Optimization for Deep Learning

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Background

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4. Solve the *training problem*:

$$\min_{\mathbf{x} \in \mathbb{R}^d} \frac{1}{N} \sum_{i=1}^{N} \ell\left(h_{\mathbf{x}}(\mathbf{d}_i), y_i\right) \tag{2}$$

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Finite-sum empirical risk minimization problem:

$$f(\mathbf{x}^\star) = \min_{\mathbf{x}\in\mathbb{R}^d} \left\{ f(\mathbf{x}) := \frac{1}{N}\sum_{i=1}^{N} \Big(f_i(\mathbf{x}) := F(\mathbf{x}, \boldsymbol{\xi}_i) \Big) \right\} \tag{3}$$

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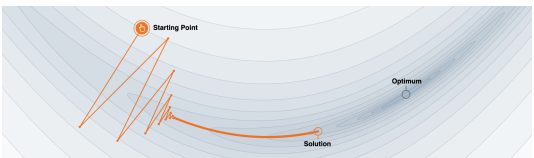

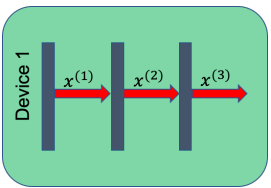

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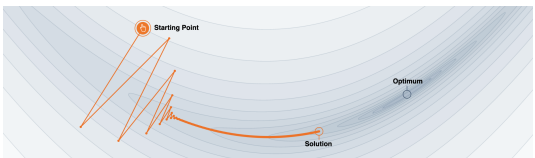

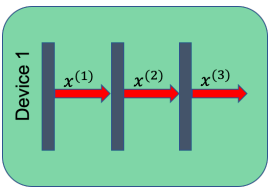

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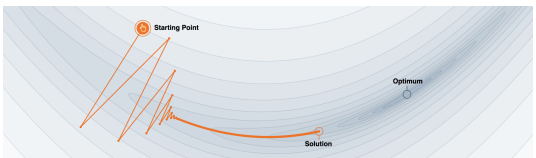

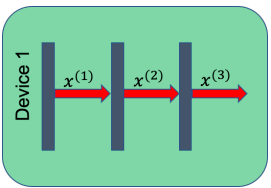

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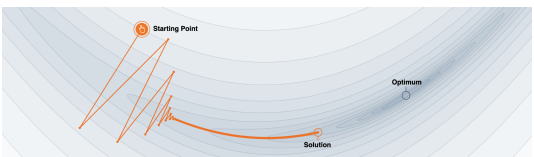

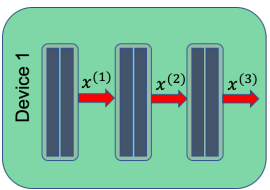

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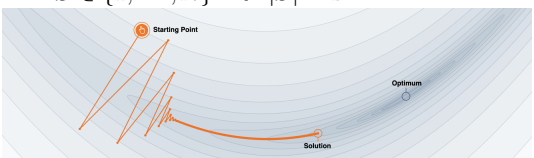
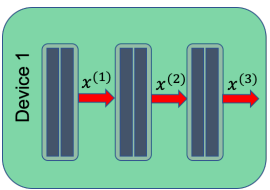
- $\mathcal{B} \in \{1, \ldots, N\}$ with $|\mathcal{B}| = B$.





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Minimizing the expectation of **random linear combinations** of original function

Background: Stochastic reformulation of finite-sum problems: SGD with arbitrary sampling

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The distribution $\mathcal{D}$ encodes any form of mini-batching / non-uniform sampling.

The convergence of mini-batch SGD

Assumption 1

- *The function* $f(\mathbf{x})$ *we are minimizing is lower bounded from below by* $f^\star := f(\mathbf{x}^\star)$*, and each* f_i *is* L*-smooth satisfying* $\|\nabla f_i(\mathbf{y}) - \nabla f_i(\mathbf{x})\| \leq L \|\mathbf{y} - \mathbf{x}\|$

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- $\mathbb{E}\left[\left\|\nabla f(\mathbf{x}^{(t)})\right\|^2\right] \to 0$ implies the sequence converges to a stationary solution

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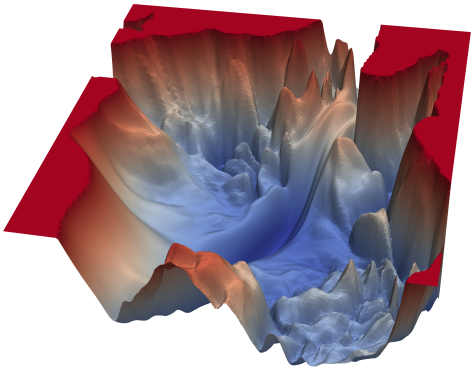
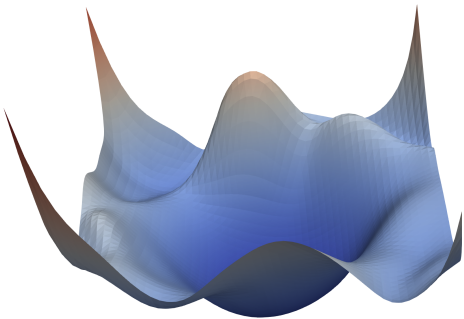
Issues of SGD—from the perspective of loss landscape



(a) ResNet w/o skip connections.

