Lecture 13: Optimization for Deep Learning

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SoE, Westlake University

December 16, 2025

1. Stochastic Gradient Descent (SGD) and Mini-batch SGD

2. Accelerated and Stabilized Optimization Methods

3. Advanced Optimization Methods
   - Lookahead
   - Sharpness-aware Minimization
   - Muon Optimizer

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Background

1. **Get data:** $\xi_1, \ldots, \xi_N$**, where** $\xi_i := (\mathbf{d}, y)_i$

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3. Choose a loss function: $\ell(h_{\mathbf{x}}(\mathbf{d}, y)) \geq 0$
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:

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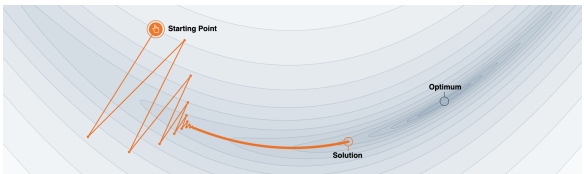

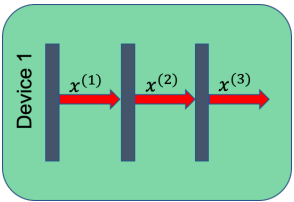

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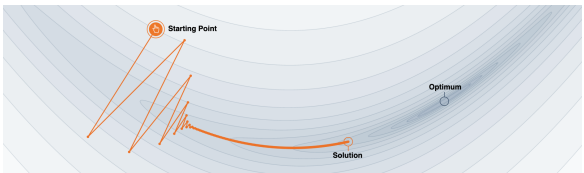

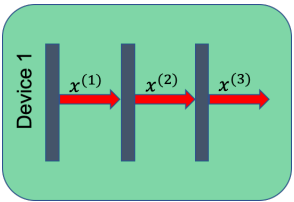

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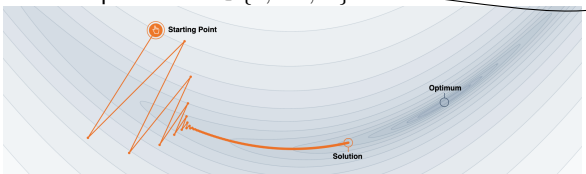

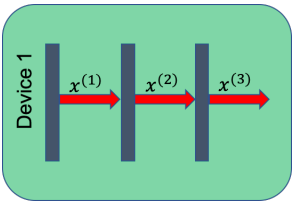

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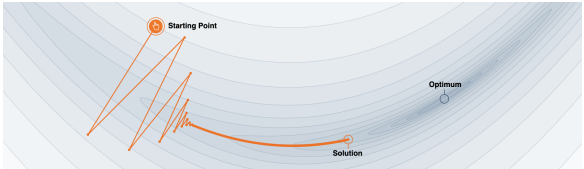

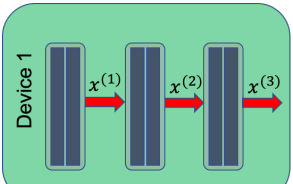

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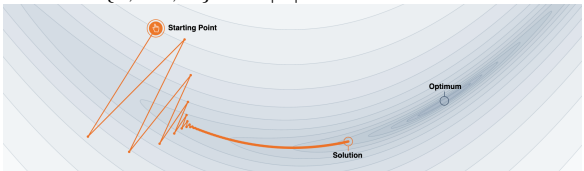
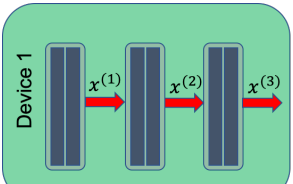
- $\mathcal{B} \in \{1, \ldots, N\}$ with $|\mathcal{B}| = B$.





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Random sampling vector $\mathbf{v} = (v_1, \ldots, v_N) \sim \mathcal{D}$ with $\mathbb{E}[v_i] = 1$ for $i = 1, \ldots, N$.

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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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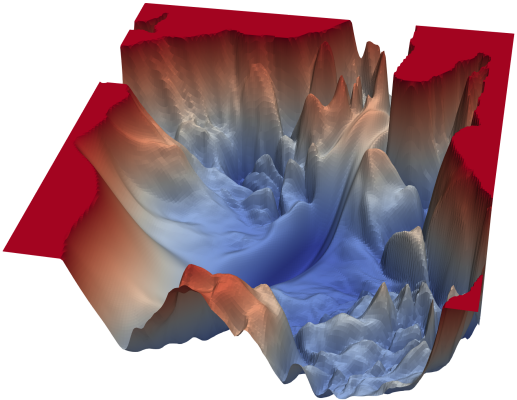
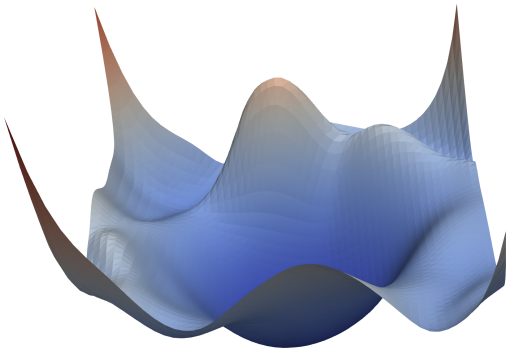
Issues of SGD—from the perspective of loss landscape



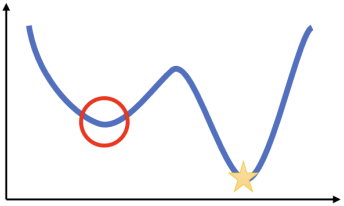
(a) ResNet w/o skip connections.



