Theoretical Insights on Training Instability in Deep Learning

NeurIPS 2025 Tutorial

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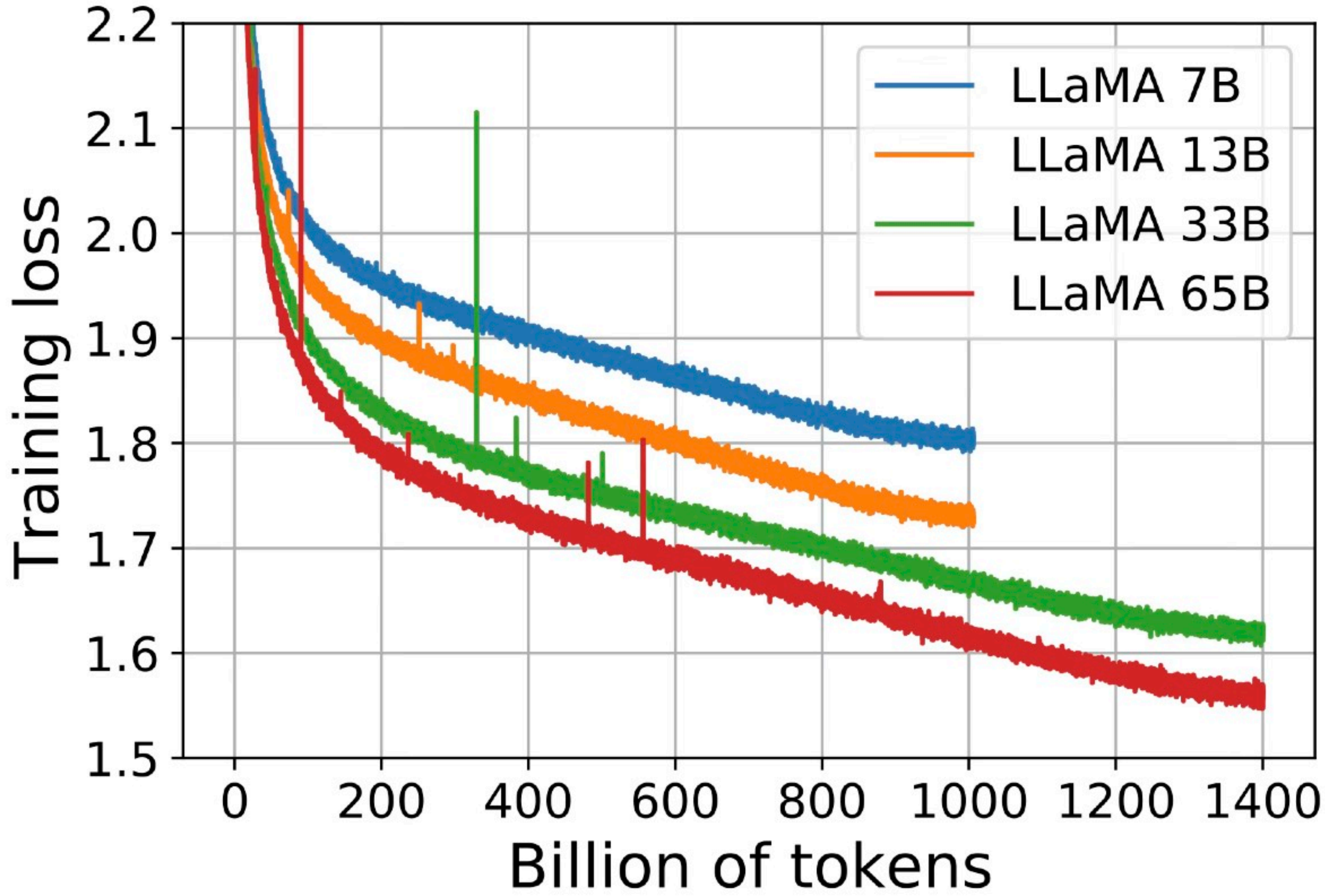
Yu-Xiang Wang — UC San Diego
Maryam Fazel — University of Washington

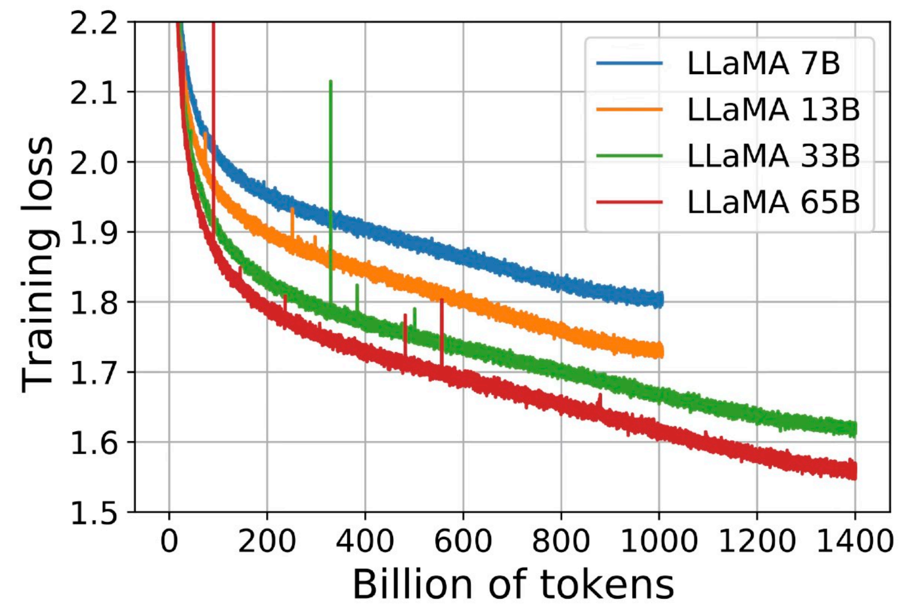
NEURAL INFORMATION PROCESSING SYSTEMS

An LLM pretraining curve



“online” AdamW, batch size = 4M, internet data, transformer

Touvron, Hugo, Izacard, et al. “LLaMA: open and efficient foundation language models.” arXiv 2023



r/MachineLearning • 12d ago
Previous-Raisin1434

[R] Why loss spikes?

Research

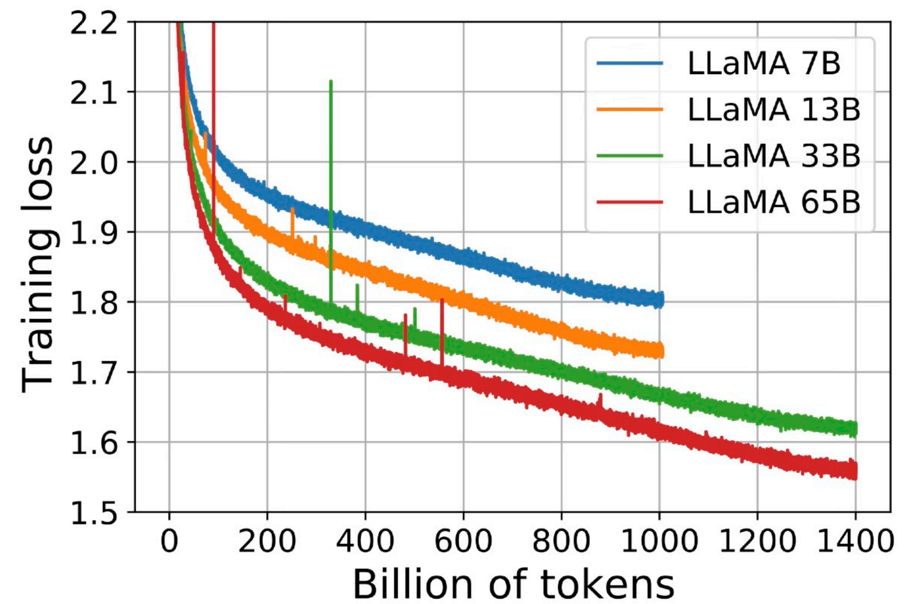
During the training of a neural network, a very common phenomenon is that of loss spikes, which can cause large gradient and destabilize training. Using a learning rate schedule with warmup, or clipping gradients can reduce the loss spikes or reduce their impact on training.

However, I realised that I don't really understand why there are loss spikes in the first place. Is it due to the input data distribution? To what extent can we reduce the amplitude of these spikes? Intuitively, if the model has already seen a representative part of the dataset, it shouldn't be too surprised by anything, hence the gradients shouldn't be that large.

Do you have any insight or references to better understand this phenomenon?

62 | 20 | Share

https://www.reddit.com/r/MachineLearning/comments/1odfuwe/r_why_loss_spikes/



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yes, we do!

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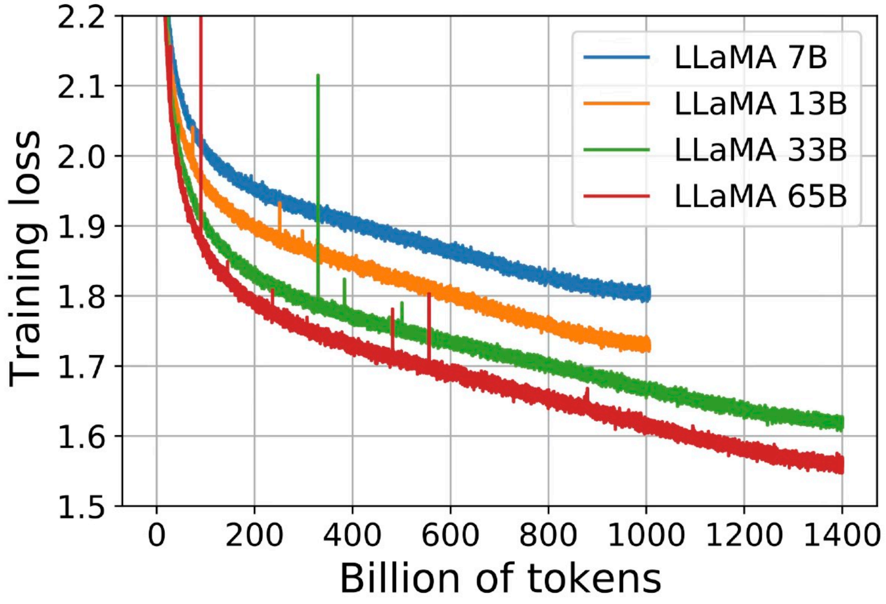
Why loss spikes

$$\theta_+ = \theta - \text{stepsize} \times \text{"gradient"}$$



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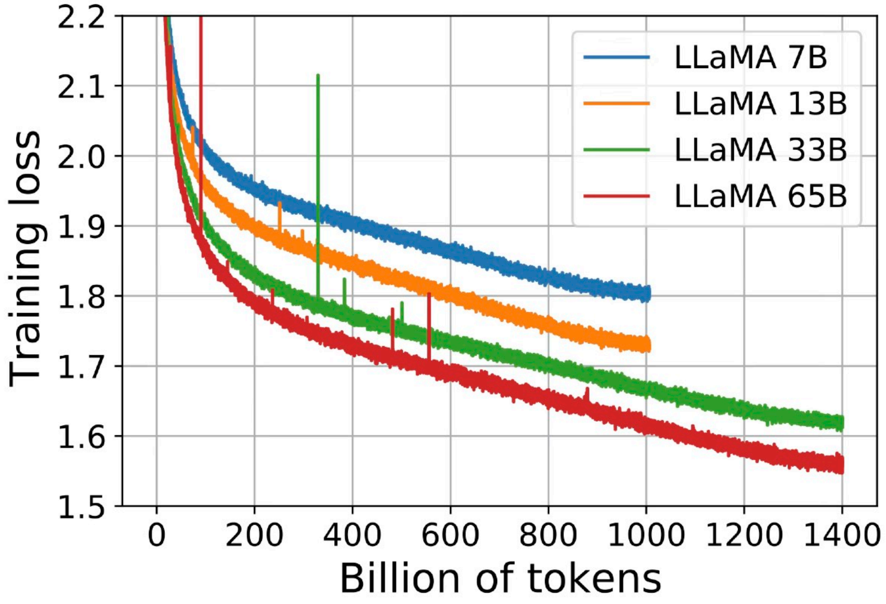

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data randomness $\leftarrow$ unlucky mini-batch

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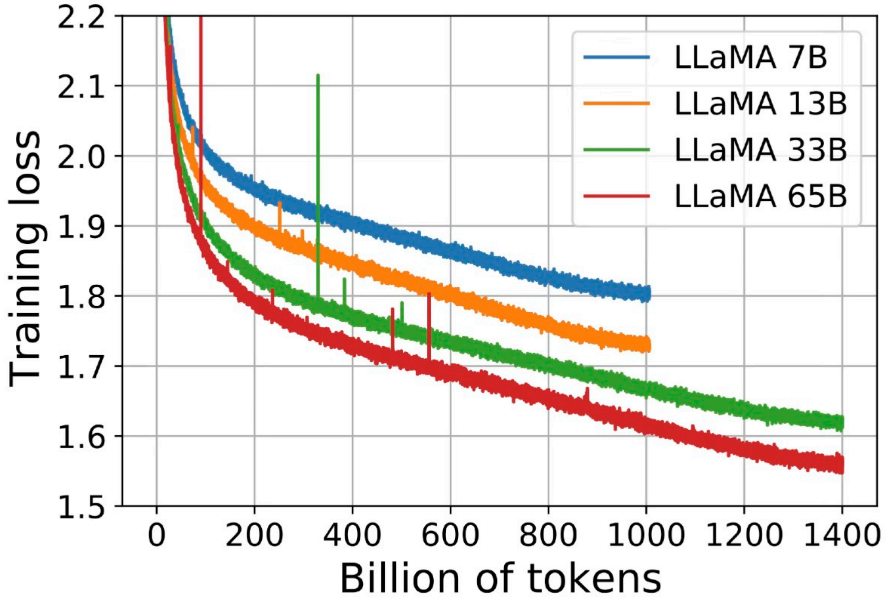

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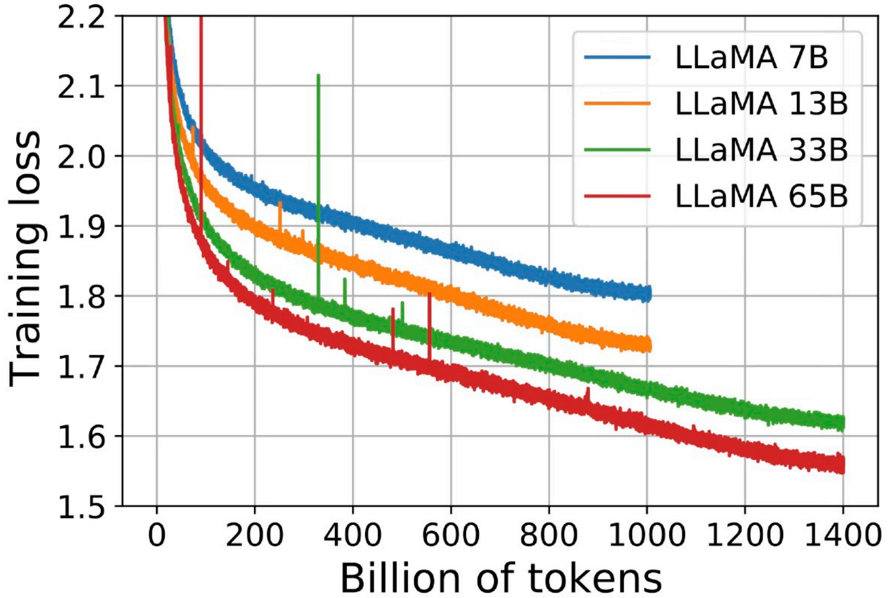