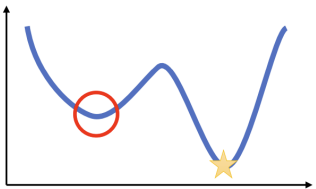


(b) ResNet w/ skip connections.

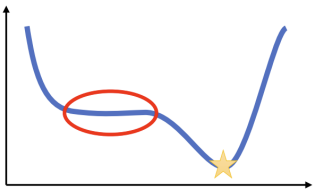
Figure: The surfaces of ResNet-56 w/ and w/o skip connections [4].

[4] *Li et al.* Visualizing the Loss Landscape of Neural Nets. NeurIPS 2018.

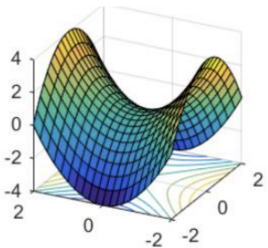
Issues of SGD—from the perspective of loss landscape



the local optimum



the plateau



the saddle point

Challenging optimization loss landscape!

Figures borrowed from https://cs182sp21.github.io/static/slides/lec-4.pdf

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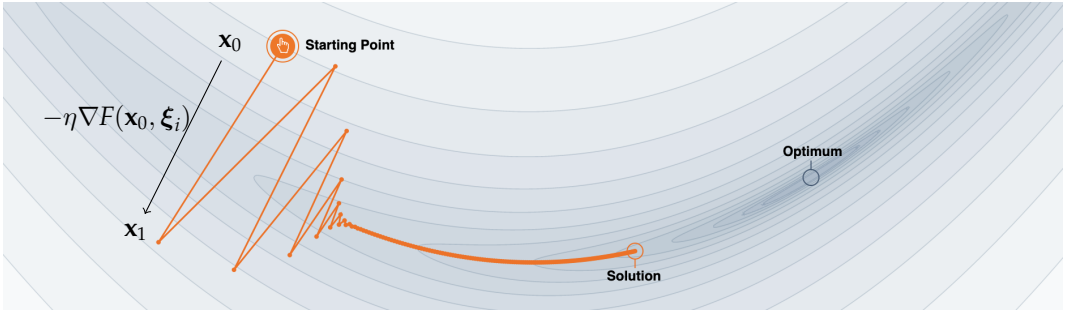
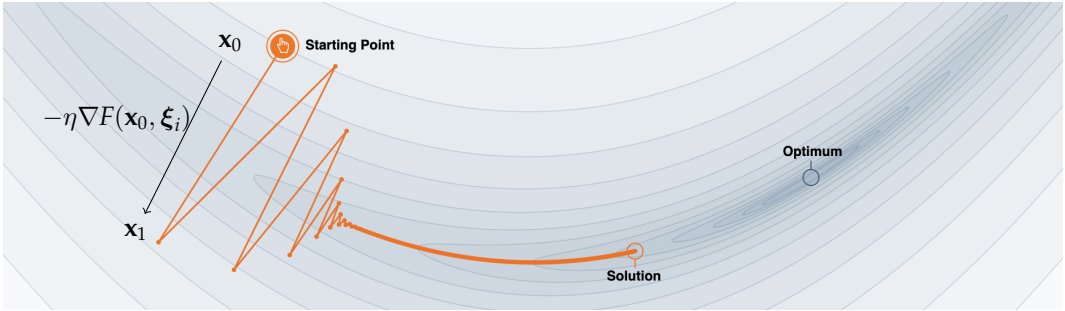


- **Challenges # 1**: loss function has high condition number.
  $\rightarrow$ very slow progress along shallow dimension, jitter along steep direction.

Visualizations based on Gabriel Goh's distill.pub article: https://distill.pub/2017/momentum/

Issues of SGD—from the perspective of loss landscape



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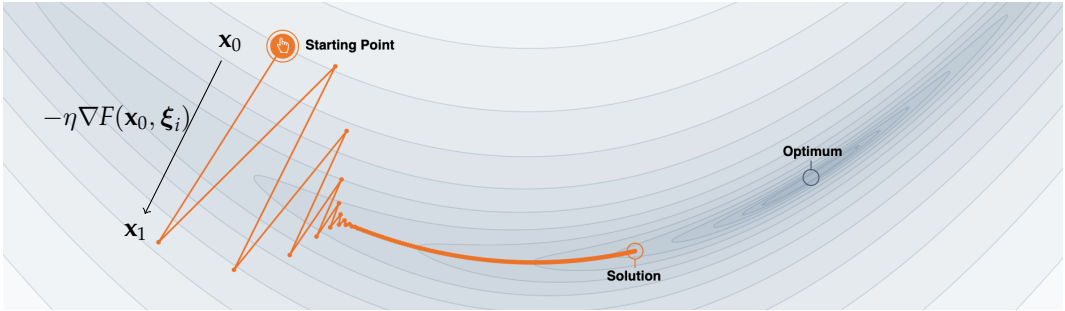