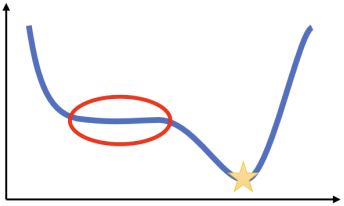
(b) ResNet w/ skip connections.

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

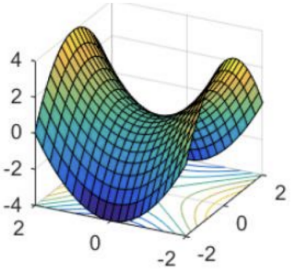
Issues of SGD—from the perspective of loss landscape



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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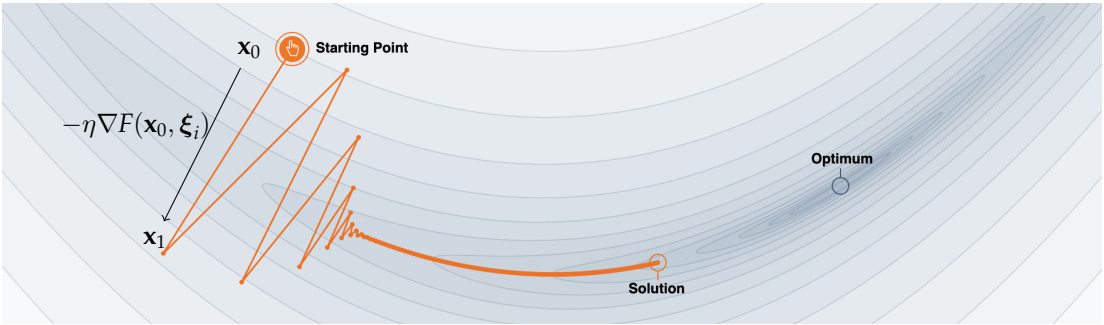
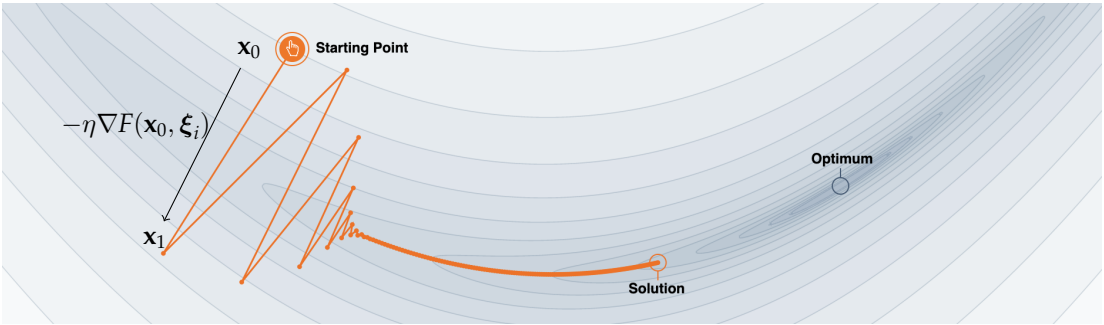


- **Challenges # 1**: loss function has high condition number.
  $\rightarrow$ very slow progress along shallow dimension, jitter along steep direction.

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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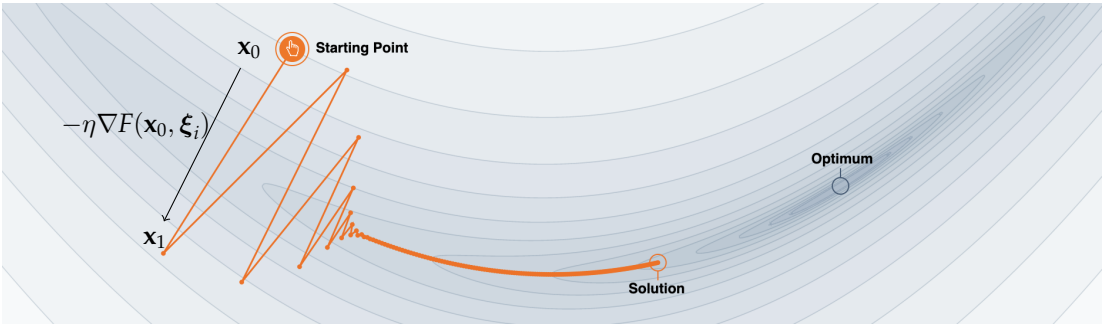

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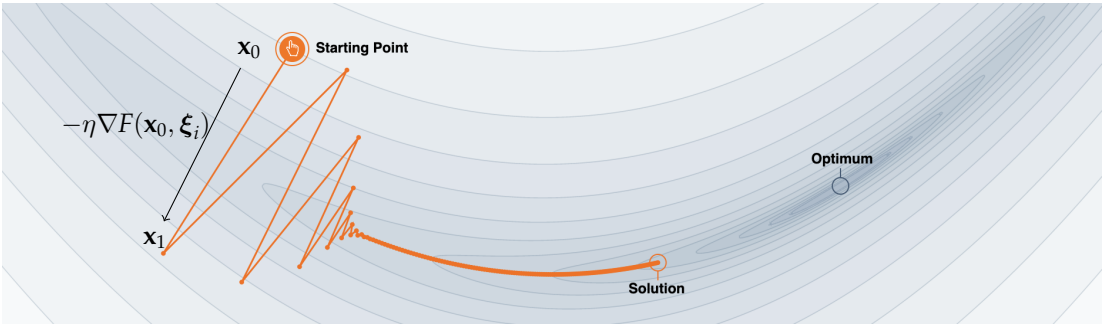