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loss landscape ← varying layer-wise curvature

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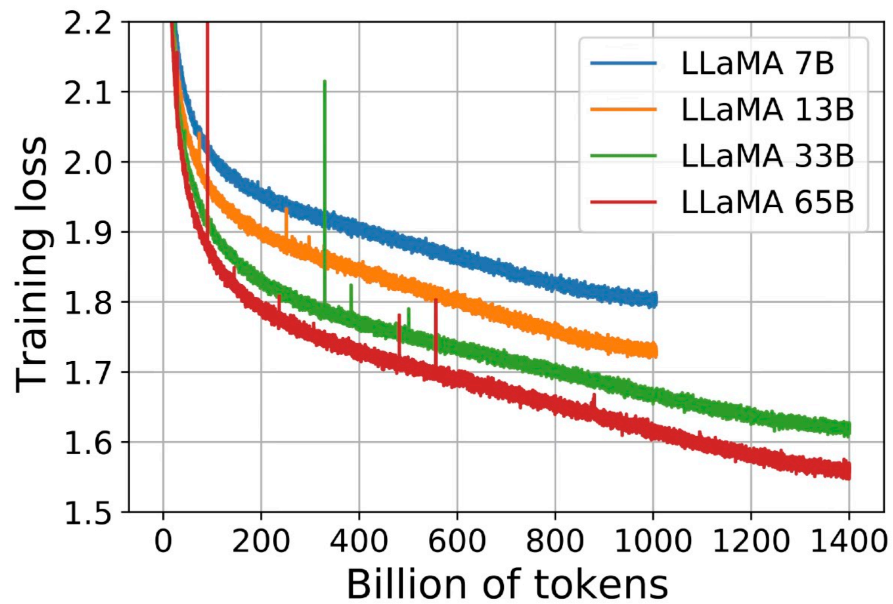

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inherent instability ← **stepsize / learning rate**

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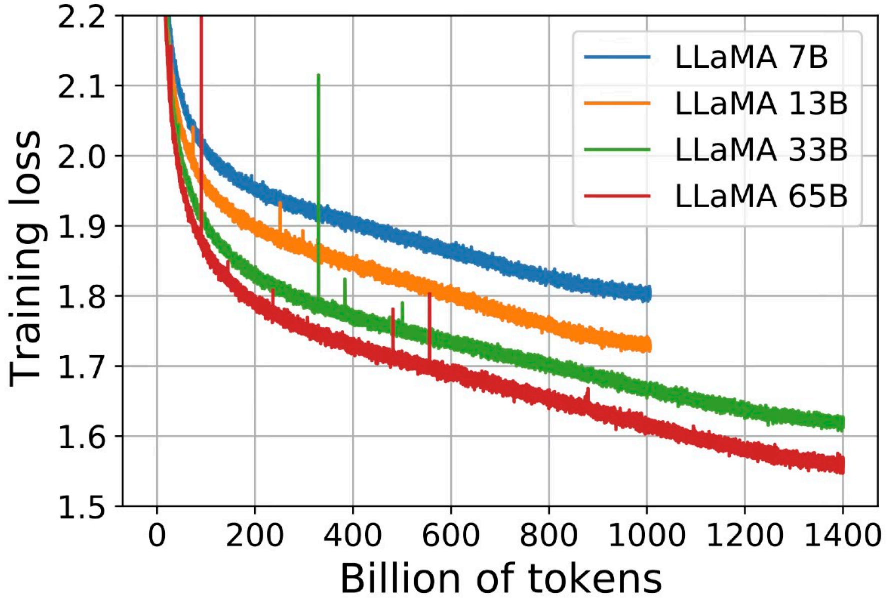

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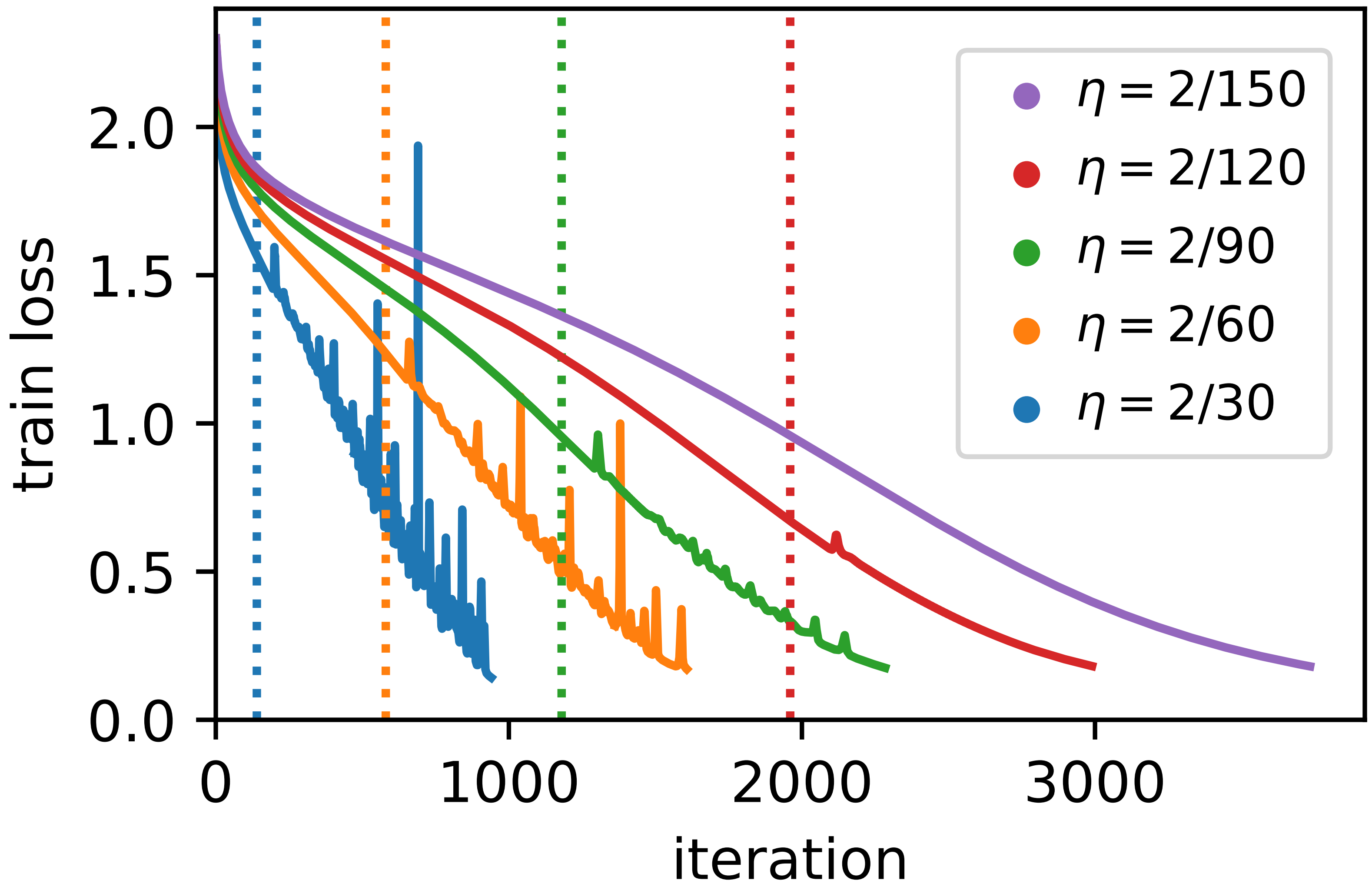
in DL, all efficient stepsizes are "large", causing training instability

Sandbox: GD + MLP



gradient descent, full batch, 5k subset of CIFAR-10, MLP

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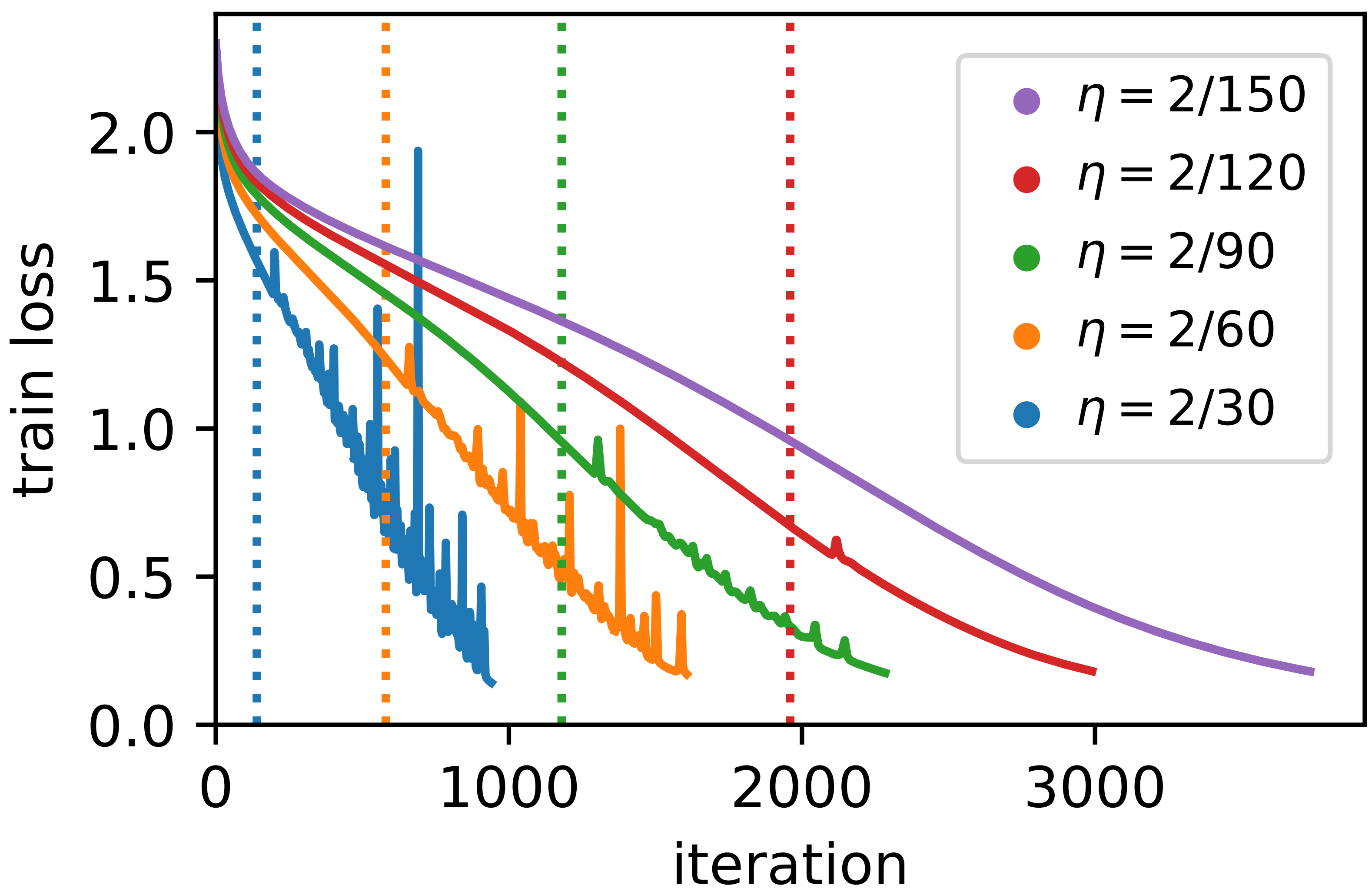

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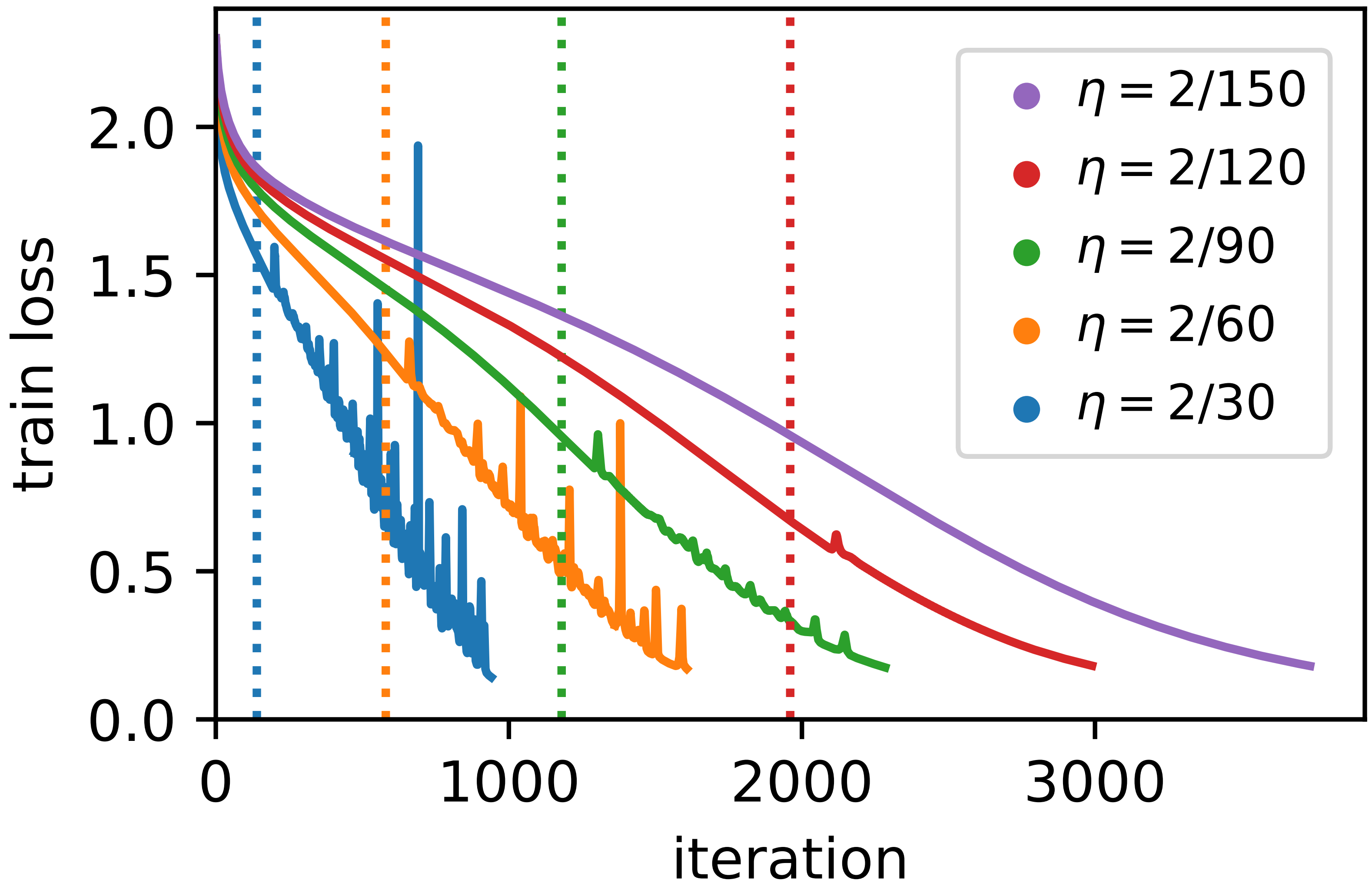