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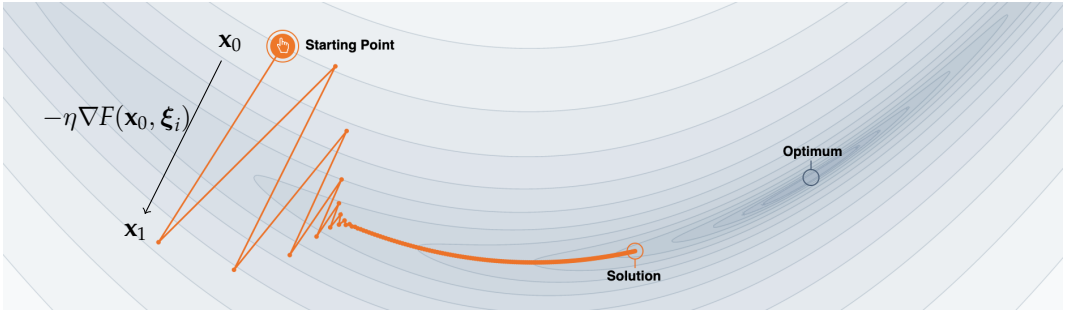

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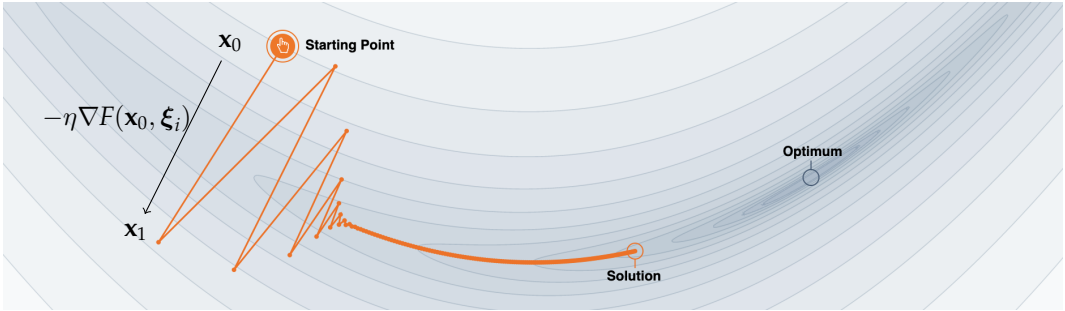

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  $\rightarrow$ saddle points have very small gradients: but much more common in high dimension.

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Improvement directions: leveraging the curvature information

Can we find a better descent direction in the loss landscape?
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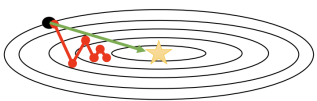

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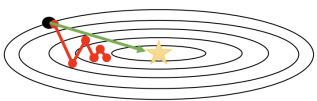

Multivariate case:

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \underbrace{\nabla_{\mathbf{x}} f(\mathbf{x}_0)}_{\text{gradient}}(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top \underbrace{\nabla^2_{\mathbf{x}} f(\mathbf{x}_0)}_{\text{Hessian}}(\mathbf{x} - \mathbf{x}_0) \tag{8}$$

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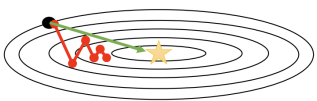

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Solution (can optimize this analytically!):

$$\mathbf{x}^\star \leftarrow \mathbf{x}_0 - \left(\nabla^2_{\mathbf{x}} f(\mathbf{x}_0)\right)^{-1} \nabla_{\mathbf{x}} f(\mathbf{x}_0) \tag{9}$$

Improvement directions: trade-offs and approximations

Q: Why is Newton's method not a viable way to improve neural network optimization?

[1] if using naive approach, though fancy methods can be much faster if they avoid forming the Hessian explicitly.

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We would prefer methods that don't require second derivatives, but somehow "stabilize" / "accelerate" gradient descent instead.

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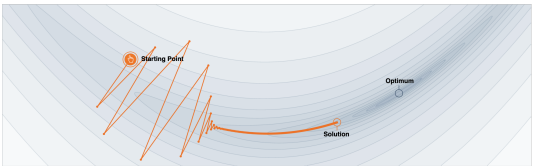
Momentum method



w/o momentum

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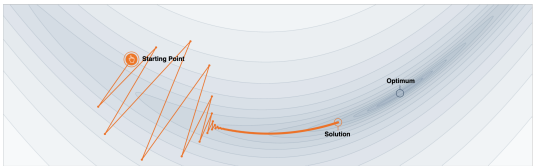

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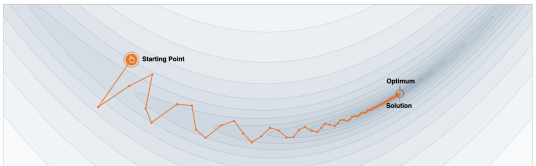

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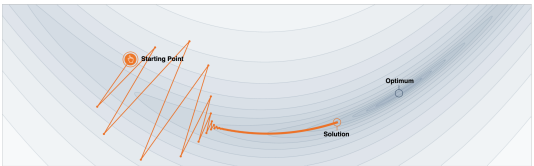

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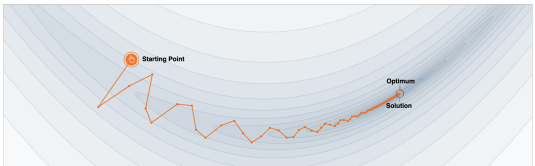

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Intuition: averaging together successive gradients yield a much better direction!