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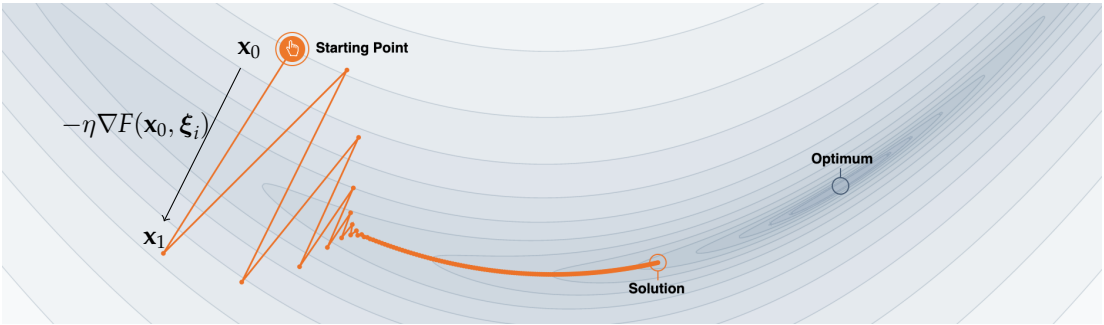

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Improvement directions: leveraging the curvature information

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

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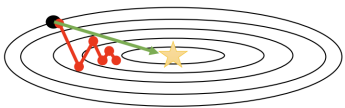

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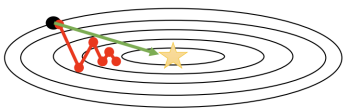

Multivariate case:

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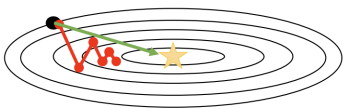

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Solution (can optimize this analytically!):

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

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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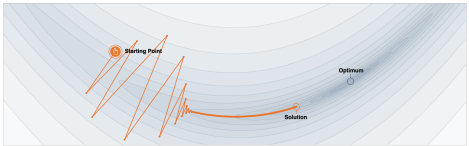
Momentum method



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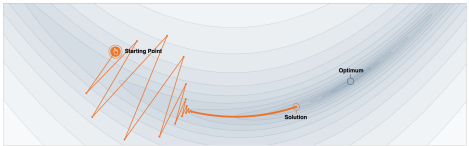

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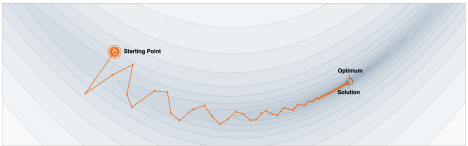

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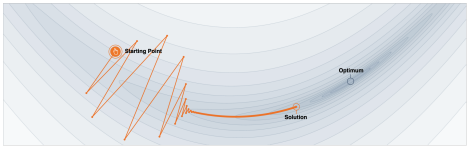

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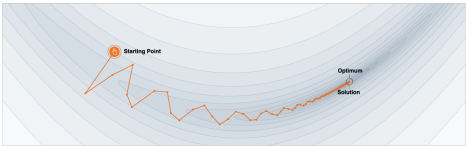

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Intuition: averaging together successive gradients yield a much better direction!

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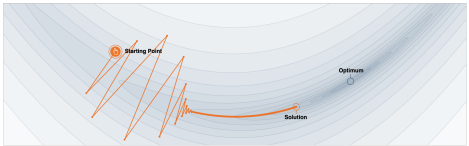

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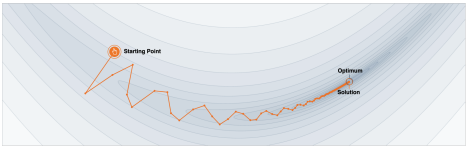

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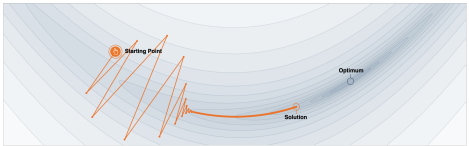

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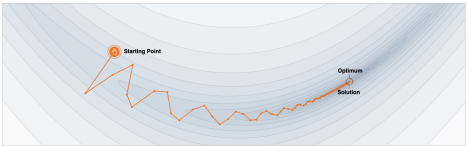

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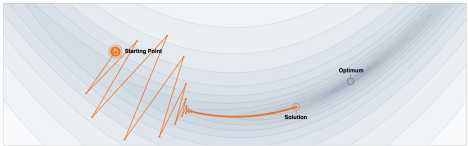

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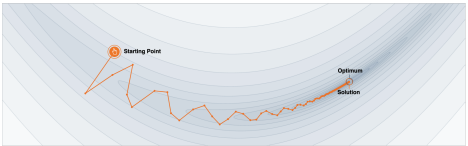

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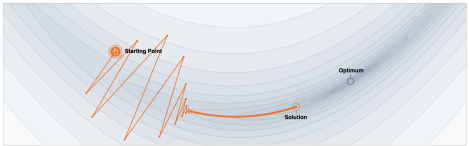

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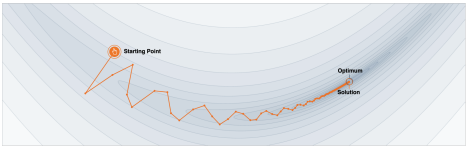

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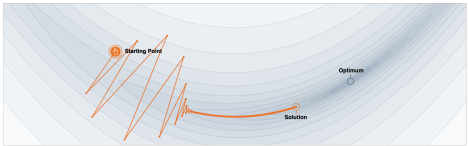

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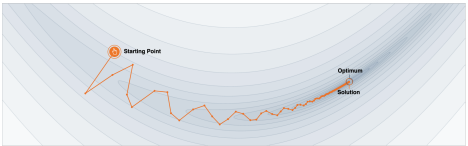

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Idea: *normalize* out the magnitude of the gradient along each dimension.