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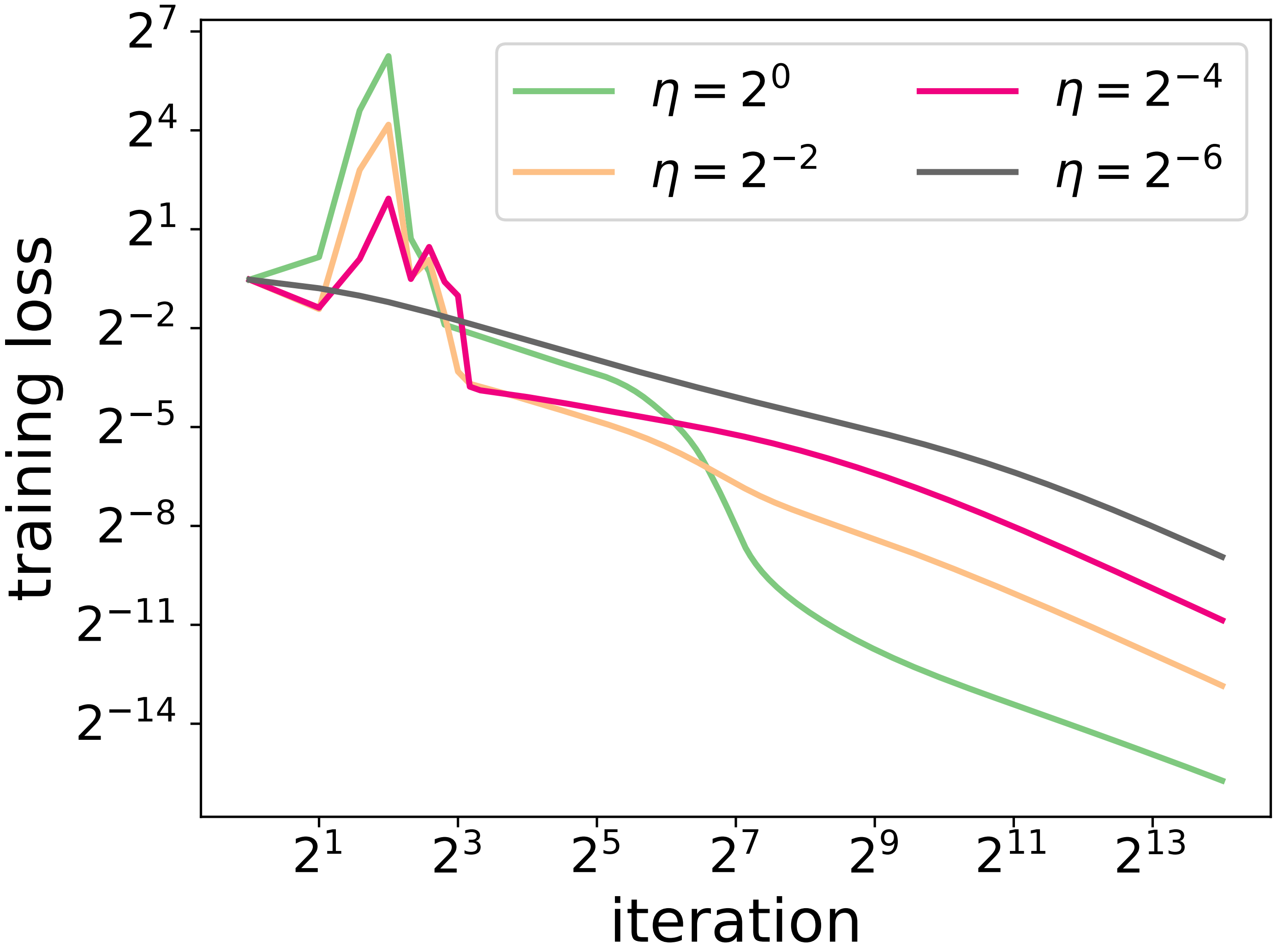

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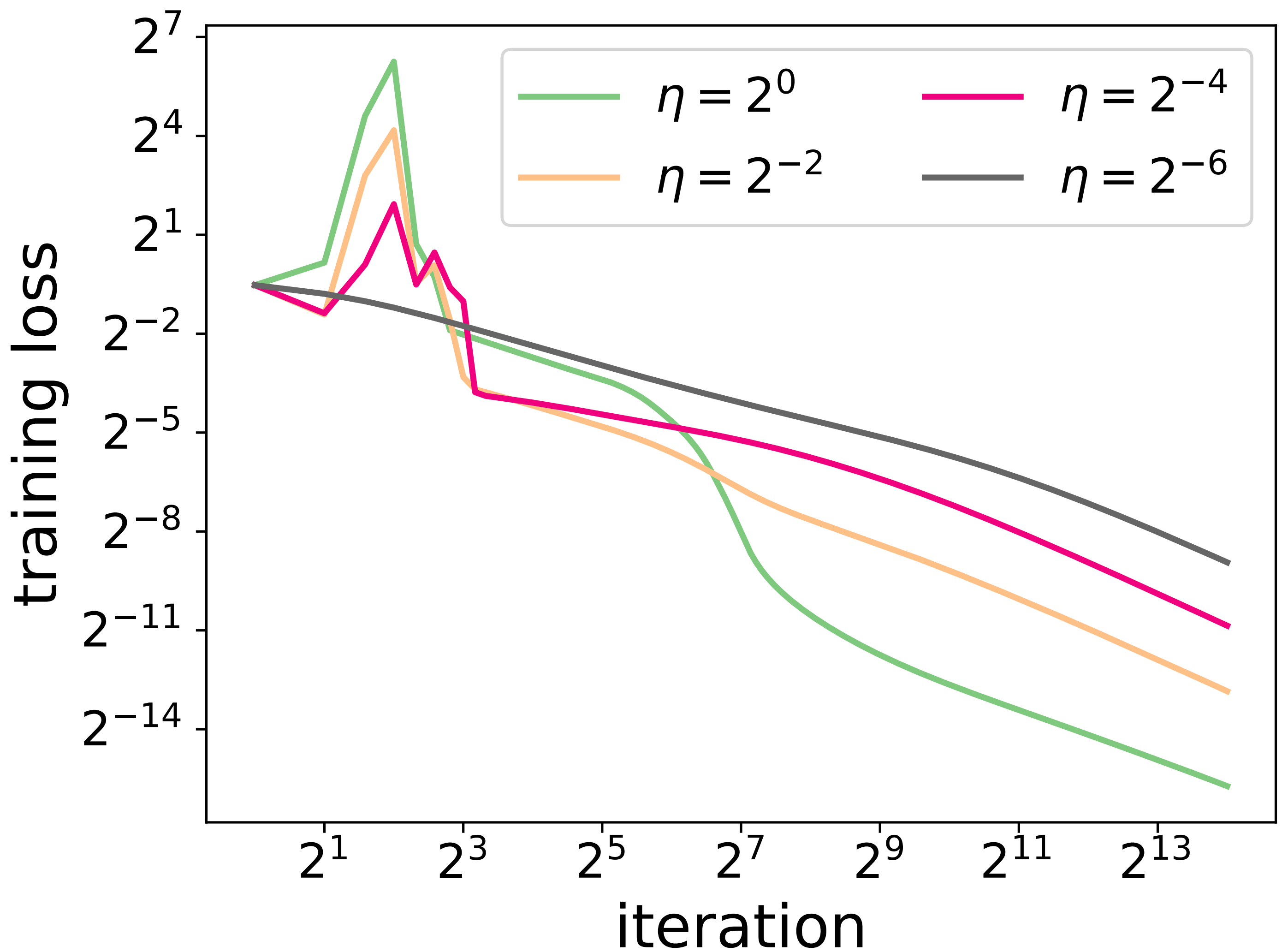

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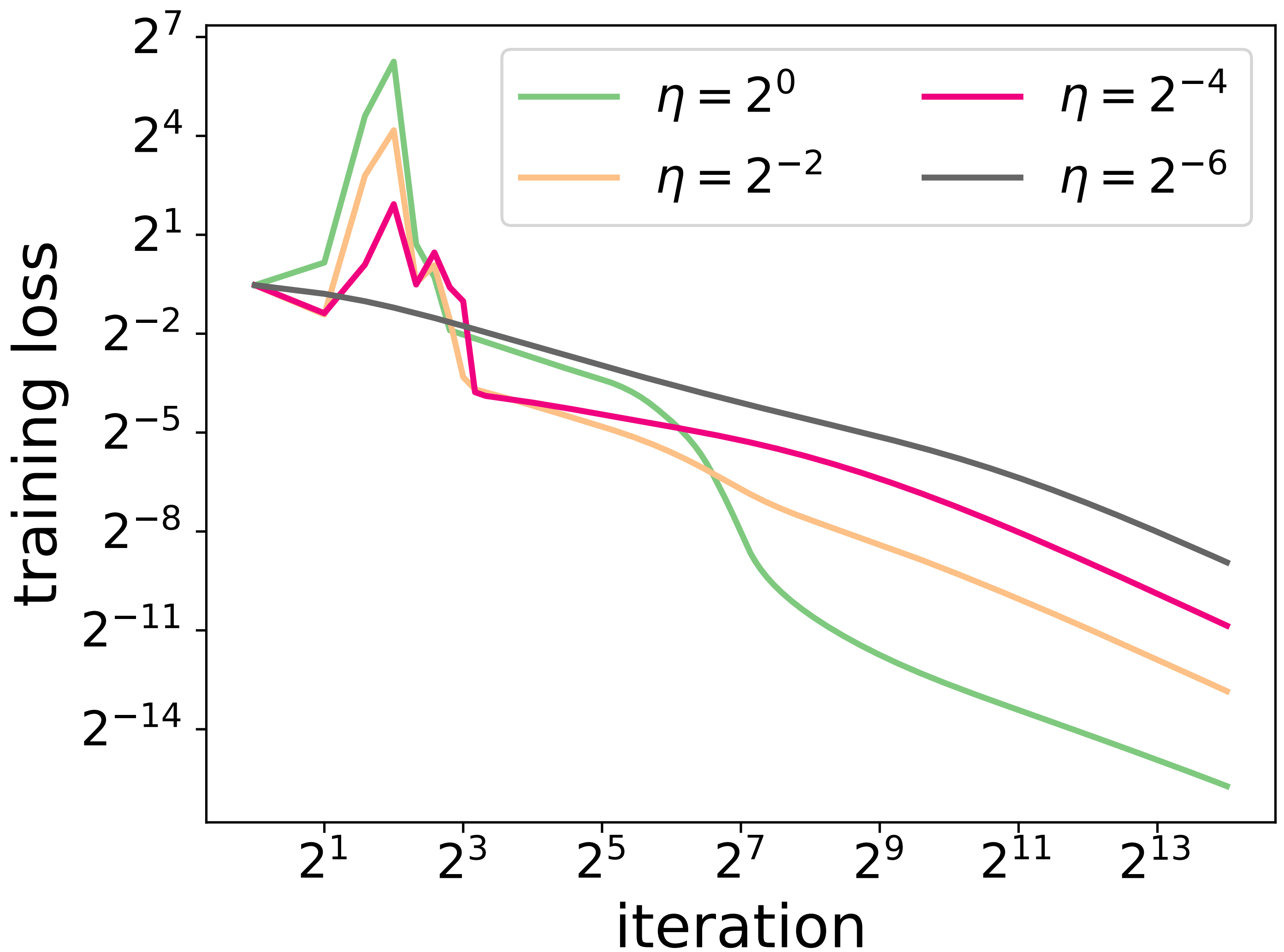

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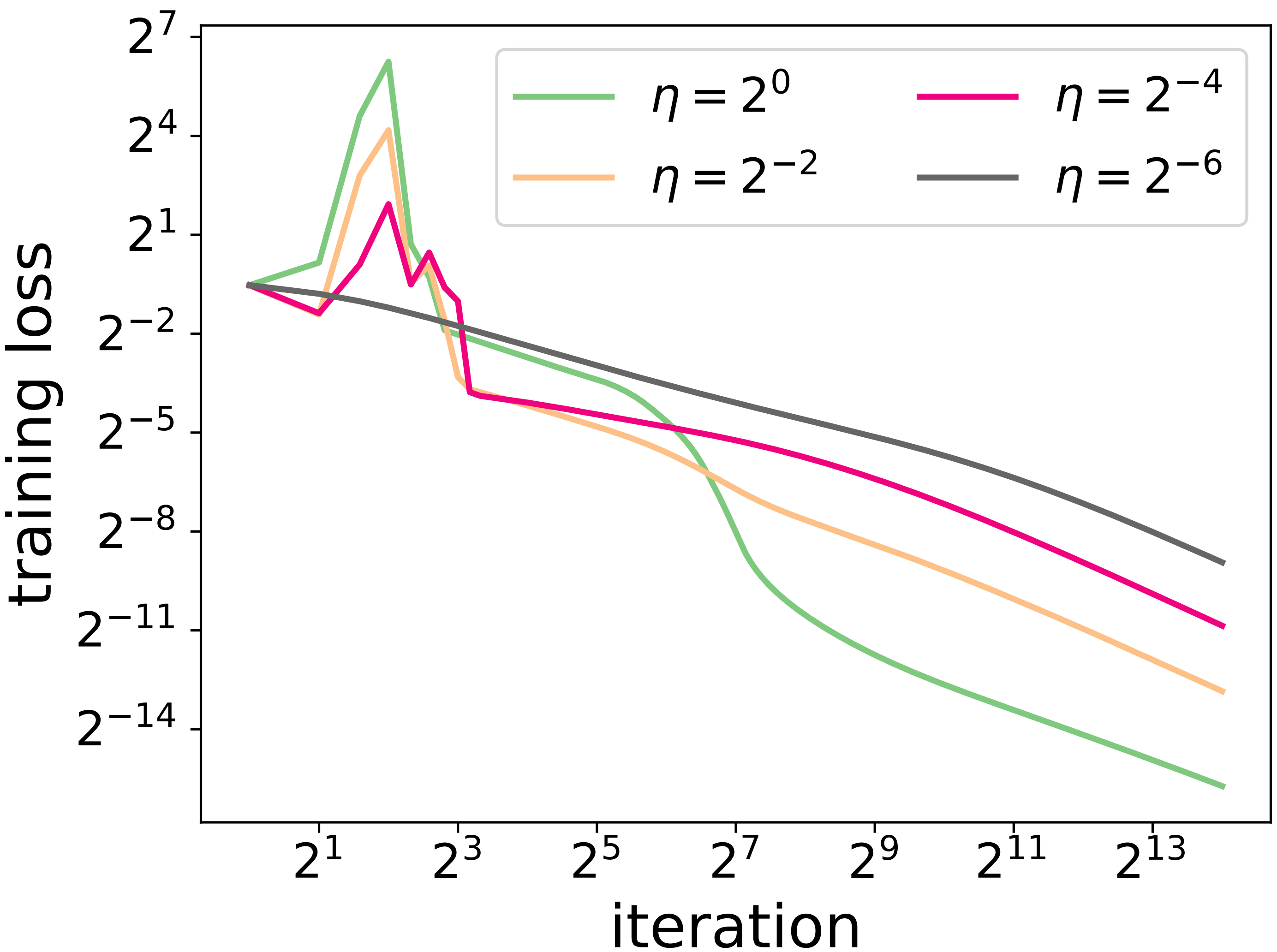