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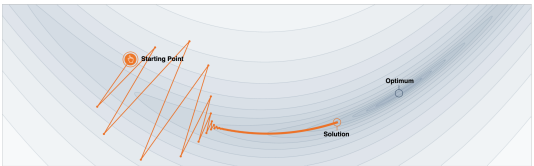

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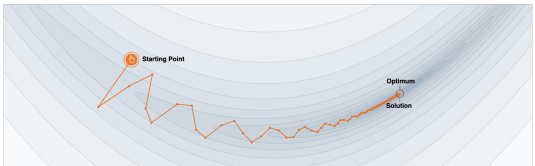

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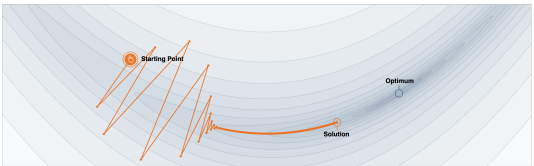

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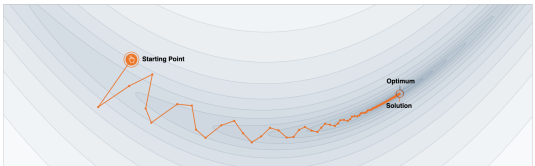

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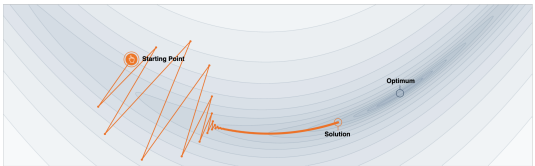

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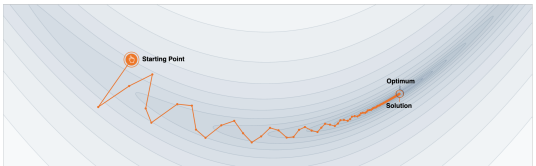

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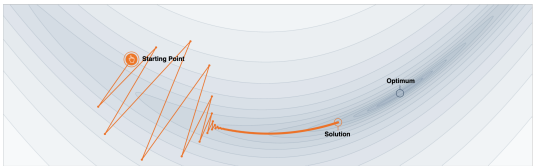

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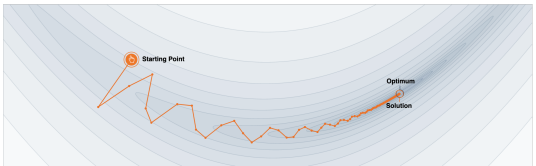

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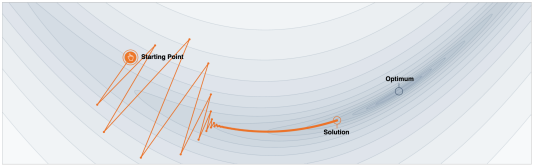

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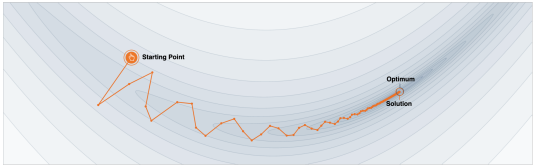

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Methods that manipulate gradient scale

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Idea: *normalize* out the magnitude of the gradient along each dimension.

Methods that manipulate gradient scale: RMSProp, AdaGrad, and their differences

AdaGrad [1] (estimate per-dimension cumulative magnitude):

$$\mathbf{v}_t = \mathbf{v}_{t-1} + (\nabla F(\mathbf{x}_t, \boldsymbol{\xi}_t))^2 \qquad \text{(roughly the squared length of each dimension)}$$

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RMSProp. https://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf.

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  → Learning rate effectively "decreases" over time: good for convex (bad for non-convex).

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- AdaGrad has some appealing guarantees for convex problems.
  → AdaGrad originally proposed to benefit from sparse data.
  → Learning rate effectively "decreases" over time: good for convex (bad for non-convex).
- RMSProp tends to be much better for deep learning (and most non-convex problems)

RMSProp. https://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf.

[1] *Duchi et al.* Adaptive subgradient methods for online learning and stochastic optimization. COLT 2010.

Adam: combining momentum and RMSProp

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[3] *Kingma et al.* Adam: A method for stochastic optimization. ICLR 2015 (Google Scholar 12w+)

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- adds bias correction (omitted in the expression above): it avoids large stepsizes in early stages of run (especially when β_2 is close to 1).

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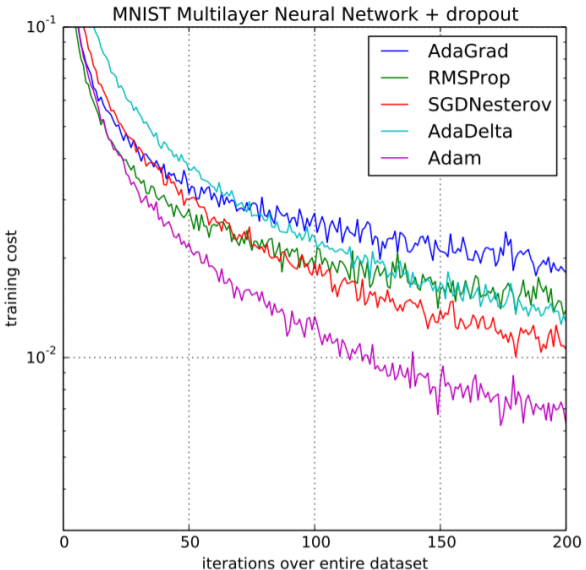