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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$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta \frac{\nabla F(\mathbf{x}_t, \boldsymbol{\xi}_t)}{\sqrt{\mathbf{v}_t}} \qquad \text{(each dimension is divided by its magnitude)}$$

Remarks:

- AdaGrad has some appealing guarantees for convex problems.
  - $\rightarrow$ AdaGrad originally proposed to benefit from sparse data.
  - $\rightarrow$ The accumulated sum of squares $\mathbf{v}_t$ in the denominator grows monotonically throughout training.
  - $\rightarrow$ Learning rate effectively "decreases" over time: good for convex (bad for non-convex).

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.

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

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- RMSProp tends to be much better for deep learning (and most non-convex problems)

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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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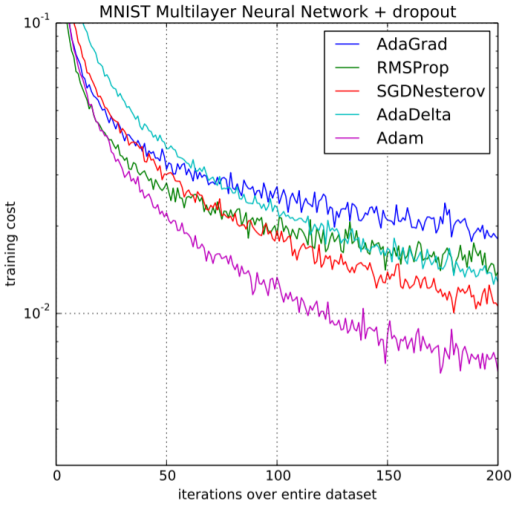

Weight decay in SGD and Adam: why AdamW matters

Many learning problems optimize the loss with L_2 norm penalty:

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

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

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

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Second-Order Optimization Methods

- **Idea:** Utilize second-derivative information (the Hessian matrix $\mathbf{H} = \nabla^2_{\mathbf{x}} F$) to get a better sense of the loss surface curvature.
- **Newton's Method Update:** $\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{H}_t^{-1} \nabla_{\mathbf{x}} F(\mathbf{x}_t)$
- **Examples:** Newton's method, Quasi-Newton methods (e.g., L-BFGS which approximates $\mathbf{H}_t^{-1}$).
- **Pros:** Can converge very rapidly (quadratically) near a good minimum.
- **Cons for Deep Learning:**
  - **Computationally Prohibitive:**
    - Computing the Hessian: $\mathcal{O}(N^2_{params})$ operations.
    - Storing the Hessian: $\mathcal{O}(N^2_{params})$ memory.
    - Inverting the Hessian: $\mathcal{O}(N^3_{params})$ operations.
  - Impractical for typical DNNs with millions/billions of parameters (N_{params}).

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- **Experimentation is Key:** It's often beneficial to try a few different optimizers and learning rate schedules.

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- Learning rate schedules are commonly used in conjunction with all types of optimizers.

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Summary: Choosing and tuning an optimizer is an art and science. It involves understanding the trade-offs and often requires empirical validation. The interplay between the optimizer, learning rate schedule, regularization, and model architecture determines the final performance.

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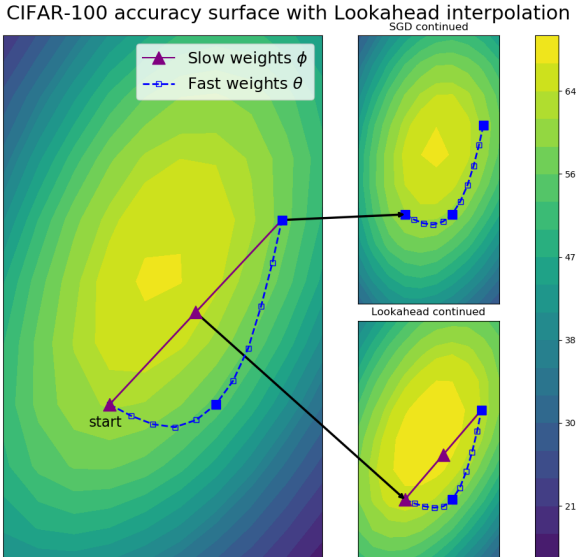

Algorithm 1: SGD

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 $\alpha \in (0, 1)$.

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[6] *Zhang et al.* Lookahead optimizer: k steps forward, 1 step back. NeurIPS 2019.

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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**

  $\boldsymbol{v}_0^{(t)} = \boldsymbol{\theta}_{t-1}$;

  for $\tau = 1, 2, ..., k$ **do**

    $\boldsymbol{v}_\tau^{(t)} = \mathcal{A}(F_{\mathcal{S}}(\boldsymbol{\theta}), \boldsymbol{v}_{\tau-1}^{(t)}, \eta_{\tau-1}^{(t)}, \mathcal{S}) = \boldsymbol{v}_{\tau-1}^{(t)} - \eta_{\tau-1}^{(t)} \boldsymbol{g}_{\tau-1}^{(t)}$

  end

  $\boldsymbol{\theta}_t = (1-\alpha)\boldsymbol{\theta}_{t-1} + \alpha \boldsymbol{v}_k^{(t)}$.

end

Output : $\boldsymbol{\theta}_{\mathcal{A},\mathcal{S}} = \boldsymbol{\theta}_T$

outer-loop optimization

- inner-loop optimization: k steps forward in SGD & LA
- outer-loop optimization: 1 step back in LA, while no step back in SGD

[6] *Zhang et al.* Lookahead optimizer: k steps forward, 1 step back. NeurIPS 2019.