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🙀 — me in 2023

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GD $\to$ gradient flow

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GD → gradient flow

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❓ **adaptivity.** Adam: unclear continuous limit

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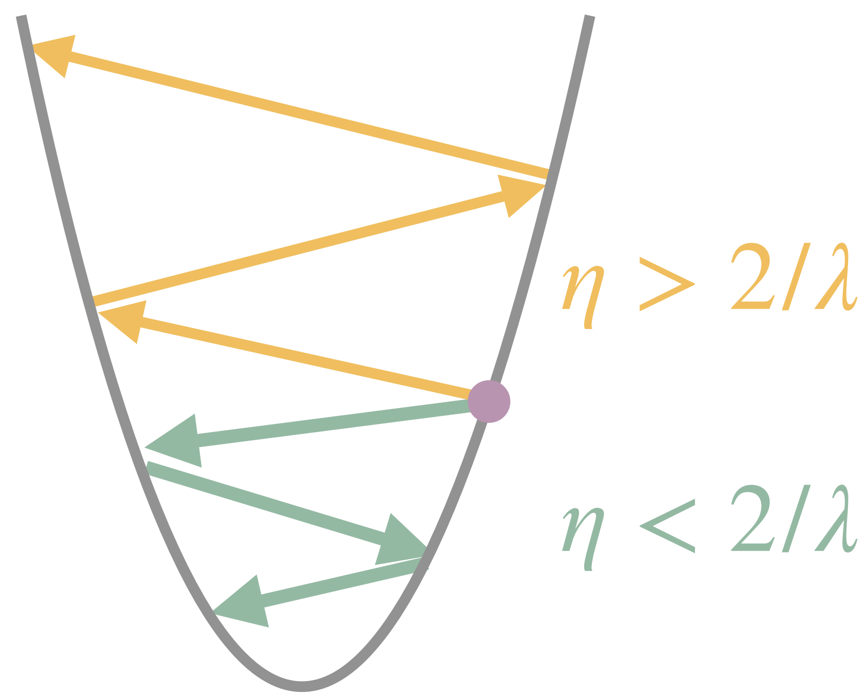

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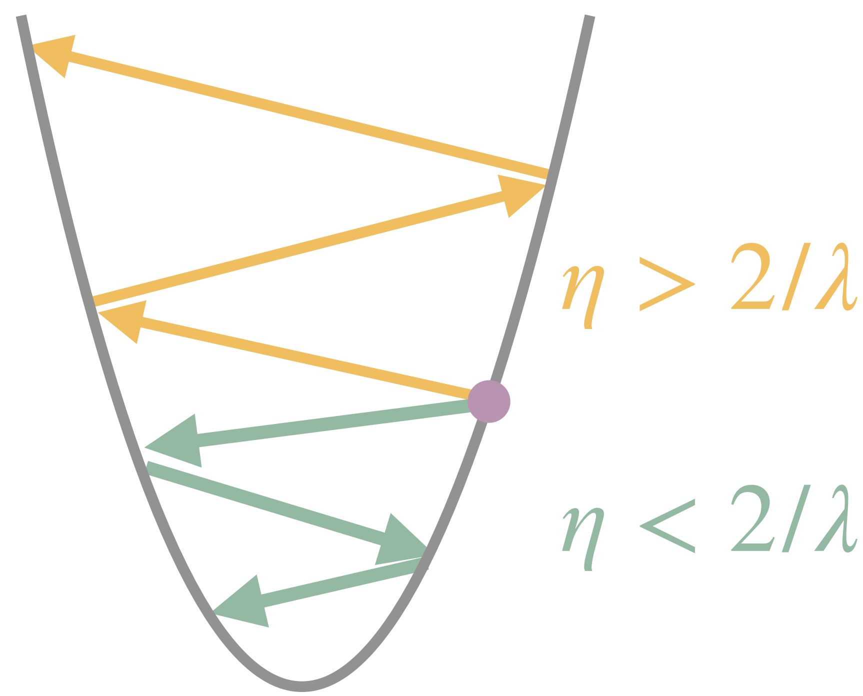

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cornerstone of optimization theory

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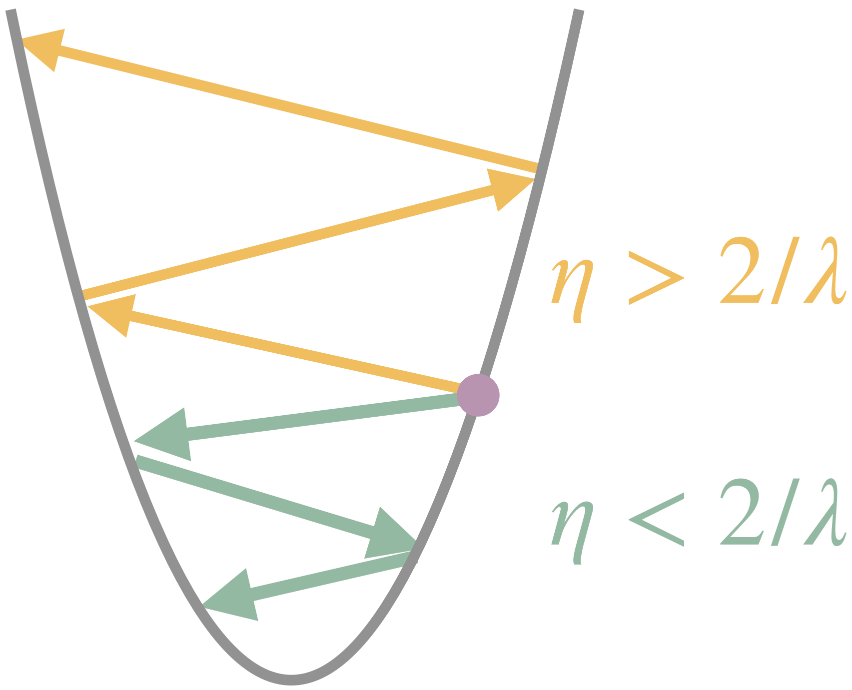

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sharpness penalty

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convergence? generalization?

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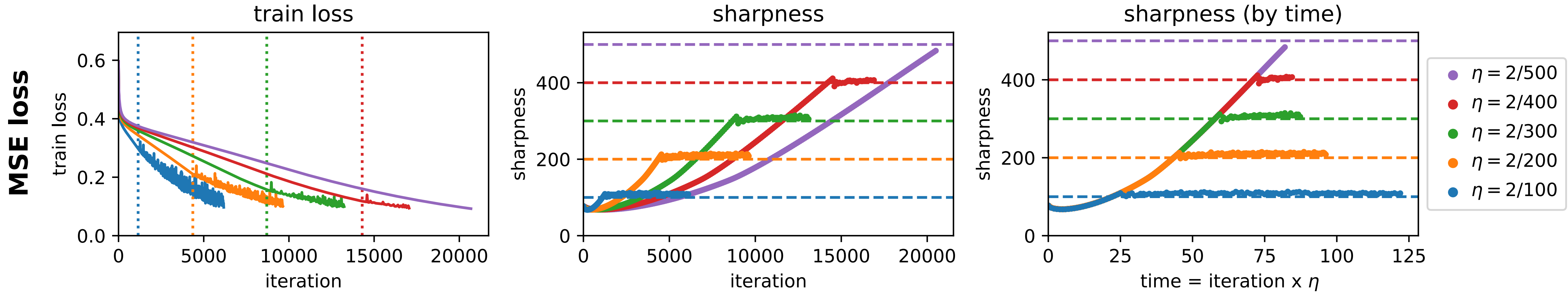
progressive sharpening

edge of stability



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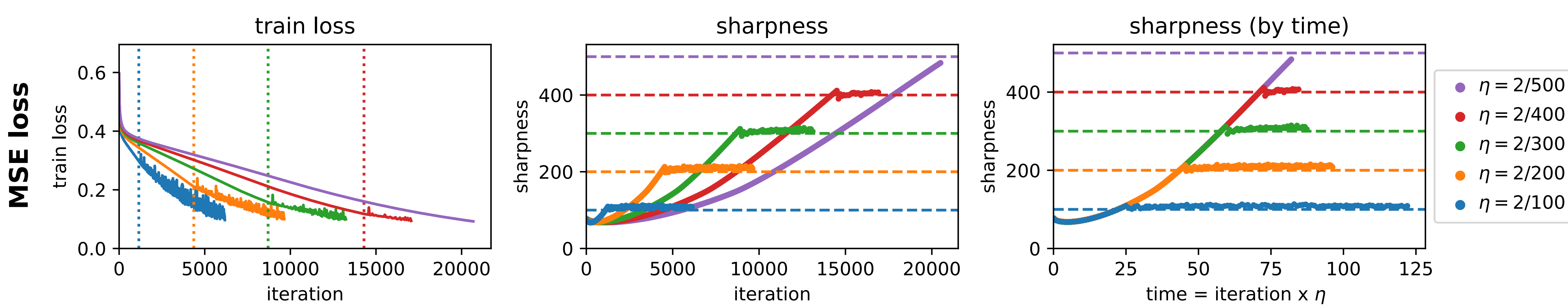

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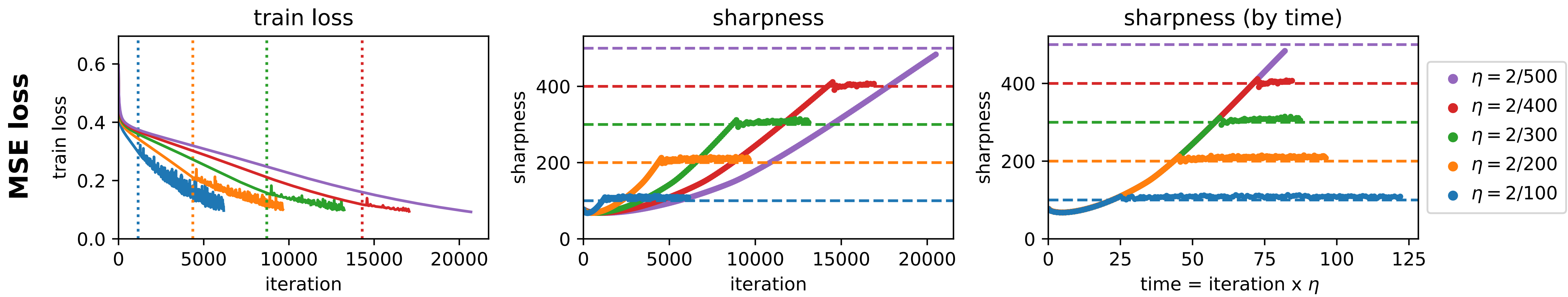
after **PS**, sharpness oscillates around $2/\eta$ for a while



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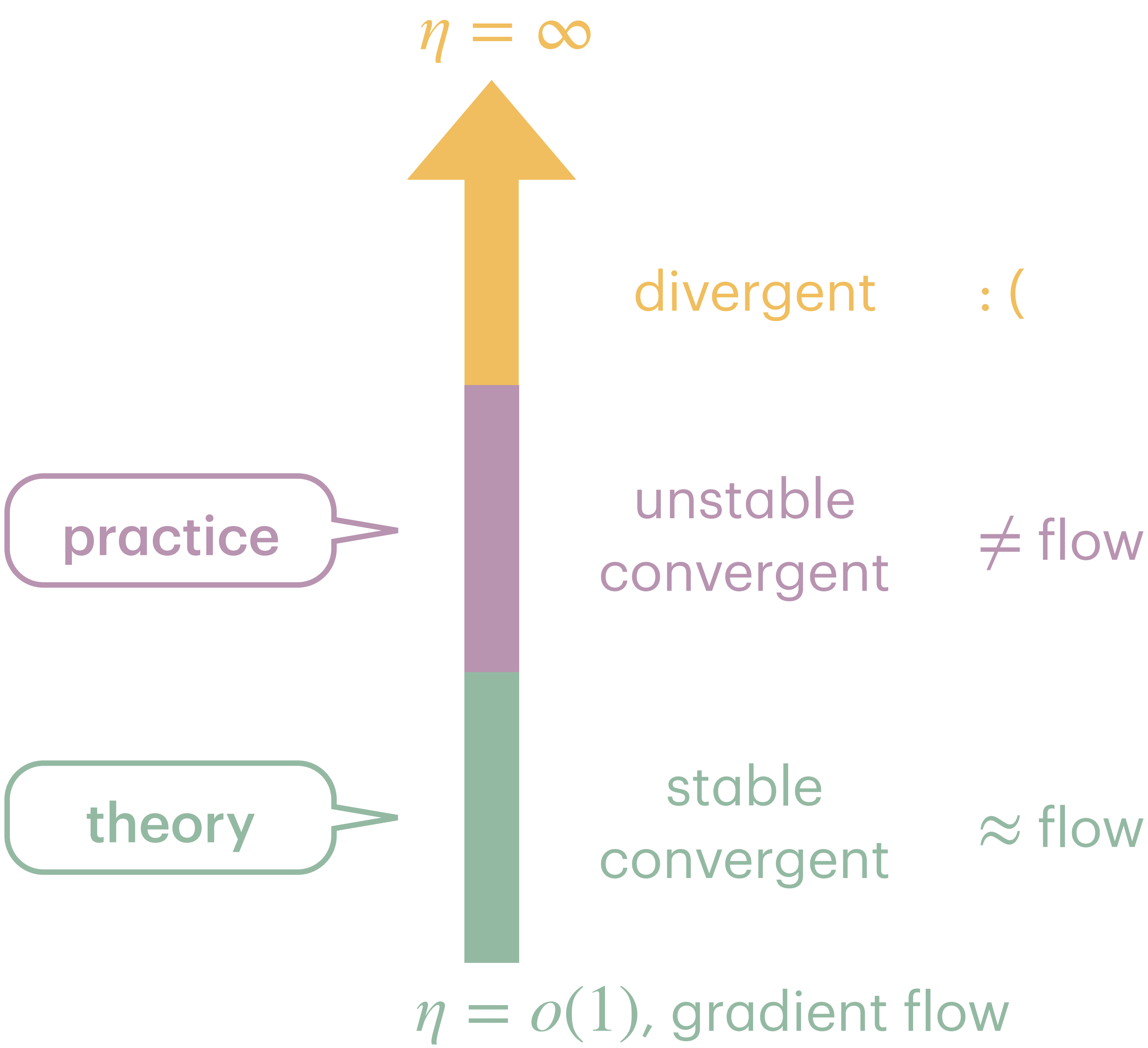

We will cover

Part 1: large stepsizes accelerate optimization

Part 2: large stepsizes prevent overfitting

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Part 1: large stepsizes accelerate optimization

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- **theory** & **insights** through clean **examples**
- known results & open problems
- why you should consider working on this!