Weight decay in SGD and Adam: why AdamW matters

Many learning problems optimize the loss with L_2 norm penalty:

$$\tilde{f}(\mathbf{x}) = f(\mathbf{x}) + \lambda \|\mathbf{x}\|_2^2 \,, \tag{10}$$

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where it is sometimes called “weight decay” in SGD, since its gradient decays weight:

$$\underbrace{\mathbf{x} - \eta \nabla_{\mathbf{x}} \left(f(\mathbf{x}) + \lambda \left\|\mathbf{x}\right\|_2^2 \right)}_{\text{SGD on } L_2\text{-norm penalty}} \underset{\nabla_{\mathbf{x}} \|\mathbf{x}\|_2^2 = 2\mathbf{x}}{\Longleftrightarrow} \underbrace{(1 - 2\eta\lambda)\mathbf{x} - \eta \nabla_x f(\mathbf{x})}_{\text{weight decay}} \tag{11}$$

Weight decay in SGD and Adam: why AdamW matters

On the discrepancy between L_2 regularization and weight decay:

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AdamW is widely used in training STOA NNs from scratch or fine-tuning on downstream tasks.

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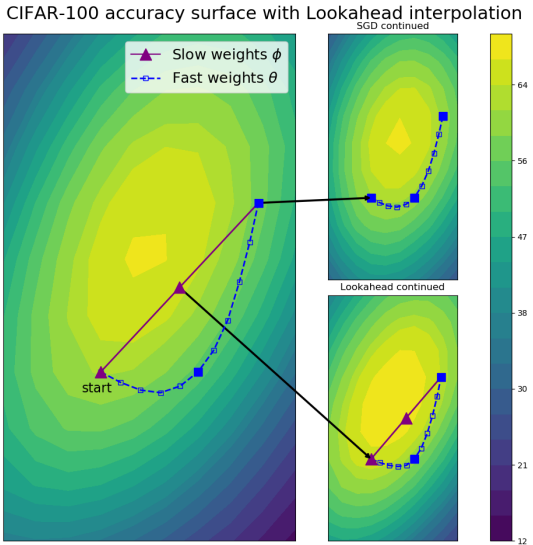

A natural way to explore and exploit the landscape!

Algorithm 1: SGD

Input : Objective $F_{\mathcal{S}}(\boldsymbol{\theta})$, dataset $\mathcal{S}$, inner-loop optimizer $\mathcal{A}$, inner-loop step number k and learning rate $\{\{\eta_\tau^{(t)}\}$, outer-loop learning rate $\alpha \in (0, 1)$.

for $t = 1, 2, ..., T$ **do**

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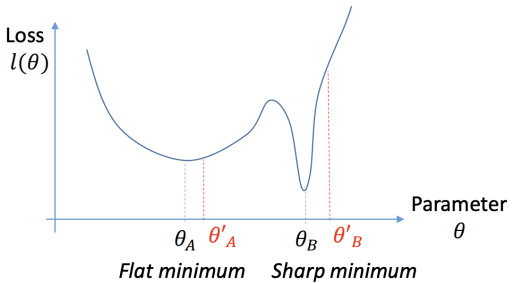

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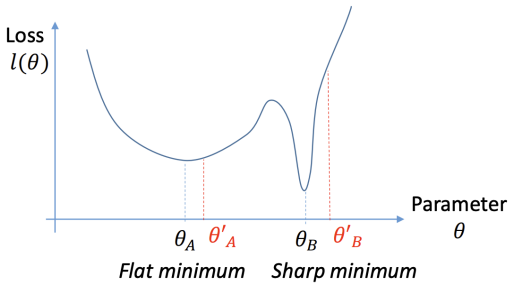

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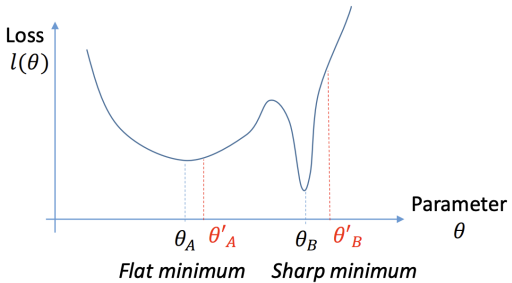

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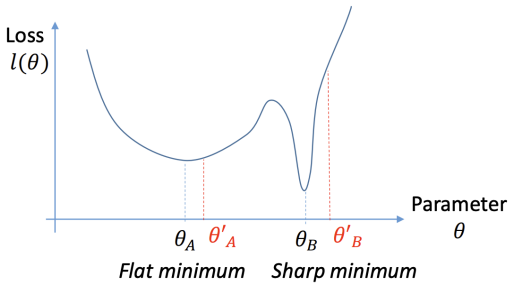

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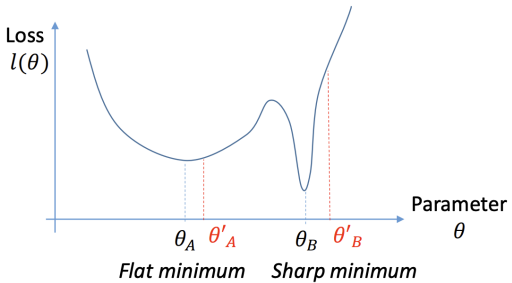