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Flat Minima in Deep Learning

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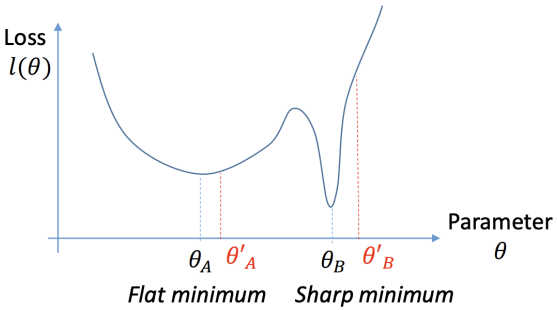

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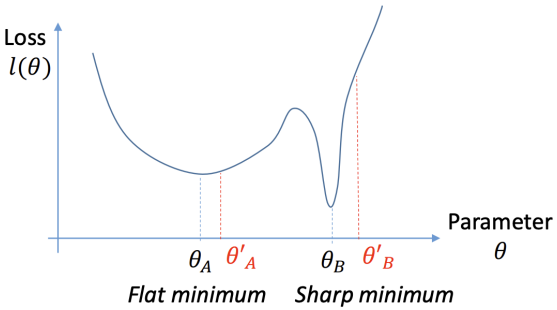

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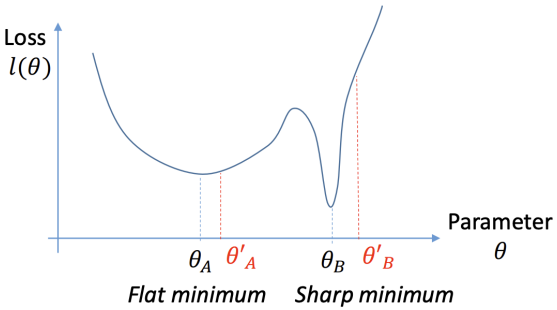

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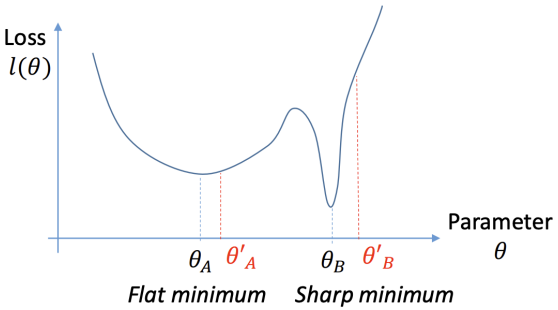

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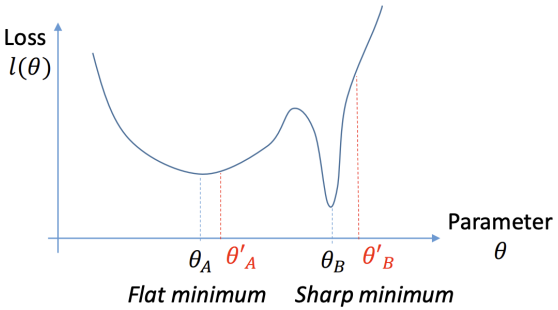

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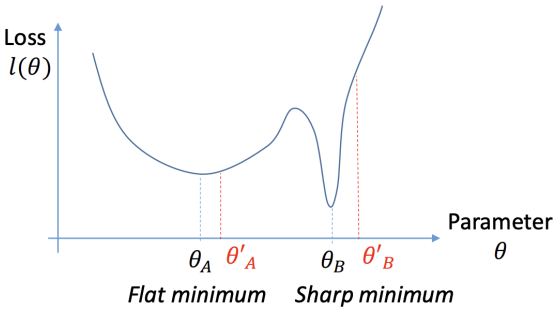

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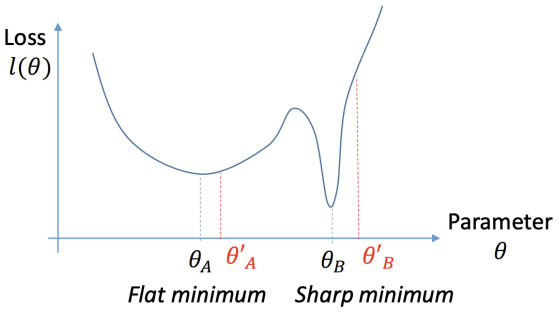