We won’t cover but worth checking

(1/many) experimental science of large stepsize

*check our website for more references

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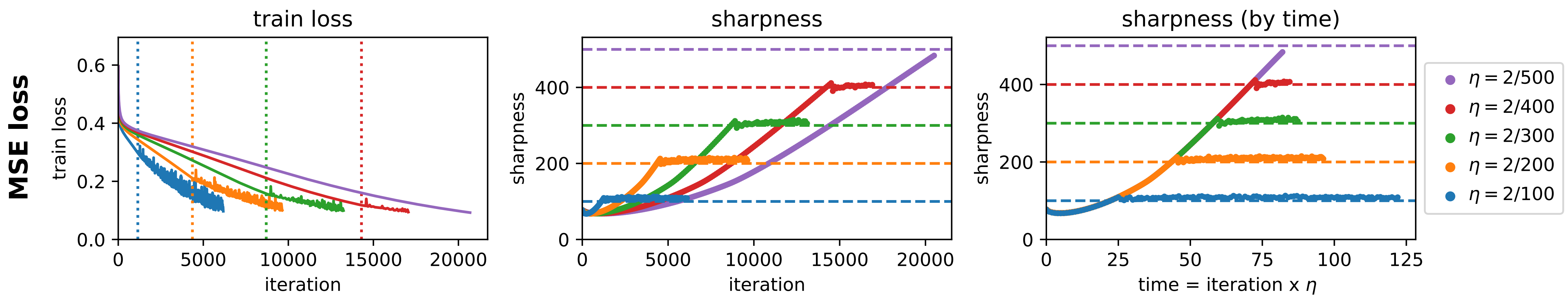
📋 progressive sharpening & edge of stability



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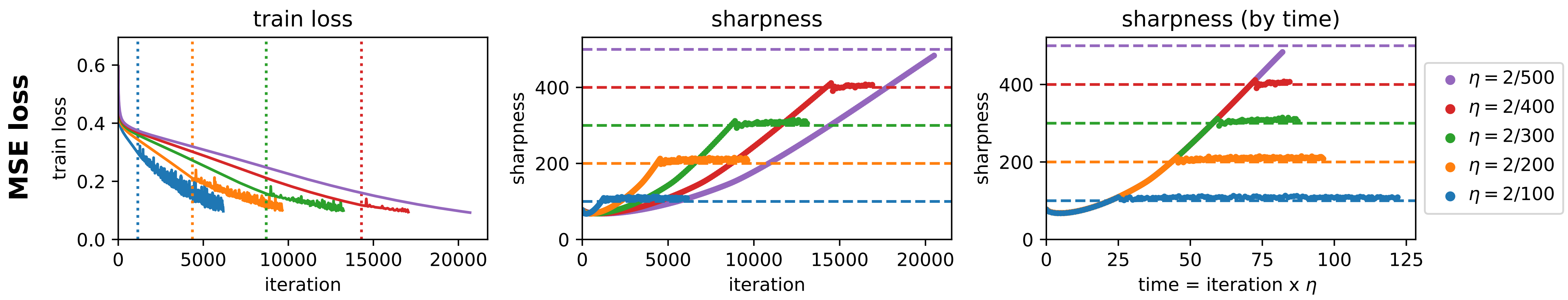
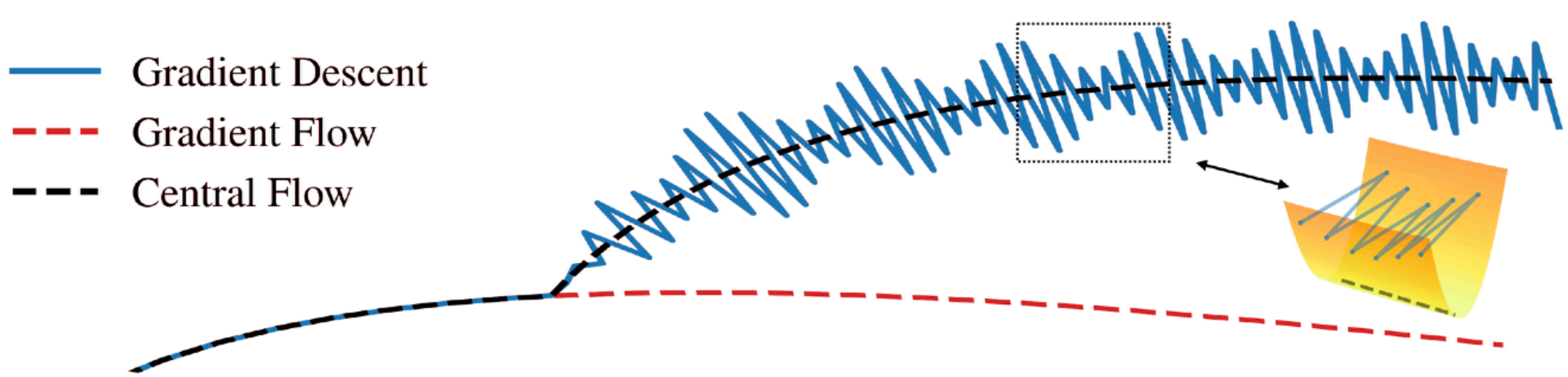


📋 central flow: an approximation of the trajectory



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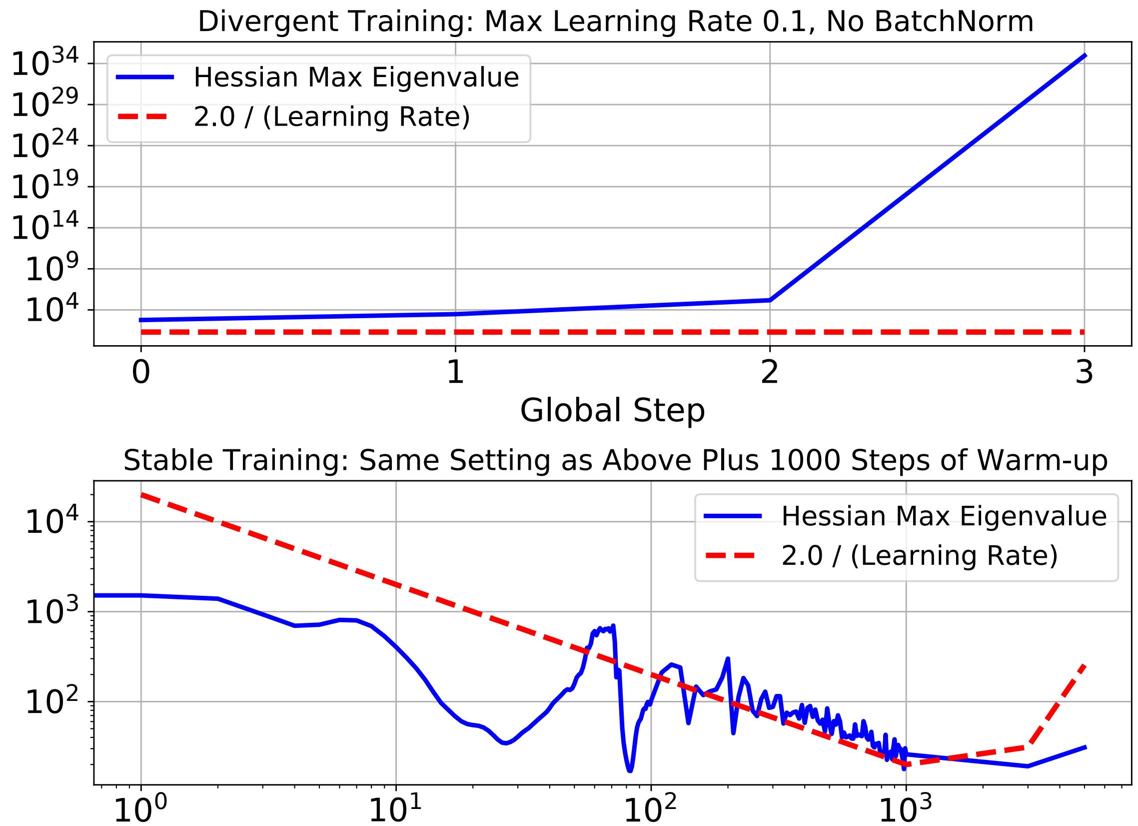
📋 learning rate warmup navigates to flatter region



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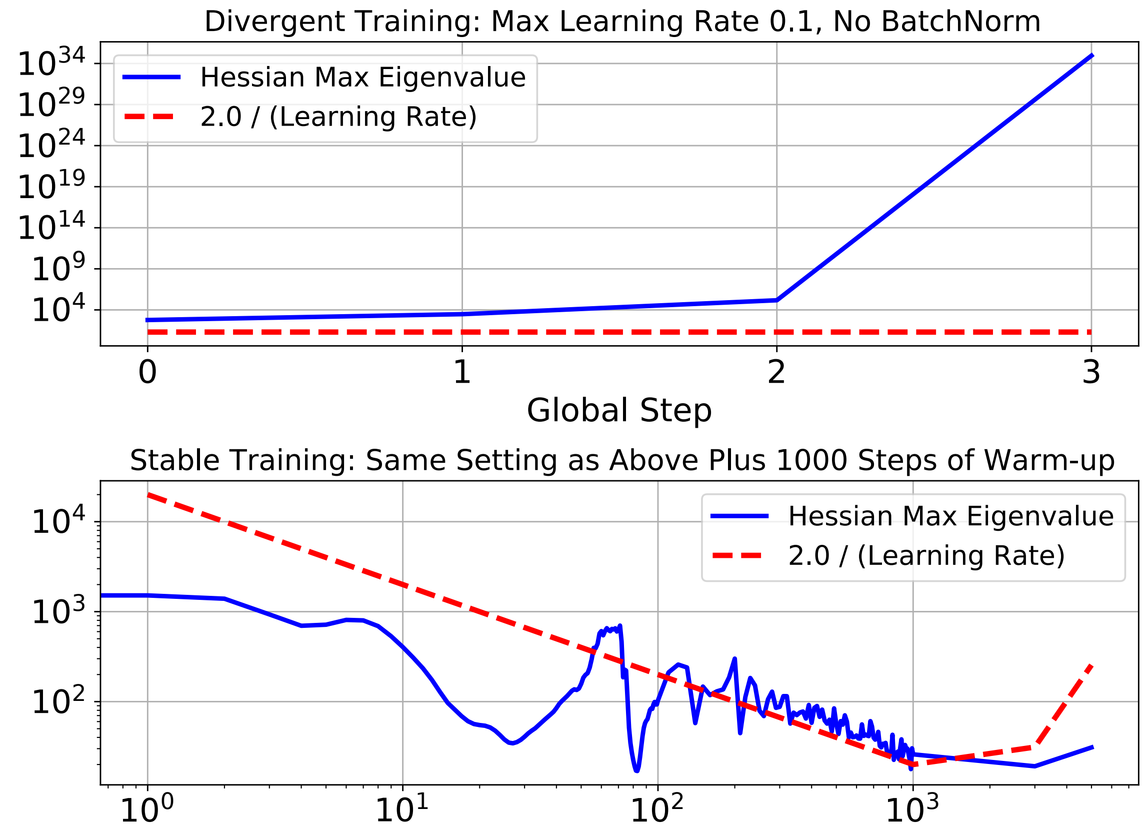
Gilmer, Ghorbani, Garg, et al. "A loss curvature perspective on training instability in deep learning." ICLR 2022

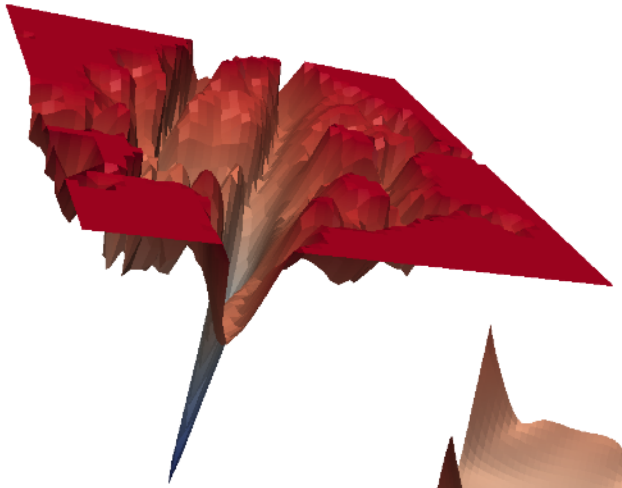
We won't cover but worth checking

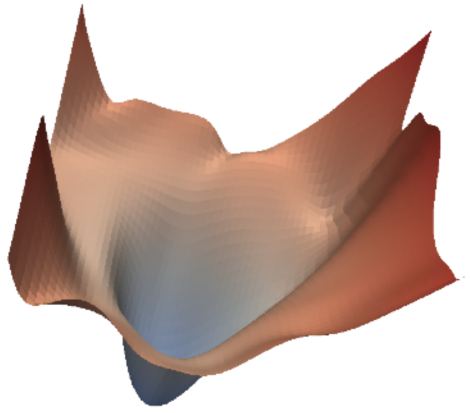
(2/many) optimizer-landscape codesign

📋 learning rate warmup navigates to flatter region



📋 sharpness-aware minimization





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Gilmer, Ghorbani, Garg, et al. "A loss curvature perspective on training instability in deep learning." ICLR 2022