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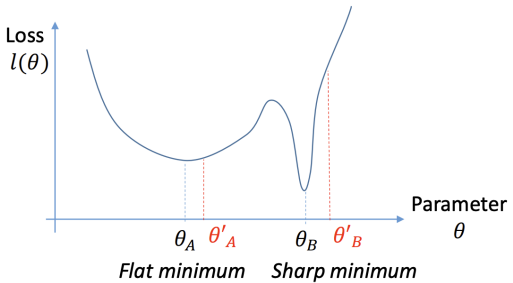

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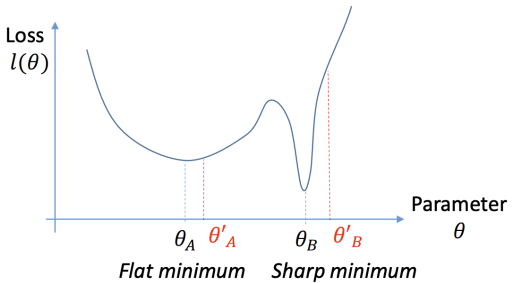

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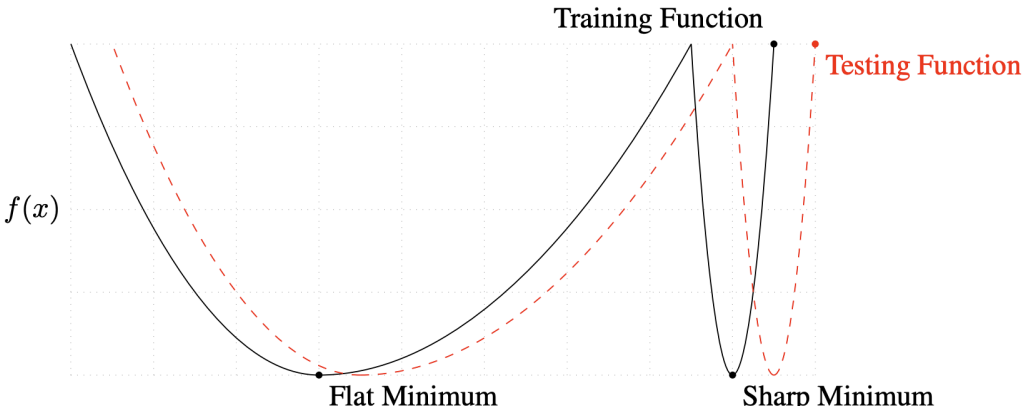
  - Imagine some perturbation: $\theta_A \rightarrow \boldsymbol{\theta}'_A, \boldsymbol{\theta}_B \rightarrow \boldsymbol{\theta}'_B \Rightarrow \ell(\boldsymbol{\theta}'_A) \ll \ell(\boldsymbol{\theta}'_B)$.


Training Function
Testing Function
$f(x)$
Flat Minimum
Sharp Minimum

Let's seek for a Flat Minimum

$$\begin{aligned} \text{Flat Minima} &= \text{Robust models} && (12)\\ &= \text{Resilient to data noise or model corruption} && (13)\\ &= \text{(often encountered in AI applications)} && (14) \end{aligned}$$

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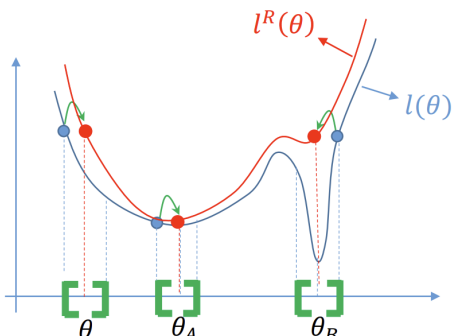
But, how?

Sharpness-Aware Minimization (SAM)

Idea of SAM:

Define a robust loss $\ell^R(\boldsymbol{\theta})$ as worst-case loss within a neighborhood of $\boldsymbol{\theta}$.



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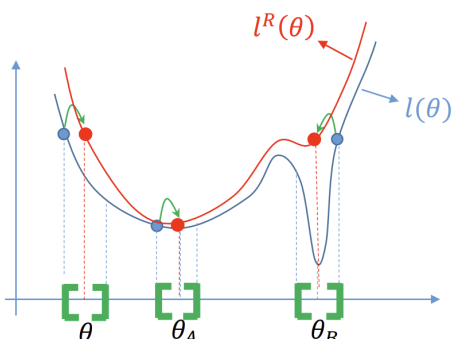

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With high probability over $\mathcal{S}$, the flatness-based bound says:

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}) \leq \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}) + \underbrace{\left[\max_{\|\boldsymbol{\epsilon}\|_2 \leq \rho} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}+\boldsymbol{\epsilon}) - \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta})\right]}_{\textit{flatness measure}} + h(\|\boldsymbol{\theta}\|_2^2/\rho^2)\,, \tag{16}$$

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Theorem 2

With high probability over $\mathcal{S}$, the flatness-based bound says:

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}) \leq \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}) + \underbrace{\left[\max_{\|\boldsymbol{\epsilon}\|_2 \leq \rho} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}+\boldsymbol{\epsilon}) - \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta})\right]}_{\textit{flatness measure}} + h(\|\boldsymbol{\theta}\|_2^2/\rho^2)\,, \tag{16}$$

where $h(\|\boldsymbol{\theta}\|_2^2/\rho^2)$ is a strictly increasing function of $\boldsymbol{\theta}$. It decreases as the number of samples $n = |\mathcal{S}|$ increases.