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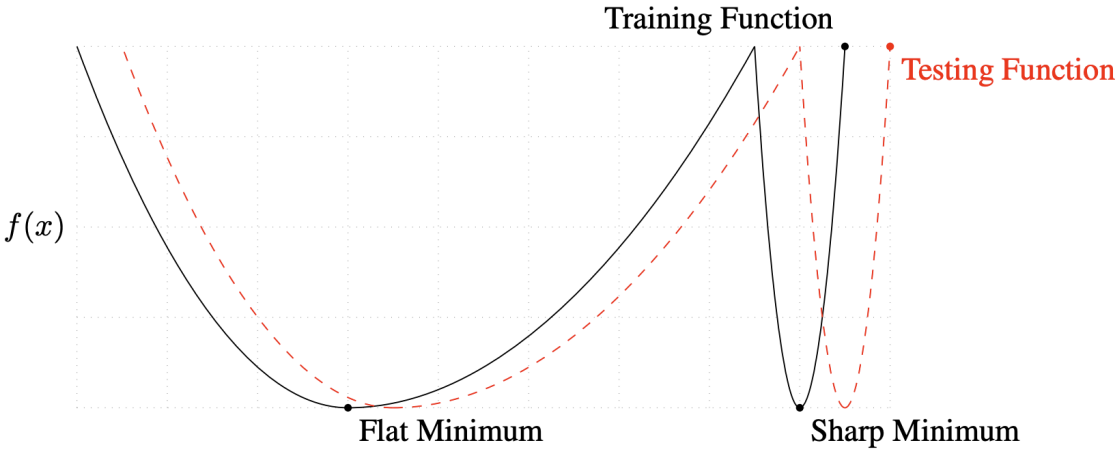
  - Why? Because θ_A is more robust.
  - Imagine some perturbation: $\theta_A \rightarrow \boldsymbol{\theta}'_A, \boldsymbol{\theta}_B \rightarrow \boldsymbol{\theta}'_B \Rightarrow \ell(\boldsymbol{\theta}'_A) \ll \ell(\boldsymbol{\theta}'_B)$.


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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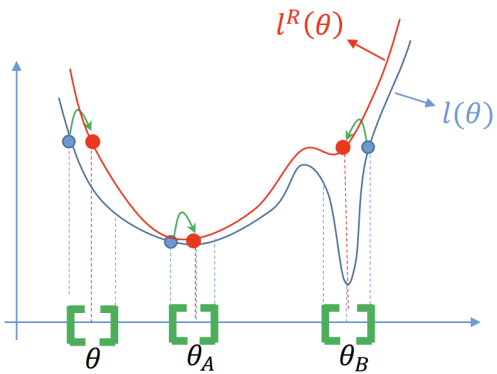
But, how?

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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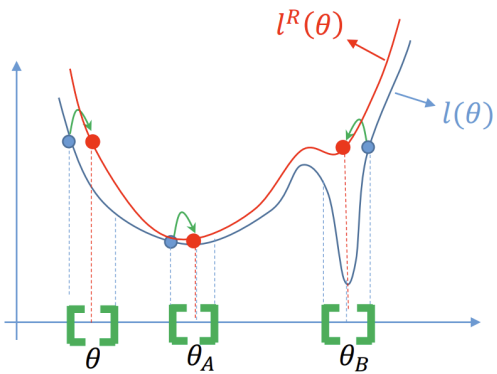

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With high probability over $\mathcal{S}$, the flatness-based bound says:

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

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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.

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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

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

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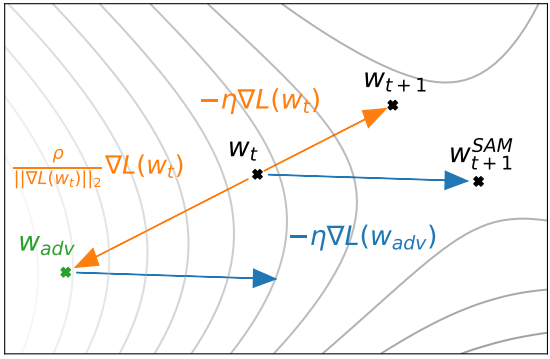

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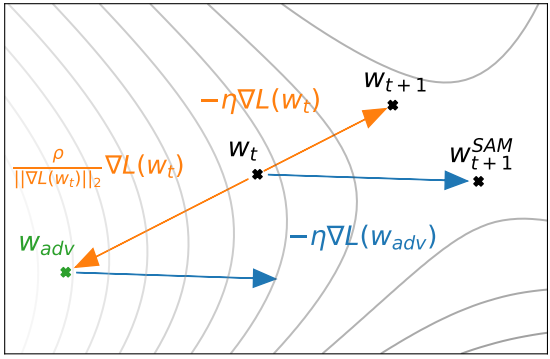

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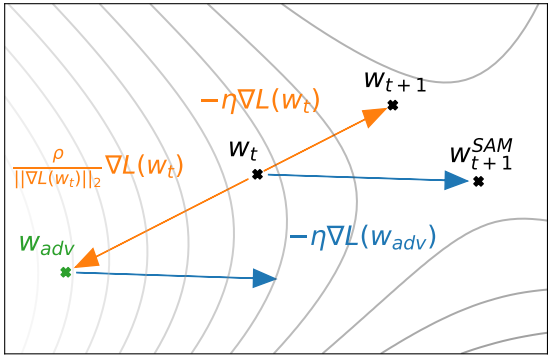

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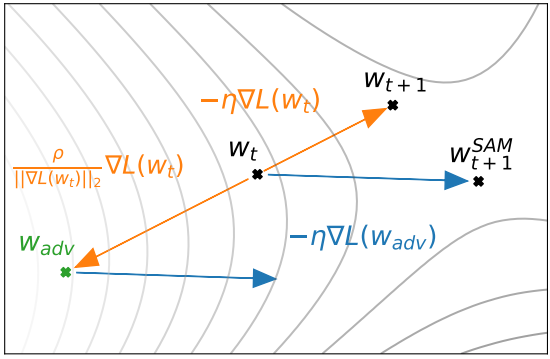

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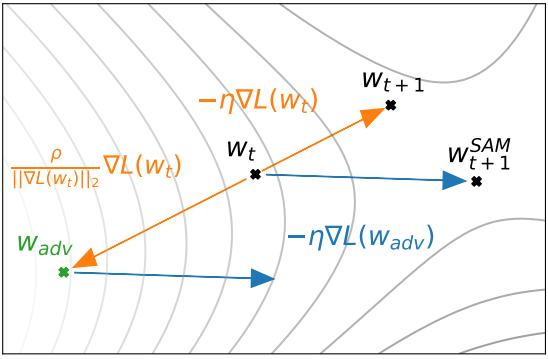
- Set $p = 2$-norm and neighborhood-size $\rho = 0.05$ as a default setup.