Foret, Kleiner, Mobahi, Neyshabur. "Sharpness-aware minimization for efficiently improving generalization." ICLR 2021

Part 1: optimization

Review: classical optimization theory

A modern take: acceleration via large stepsizes

Summary, open problems, Q&A

Part 2: generalization

Review: descent lemma

For GD, $L(\theta_t)$ decreases monotonically for small η such that

$$\eta < \frac{2}{\sup \|\nabla^2 L(\,\cdot\,)\|}$$

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Proof.

$$
\begin{aligned}
L(\theta_+) &= L(\theta - \eta \nabla L(\theta)) \\
&= L(\theta) - \eta \|\nabla L(\theta)\|^2 + \frac{\eta^2}{2} \nabla L(\theta)^\top \nabla^2 L(\nu) \nabla L(\theta) \\
&\leq L(\theta) - \eta \|\nabla L(\theta)\|^2 \left(1 - \frac{\eta}{2} \|\nabla^2 L(\nu)\|\right) \\
&\leq L(\theta)
\end{aligned}
$$

Review: descent lemma

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GD step

$$= L(\theta) - \eta \|\nabla L(\theta)\|^2 + \frac{\eta^2}{2} \nabla L(\theta)^\top \nabla^2 L(\nu) \nabla L(\theta)$$

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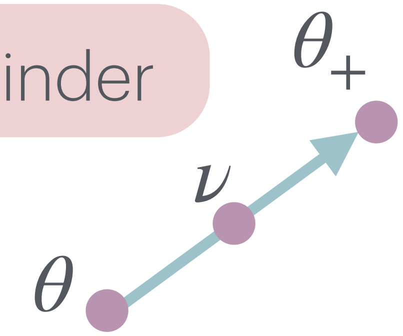
GD step

Taylor remainder

$$= L(\theta) - \eta \|\nabla L(\theta)\|^2 + \frac{\eta^2}{2} \nabla L(\theta)^\top \nabla^2 L(\nu) \nabla L(\theta)$$



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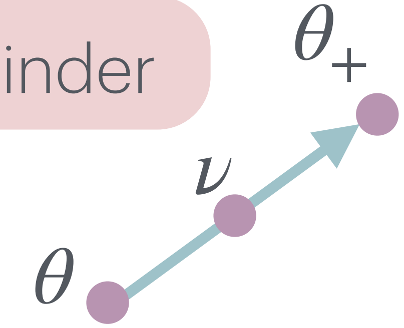

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operator norm

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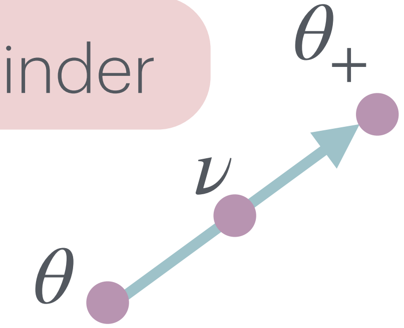

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small stepsize

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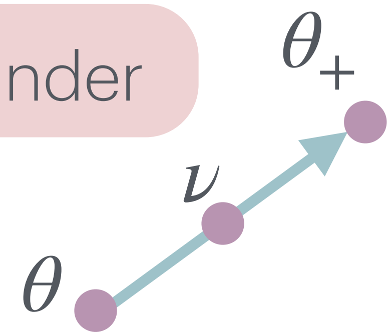

this descent lemma can be generalized

Review: convergence rates

Let L be 1-smooth ($\|\nabla^2 L\| \leq 1$) with finite minimizer $w*$. For GD with $\eta = 1$, we have

descent lemma $L(\theta_t) \downarrow$

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number of steps to get ϵ-error:

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$\kappa = 1/\alpha$, condition number

Review: gradient flow analysis

For **convex** L and **gradient flow** $\mathrm{d}\theta_t = -\nabla L(\theta_t)\mathrm{d}t$, we have

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step 1:

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step 2:

$$\frac{1}{2}\|\theta_t - \nu\|^2 - \frac{1}{2}\|\theta_0 - \nu\|^2 \leq \int_0^t L(\nu) - L(\theta_s)\mathrm{d}s \leq t\big(L(\theta) - L(\theta_t)\big)$$

step 3: rearranging terms

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chain rule

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step 3: rearranging terms

for small stepsize, discretize this => GD analysis

Review: acceleration

number of steps to get ϵ-error

GD

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$$O\left(1/\epsilon\right) \text{ \& } O\left(\kappa \log(1/\epsilon)\right)$$

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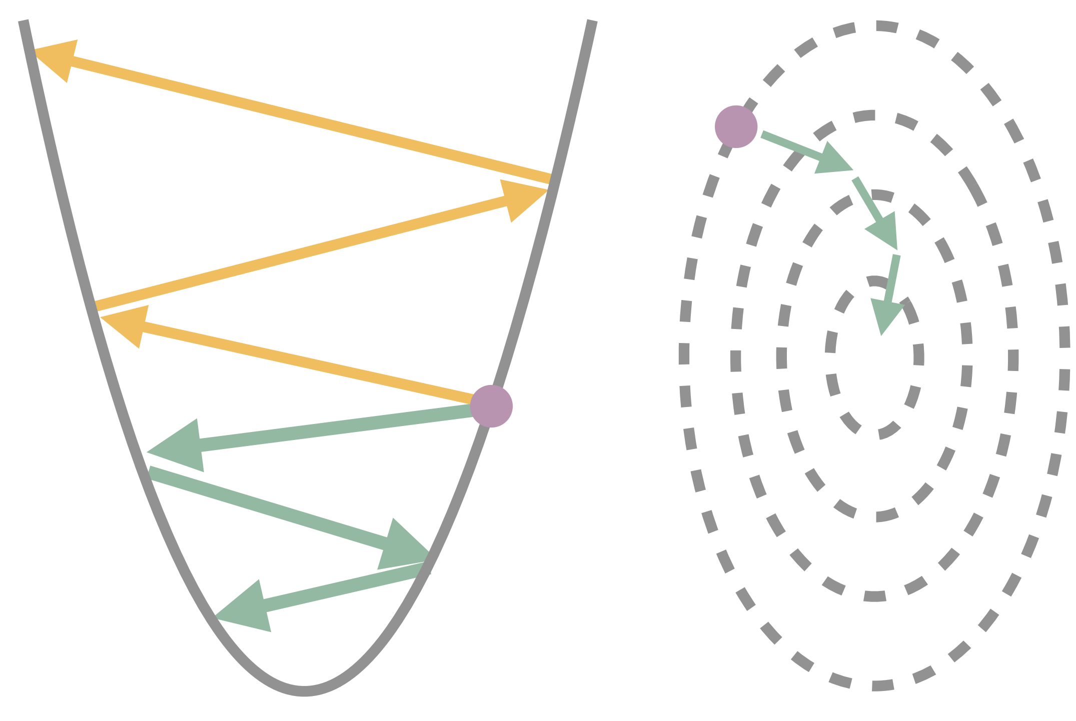
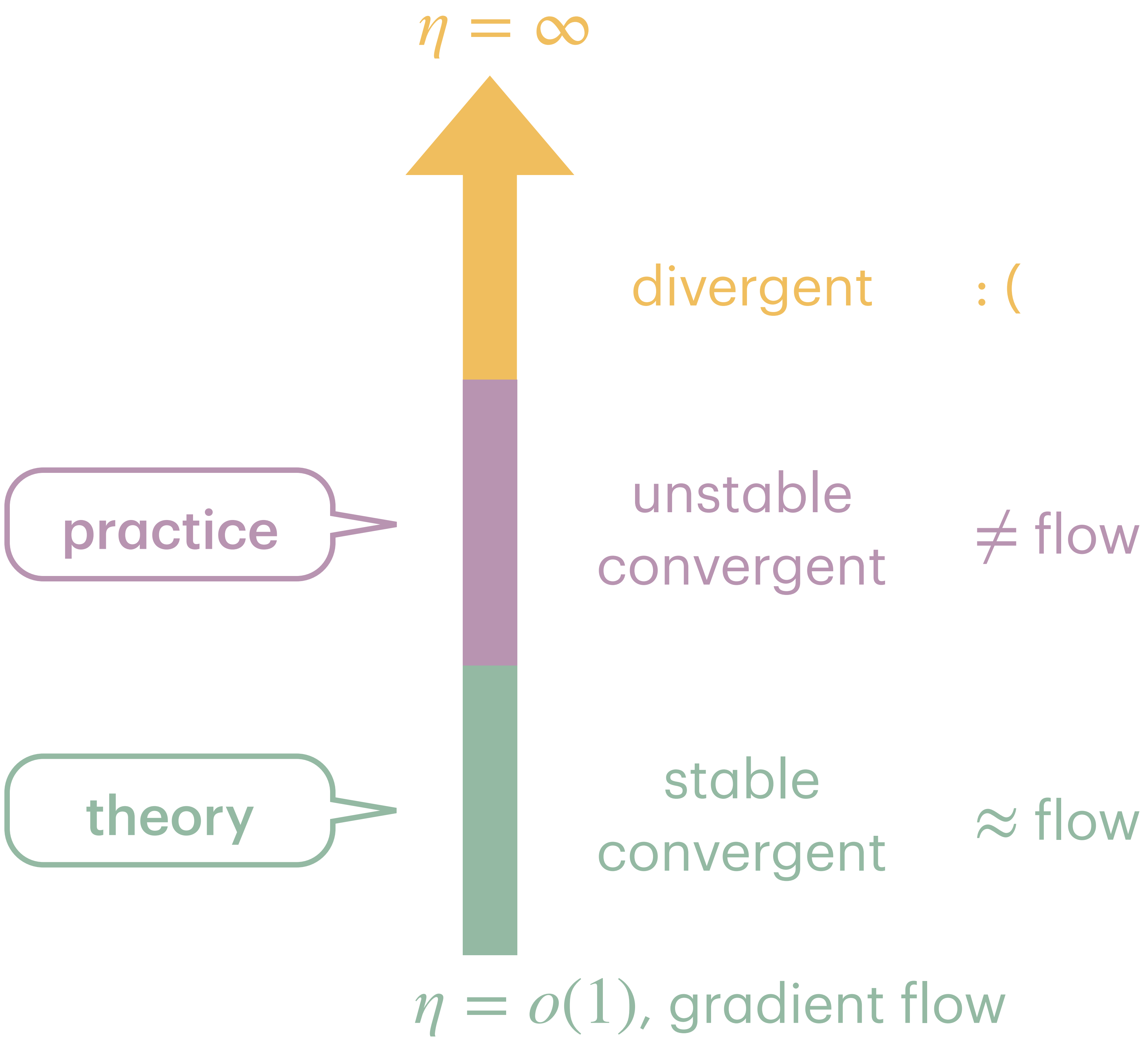
hard case: quadratics in high-dim



From small to large stepsize



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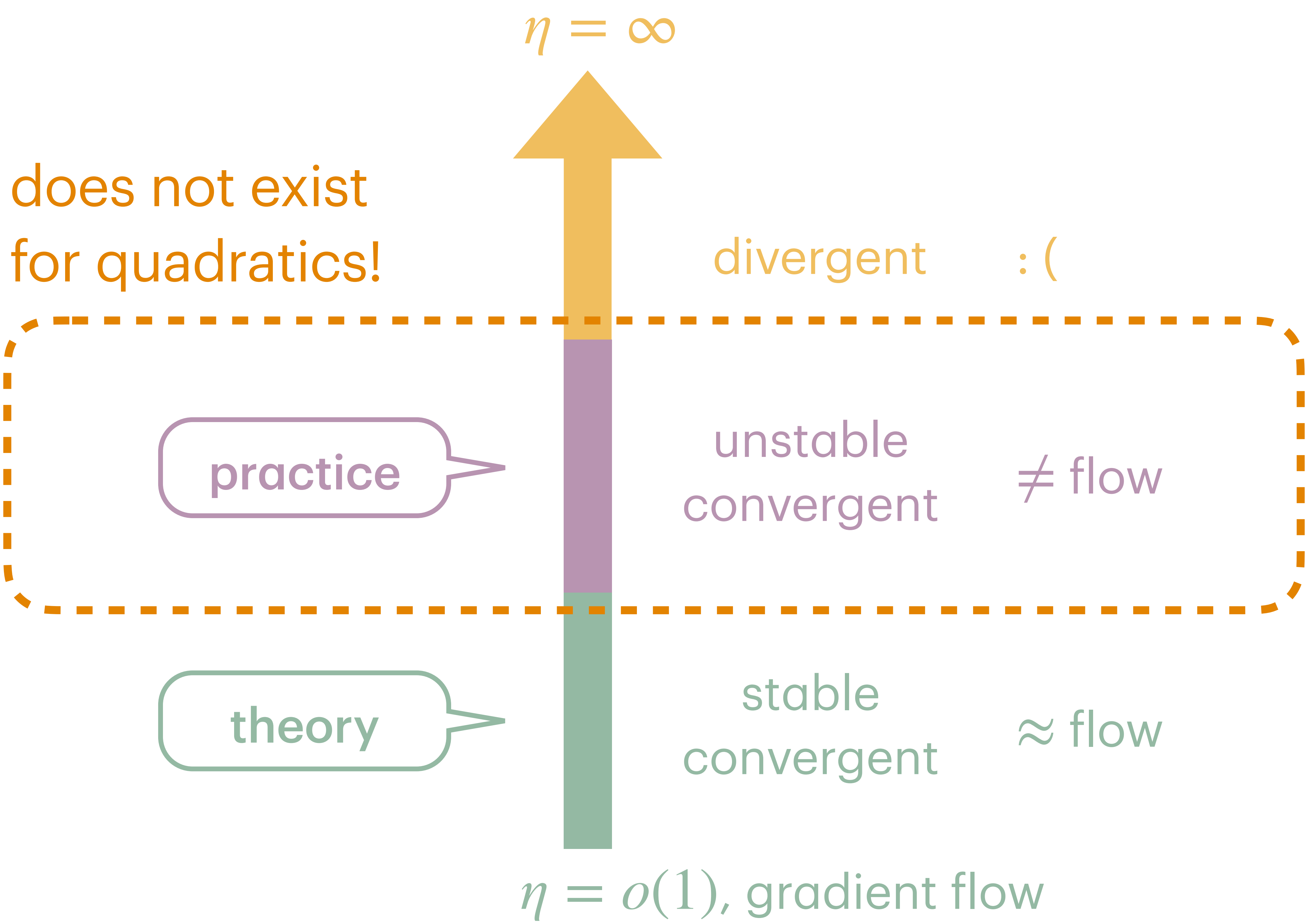
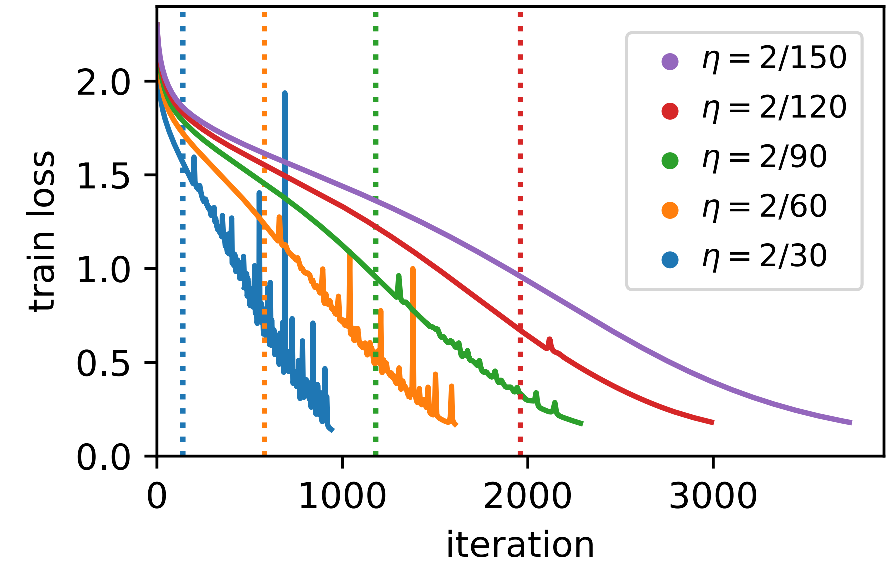