Sharpness-Aware Minimization (SAM)

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}) \leq \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}) + \underbrace{\left[\max_{\|\boldsymbol{\epsilon}\|_2 \leq \rho} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}+\boldsymbol{\epsilon}) - \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta})\right]}_{\text{flatness measure}} + h(\|\boldsymbol{\theta}\|_2^2/\rho^2) \tag{17}$$

$$= \max_{\|\boldsymbol{\epsilon}\|_2 \leq \rho} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta}+\boldsymbol{\epsilon}) + h(\|\boldsymbol{\theta}\|_2^2/\rho^2) \tag{18}$$

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The objective of SAM becomes:

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  where $1/p + 1/q = 1$ and the solution to a classical dual norm problem can solve this approximation.
- substituting $\hat{\boldsymbol{\epsilon}}$ gives a gradient estimator

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{S}}^{\text{SAM}}(\boldsymbol{\theta}) := \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta} + \hat{\boldsymbol{\epsilon}}) \approx \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta})|_{\boldsymbol{\theta} + \hat{\boldsymbol{\epsilon}}} \tag{19}$$

- The gradient estimator of SAM is given by:

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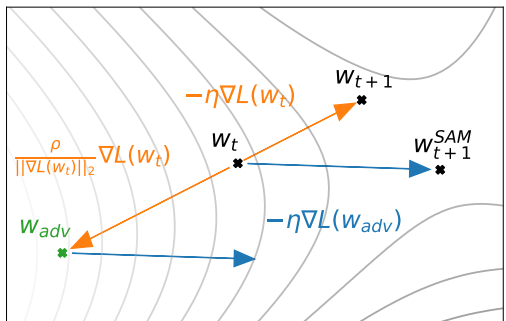

From original SAM paper.

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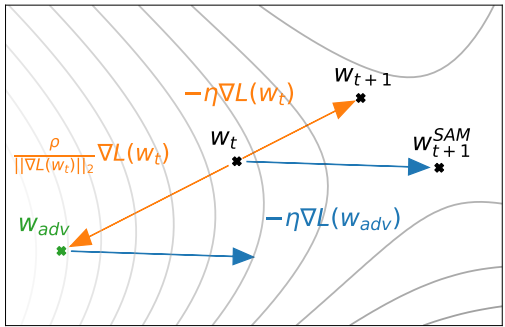
- Recall that SAM requires *2-step* gradient descent (thus, twice slow)



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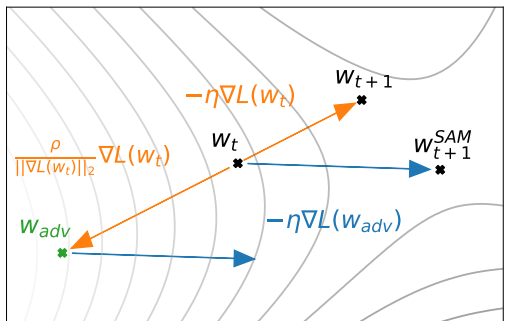

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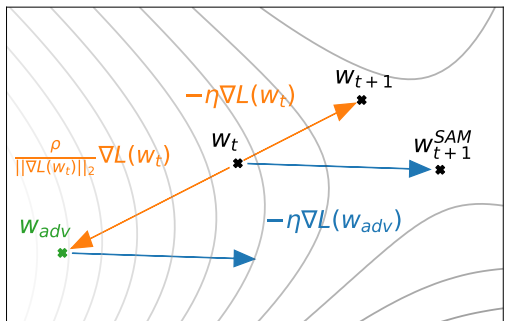

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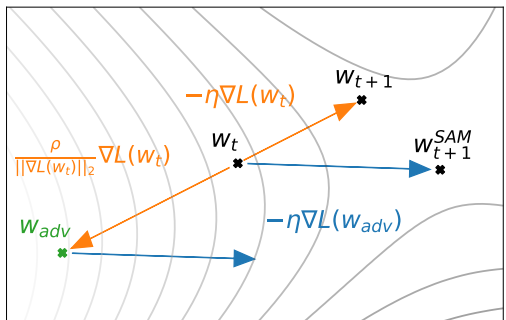
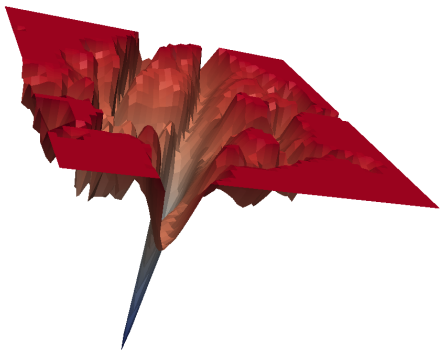
  - 2nd for computing $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{S}}(\boldsymbol{\theta})|_{\boldsymbol{\theta}+\hat{\boldsymbol{\epsilon}}}$
- Set $p = 2$-norm and neighborhood-size $\rho = 0.05$ as a default setup.

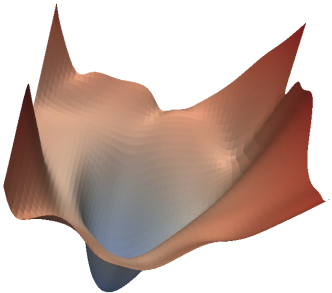


From original SAM paper.

