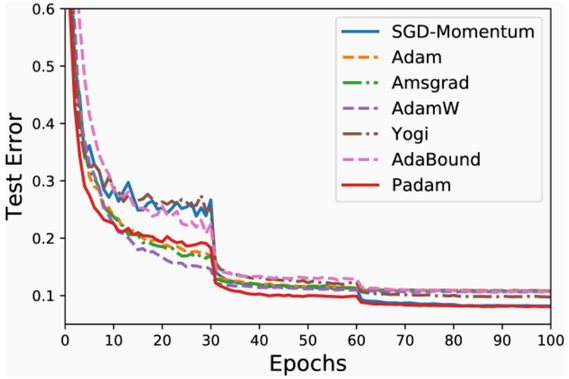
(a) Top-1 Error, VGGNet



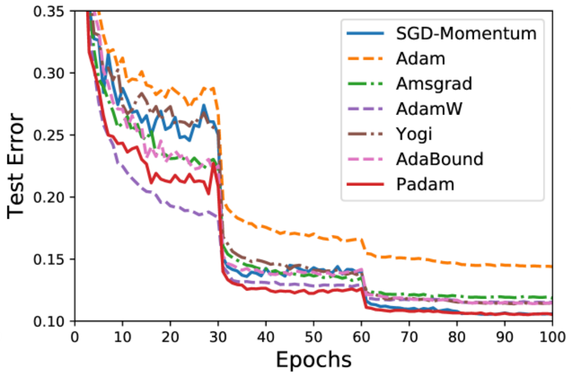
(b) Top-1 Error, ResNet



(c) 2-layer LSTM



(d) Top-5 Error, VGGNet



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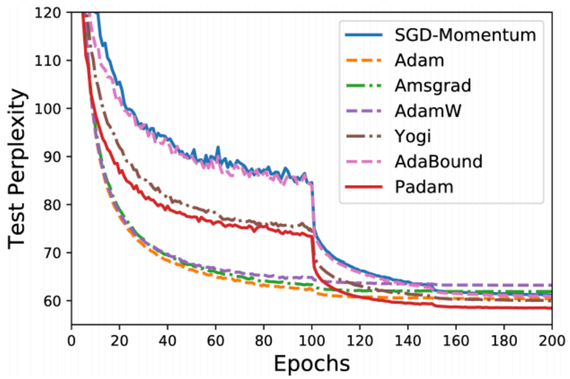

(f) 3-layer LSTM

Experimental Results

Test Accuracy on the CIFAR10 dataset after 200 epochs

Models	SGD-Momentum	Adam	Amsgrad	AdamW	Yogi	AdaBound	Padam
VGGNet	93.71	92.21	92.54	93.54	92.94	93.28	**93.78**
ResNet	**95.00**	92.89	93.53	94.56	93.92	94.16	94.94
WideResNet	95.26	92.27	92.91	95.08	94.23	93.85	**95.34**

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	Top-5	89.40	85.61	88.15	88.47	88.59	88.55	**89.47**
VGGNet	Top-1	73.93	69.52	69.61	69.89	71.56	70.00	**74.04**
	Top-5	91.82	89.12	89.19	89.35	90.25	89.27	**91.93**

Test Perplexity on the Penn Treebank dataset after 200 epochs

Models	SGD-Momentum	Adam	Amsgrad	AdamW	Yogi	AdaBound	Padam
2-layer LSTM	63.37	61.58	62.56	63.93	64.13	63.14	**61.53**
3-layer LSTM	61.22	60.44	61.92	63.24	60.01	60.89	**58.48**

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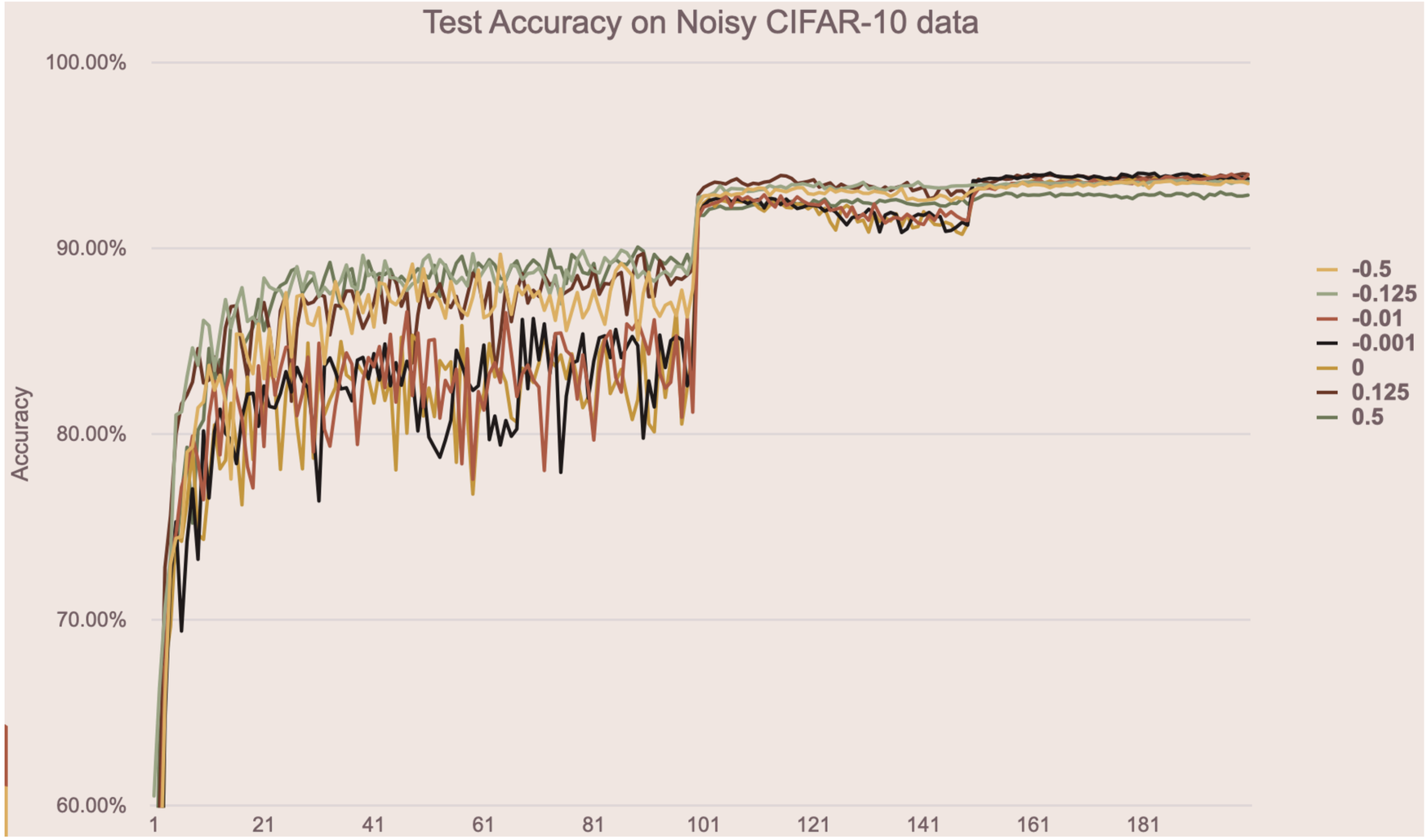
Sometimes, “Extrapolation” Also Works!



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Thank you!