Alternative mental model

......

deep learning

unstable convergence observed



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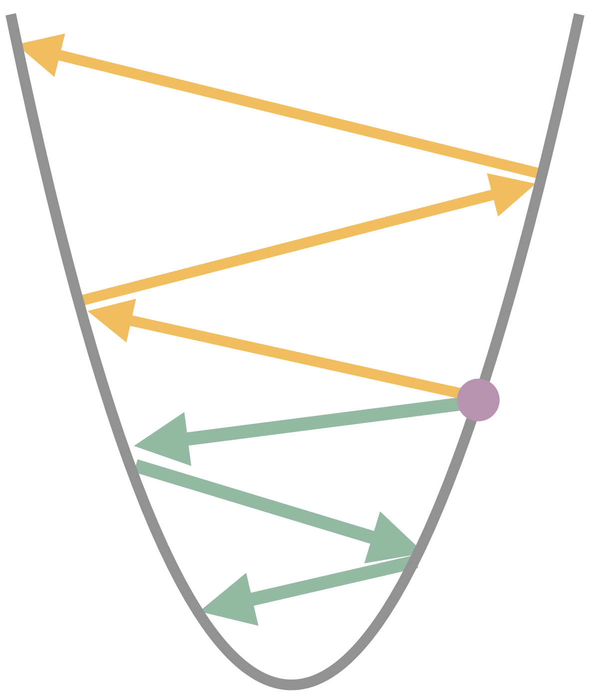
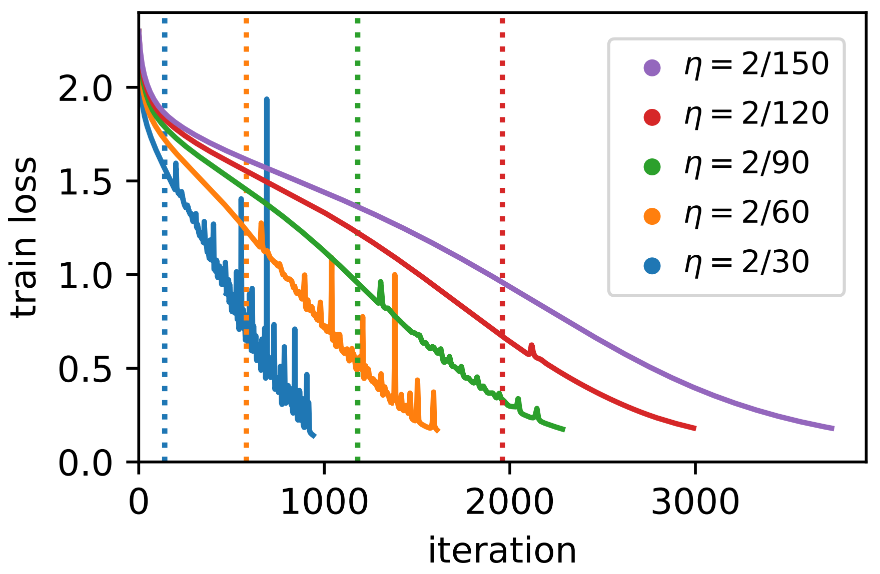
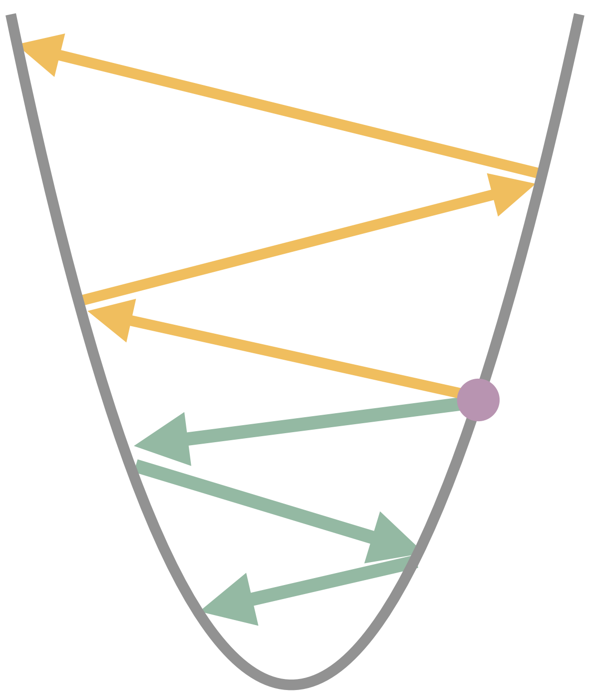
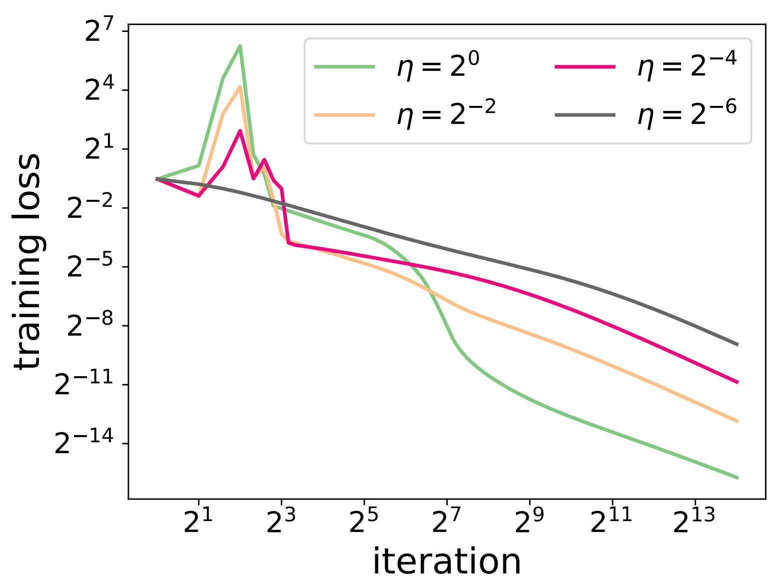


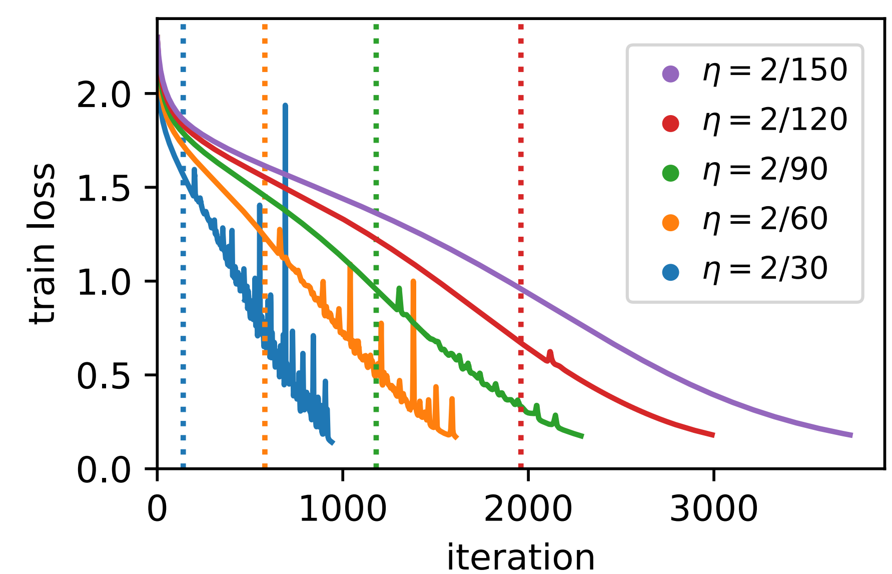


Alternative mental model

linear regression	logistic regression	......	deep learning
unstable convergence impossible	**observable & provable**		unstable convergence observed







(1/3) Logistic regression

$$L(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ln\left(1 + \exp(-y_i x_i^\top \theta)\right)$$

$$\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t)$$

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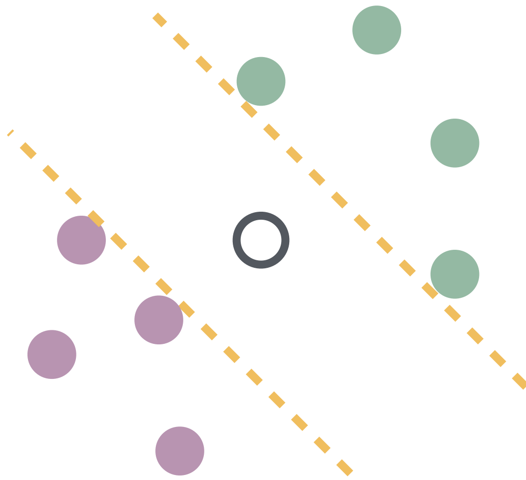
Assumption (bounded + separable)

- $\|x_i\| \leq 1,\ y_i \in \{\pm 1\},\ i = 1,\ldots,n$
- $\exists$ unit vector θ^*, $\min_i y_i x_i^\top \theta^* \geq \gamma > 0$



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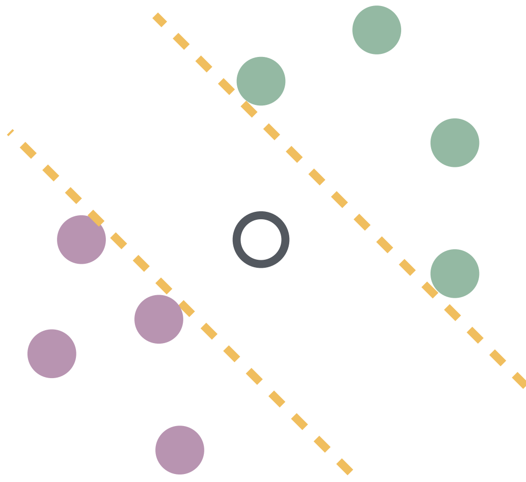

"almost surely" if overparameterized

(1/3) Logistic regression

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ln\left(1 + \exp(-y_i x_i^\top \theta)\right)$$

smooth, convex
non-strongly convex

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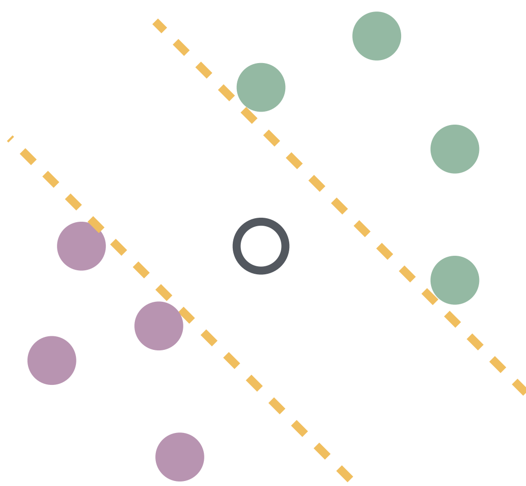

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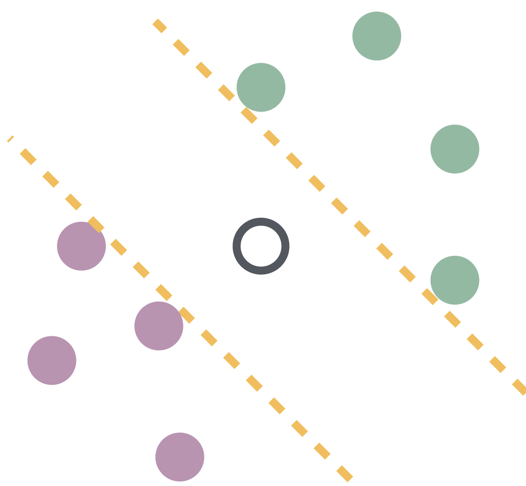

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"almost surely" if overparameterized

Classical theory

For $\eta = \Theta(1)$, $L(\theta_t) \downarrow$ and $L(\theta_t) = \tilde{O}(1/t)$

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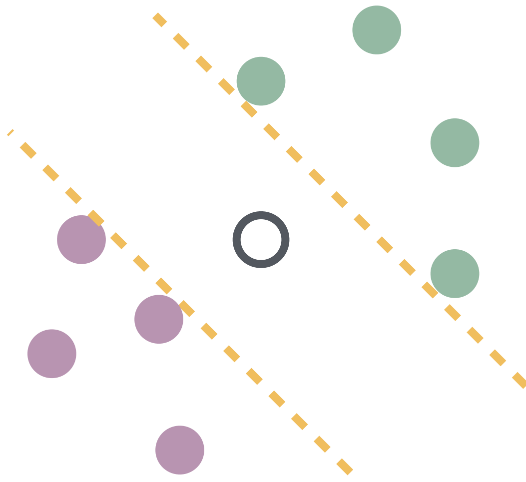