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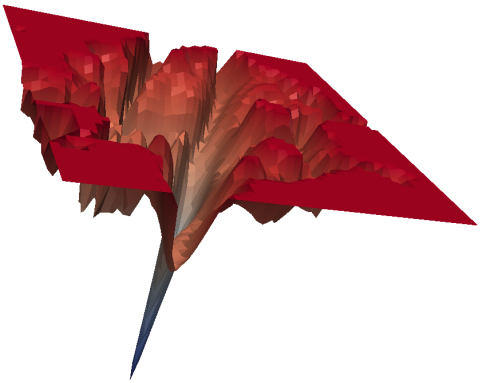
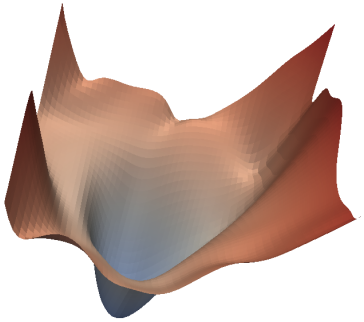
Verification of the flatness



(a) ERM.



(b) SAM.

Loss surface visualization.

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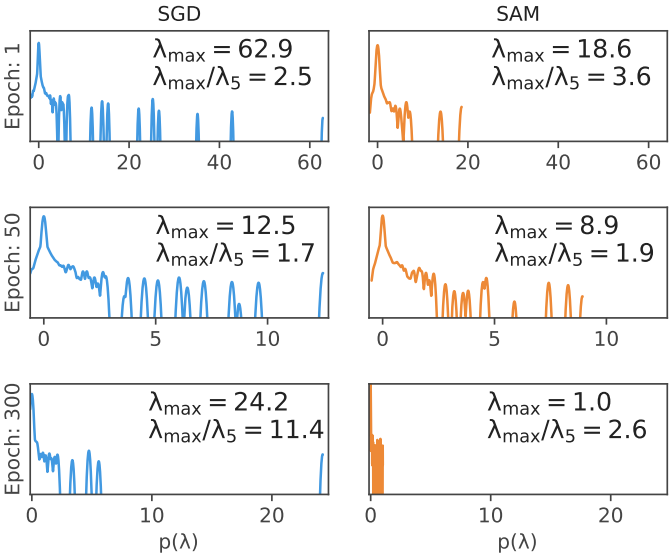


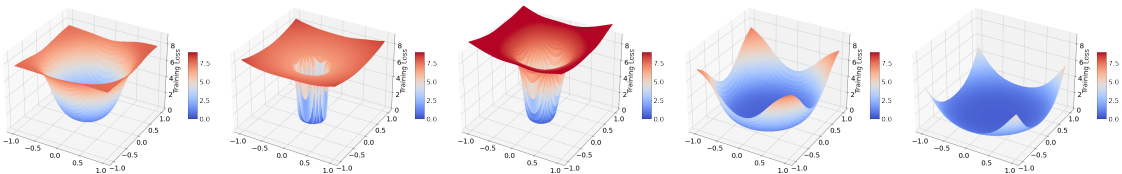
Results (i.e., SAM $>$ ERM)

- 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**

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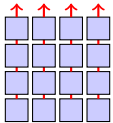
Muon: From Vector to Matrix Optimization

Element-wise Updates
(SGD, Adam, AdaGrad)



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Matrix-aware Updates
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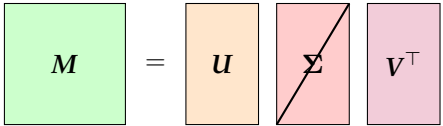

Muon: From Vector to Matrix Optimization

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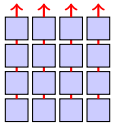

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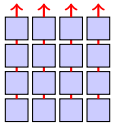

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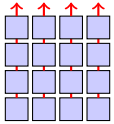

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Key Insight: Neural networks are built on matrix multiplications.
Matrix parameters have inherent structure that element-wise optimizers ignore!

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Optimization Principle:

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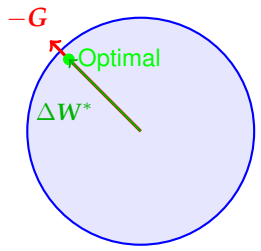

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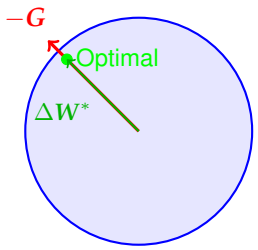

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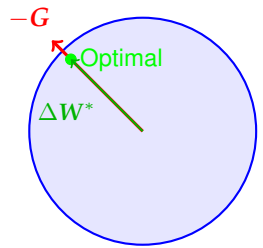

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Key Insight

Spectral norm precisely measures how much ΔW changes the output $y = xW$, while Frobenius norm (used by SGD) is looser!