Verification of the flatness



(a) ERM.



(b) SAM.

Loss surface visualization.

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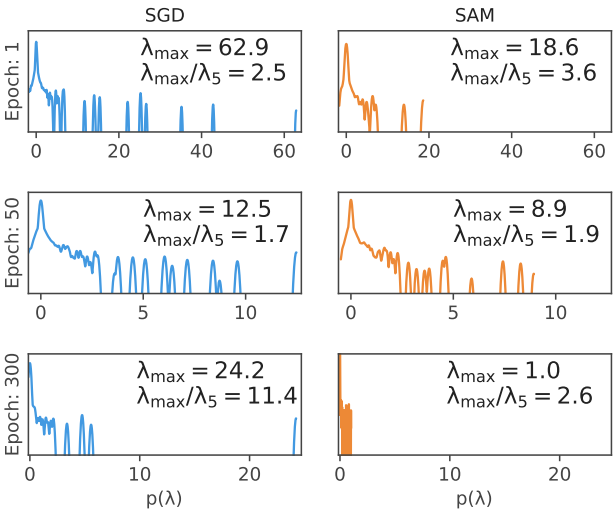


Hessian spectra.

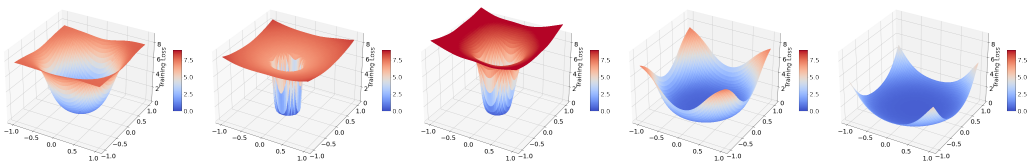
Results (i.e., SAM $>$ ERM)

- SAM *consistently improves* classification tasks, particularly with label noises

Model	Epoch	SAM		Standard Training (No SAM)	
		Top-1	Top-5	Top-1	Top-5
ResNet-50	100	**22.5**$_{\pm 0.1}$	6.28$_{\pm 0.08}$	22.9$_{\pm 0.1}$	6.62$_{\pm 0.11}$
	200	**21.4**$_{\pm 0.1}$	5.82$_{\pm 0.03}$	22.3$_{\pm 0.1}$	6.37$_{\pm 0.04}$
	400	**20.9**$_{\pm 0.1}$	5.51$_{\pm 0.03}$	22.3$_{\pm 0.1}$	6.40$_{\pm 0.06}$
ResNet-101	100	**20.2**$_{\pm 0.1}$	5.12$_{\pm 0.03}$	21.2$_{\pm 0.1}$	5.66$_{\pm 0.05}$
	200	**19.4**$_{\pm 0.1}$	4.76$_{\pm 0.03}$	20.9$_{\pm 0.1}$	5.66$_{\pm 0.04}$
	400	**19.0**$_{\pm <0.01}$	4.65$_{\pm 0.05}$	22.3$_{\pm 0.1}$	6.41$_{\pm 0.06}$
ResNet-152	100	**19.2**$_{\pm <0.01}$	4.69$_{\pm 0.04}$	20.4$_{\pm <0.0}$	5.39$_{\pm 0.06}$
	200	**18.5**$_{\pm 0.1}$	4.37$_{\pm 0.03}$	20.3$_{\pm 0.2}$	5.39$_{\pm 0.07}$
	400	**18.4**$_{\pm <0.01}$	4.35$_{\pm 0.04}$	20.9$_{\pm <0.0}$	5.84$_{\pm 0.07}$

Table: Test error rates for ResNets trained on ImageNet, with and without SAM.

Results on ViT (and MLP-Mixer)



(c) ResNet (d) ViT (e) Mixer (f) ViT-SAM (g) Mixer-SAM

Figure: **Cross-entropy loss landscapes of ResNet-152, ViT-B/16, and Mixer-B/16.** ViT and MLP-Mixer converge to sharper regions than ResNet when trained on ImageNet with the basic Inception-style preprocessing. SAM significantly smooths the landscapes.

Results on ViT (and MLP-Mixer)

Table: Number of parameters, Hessian dominate eigenvalue λ_{max}, training error at convergence L_{train}, average flatness $L_{train}^{\mathcal{N}}$, accuracy on ImageNet, and accuracy/robustness on ImageNet-C. ViT and MLP-Mixer suffer divergent κ and converge at sharp regions; SAM rescues that and leads to better generalization.

	ResNet-152	ResNet-152-SAM	ViT-B/16	ViT-B/16-SAM	Mixer-B/16	Mixer-B/16-SAM
#Params	60M		87M		59M	
Hessian λ_{max}	179.8	**42.0**	738.8	**20.9**	1644.4	**22.5**
L_{train}	**0.86**	0.90	**0.65**	0.82	**0.45**	0.97
$L_{train}^{\mathcal{N}}$ *	2.39	**2.16**	6.66	**0.96**	7.78	**1.01**
ImageNet (%)	78.5	**79.3**	74.6	**79.9**	66.4	**77.4**
ImageNet-C (%)	50.0	**52.2**	46.6	**56.5**	33.8	**48.8**

Thanks & Question Time!

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