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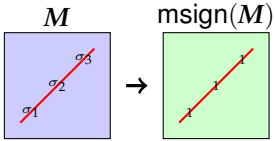

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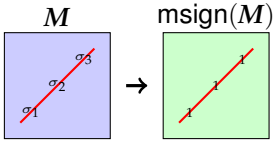

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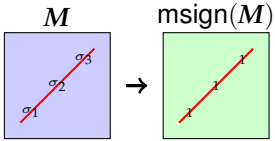

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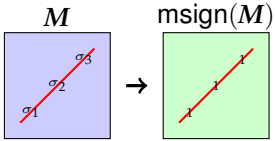

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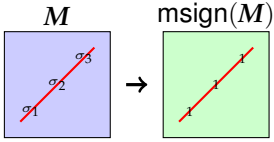

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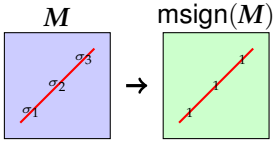

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Alternative Form: $\text{msign}(M) = M(M^\top M)^{-1/2}$
Interpretation: "Optimal orthogonal approximation" - closest orthogonal matrix to M

Muon Update Rule

Muon (MomentUm Orthogonalized by Newton-schulz):

$$\boldsymbol{M}_t = \beta \boldsymbol{M}_{t-1} + \boldsymbol{G}_t \qquad \text{(Momentum)}$$

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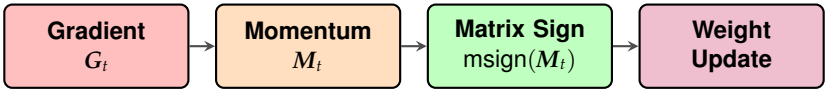

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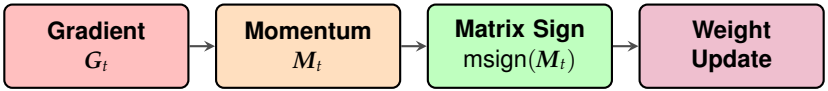

- msign$(\cdot)$: **Matrix sign function** (not element-wise sign!)
- λ: Weight decay coefficient
- β: Momentum parameter (typically 0.95)

Muon vs Other Optimizers

Optimizer	Update Rule	Constraint	Scale Inv.	Memory
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Muon Advantages

- Spectral norm = tightest constraint for matrix stability
- Captures parameter correlations via SVD
- Lower memory than Adam (no second moment)

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2. Isotropy

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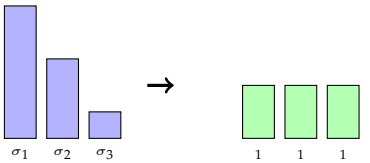

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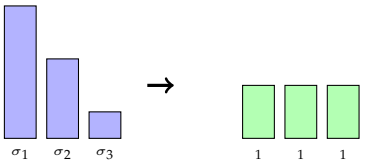

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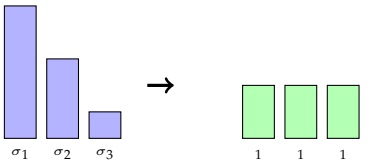

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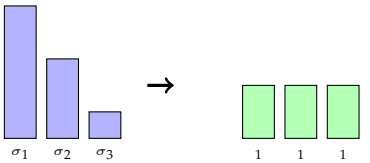

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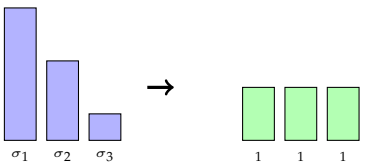

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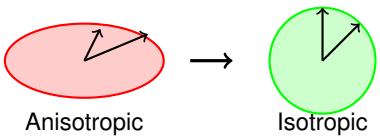

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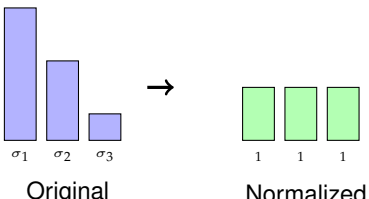

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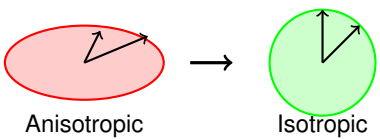

Connection: Similar to BERT-whitening, Muon "whitens" the gradient distribution!

Efficient Implementation via Newton-Schulz

Challenge:

- Direct SVD is expensive: $\mathcal{O}(n^3)$

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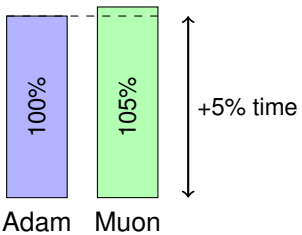

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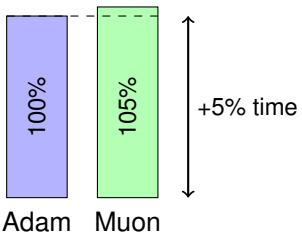

Memory Comparison:

- Adam: 2 states ($\boldsymbol{M}, \boldsymbol{V}$)
- Muon: 1 state ($\boldsymbol{M}$)

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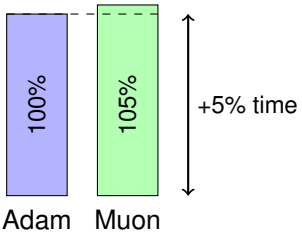

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Practical Consideration

Matrix multiplications happen during idle time (between gradient computations), so actual wall-clock overhead is minimal ($\approx$ 2-5%)!

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