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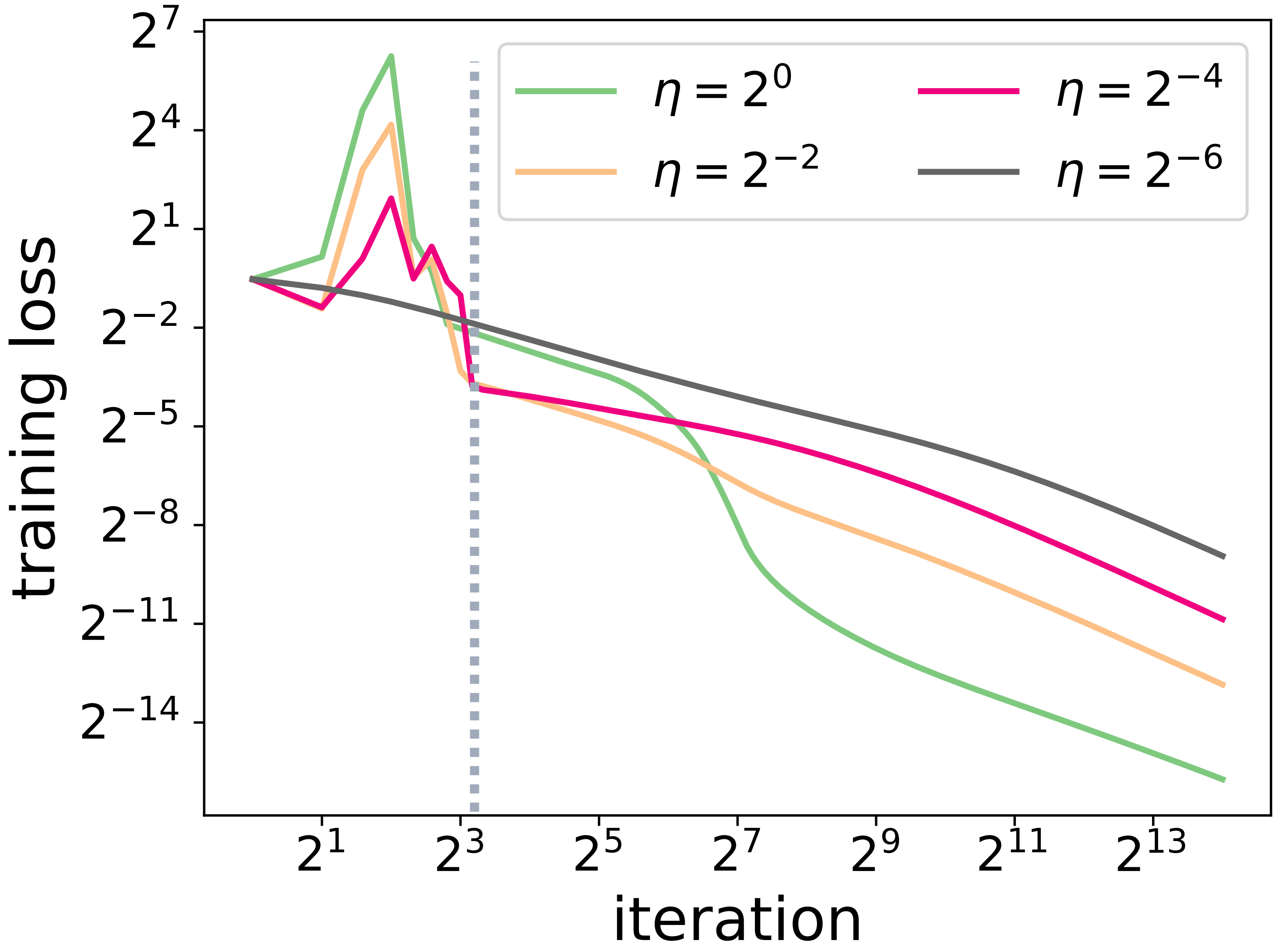
"almost surely" if overparameterized

Classical theory

For $\eta = \Theta(1)$, $L(\theta_t) \downarrow$ and $L(\theta_t) = \tilde{O}(1/t)$

improved to $\tilde{O}(1/t^2)$ by Nesterov

(1/3) Logistic regression



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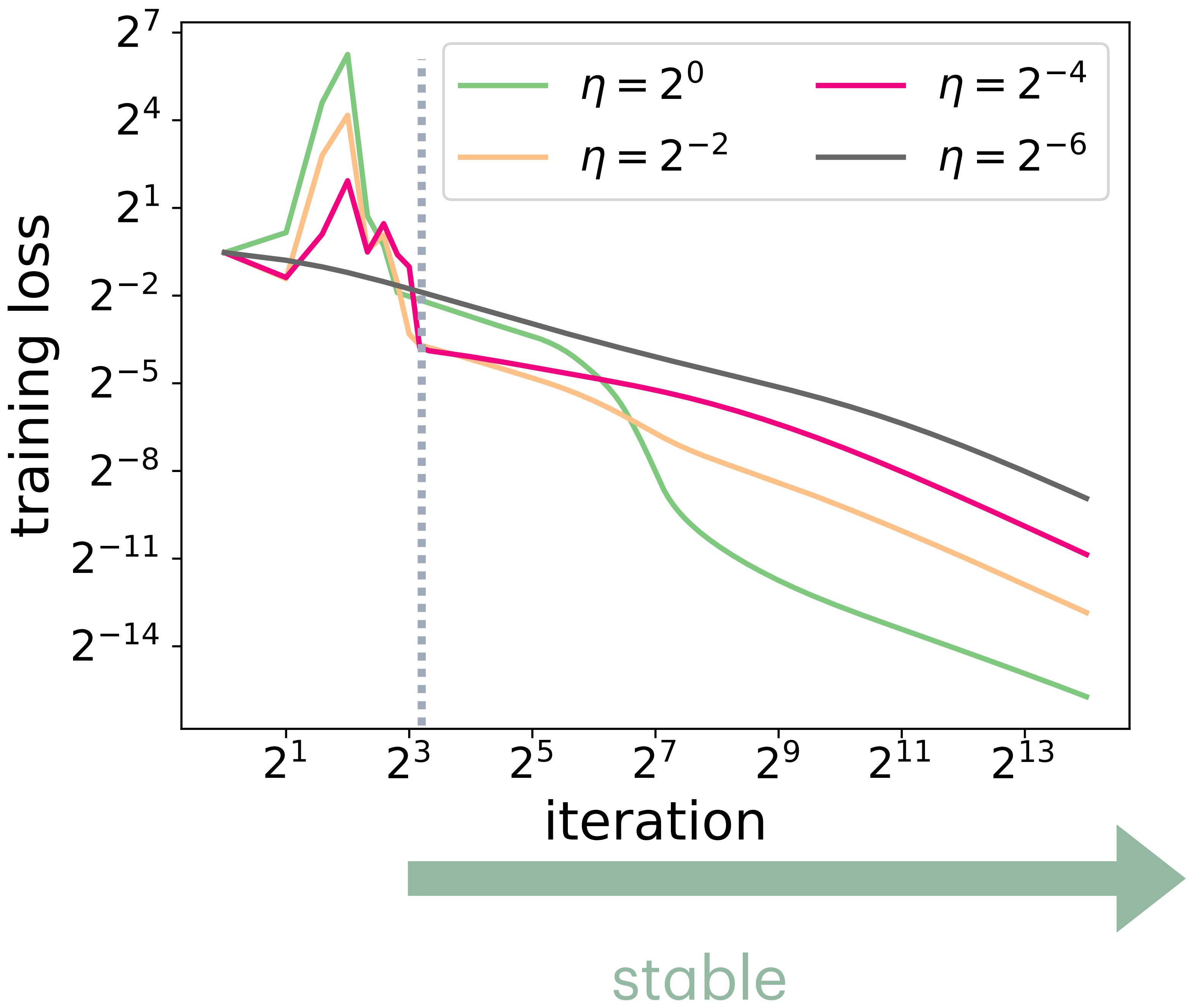
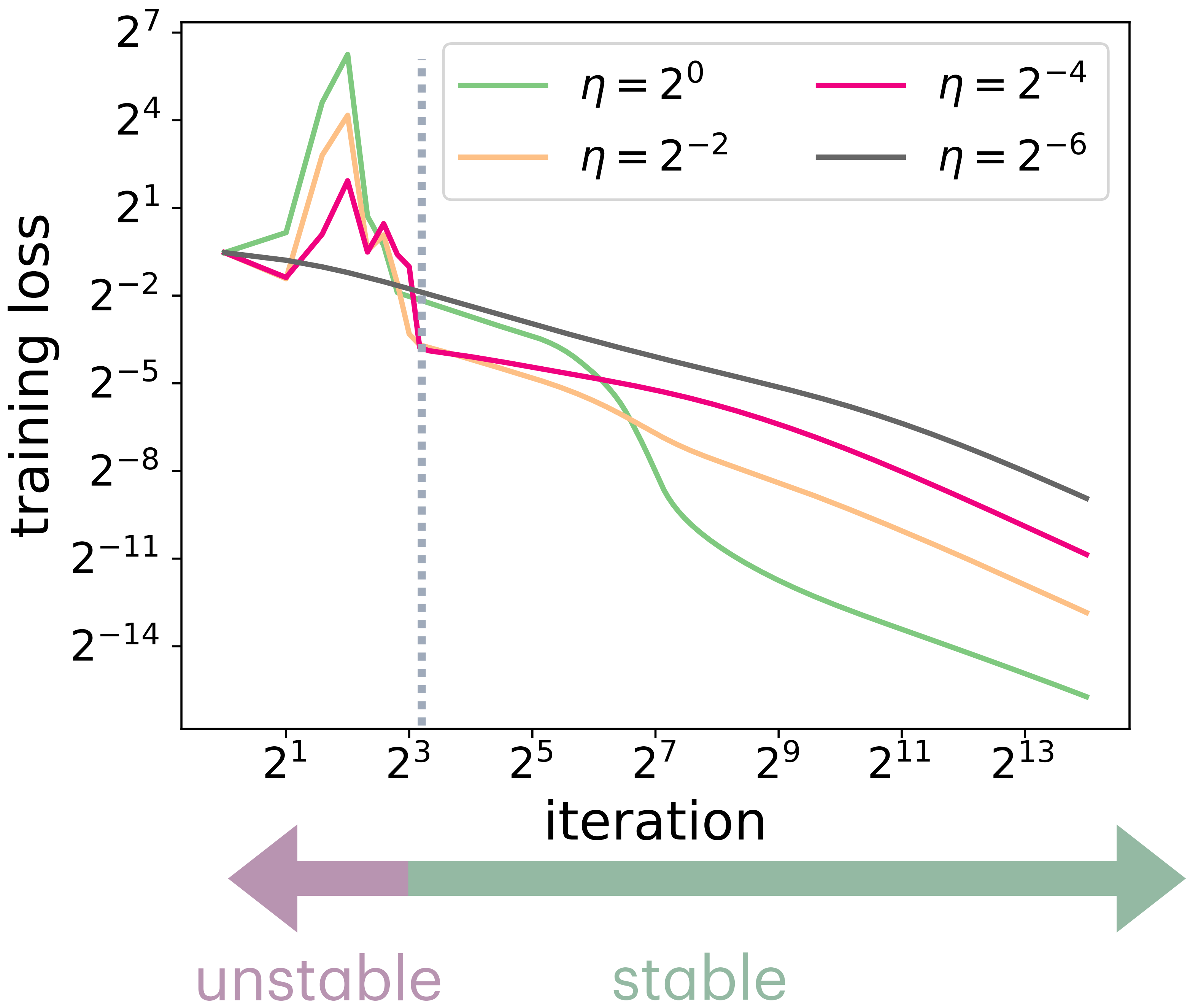


s-th step is in stable phase if $L(\theta_t) \downarrow$ for all $t \geq s$

(1/3) Logistic regression



s-th step is in stable phase if $L(\theta_t) \downarrow$ for all $t \geq s$

unstable phase if otherwise

(1/3) Theorem

Unstable phase.

Phase transition.

Stable phase.

Wu, Bartlett, Telgarsky, Yu. “Large stepsize gradient descent for logistic loss: non-monotonicity of the loss improves optimization efficiency.” COLT 2024

(1/3) Theorem

Unstable phase.

$$\text{for any } \eta \text{ and } t, \quad \frac{1}{t}\sum_{k=0}^{t-1} L(\theta_k) = \tilde{O}\left(\frac{1+\eta^2}{\eta t}\right)$$

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"flow rate"

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(1/3) Effects of large stepsize

1. Asymptotic $1/(\eta t)$ rate $\Rightarrow$ 2x stepsize 2x faster

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acceleration by large stepsize

Wu, Bartlett, Telgarsky, Yu. "Large stepsize gradient descent for logistic loss: non-monotonicity of the loss improves optimization efficiency." COLT 2024

(1/3) A “non-quadratic” picture

$\exists$ unit vector θ^*, $\min_i y_i x_i^\top \theta^* > \gamma > 0$

$L(\theta) = \hat{\mathbb{E}} \ln\big(1 + \exp(-y x^\top \theta)\big)$

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***minimizer at* ∞**

$\lim_{\lambda \to \infty} L(\lambda\theta^*) = 0$

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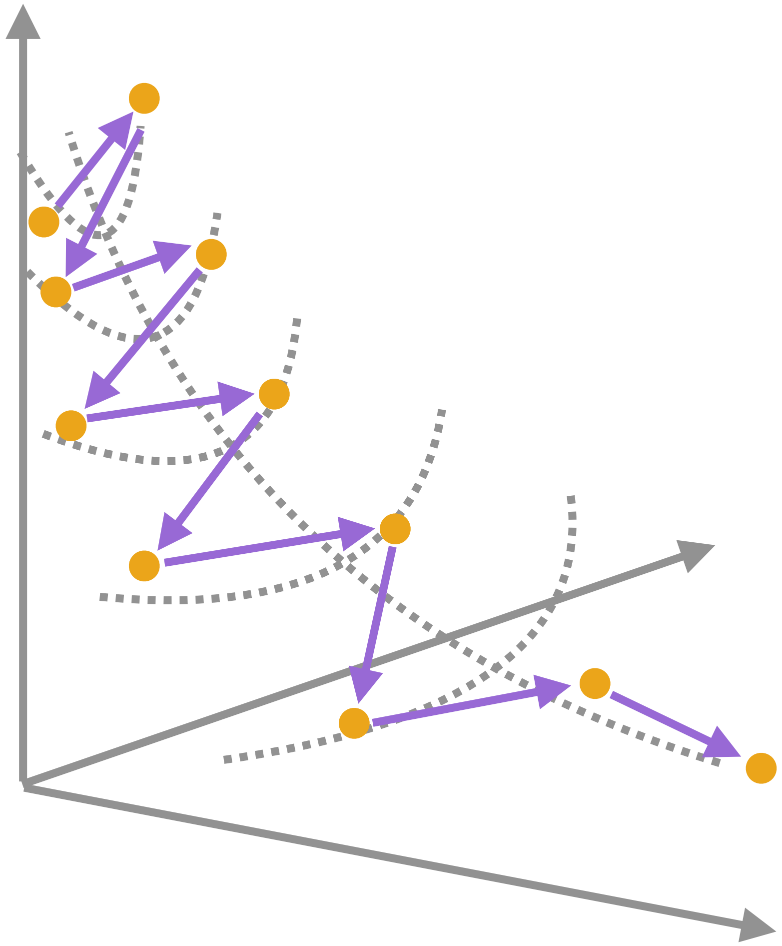

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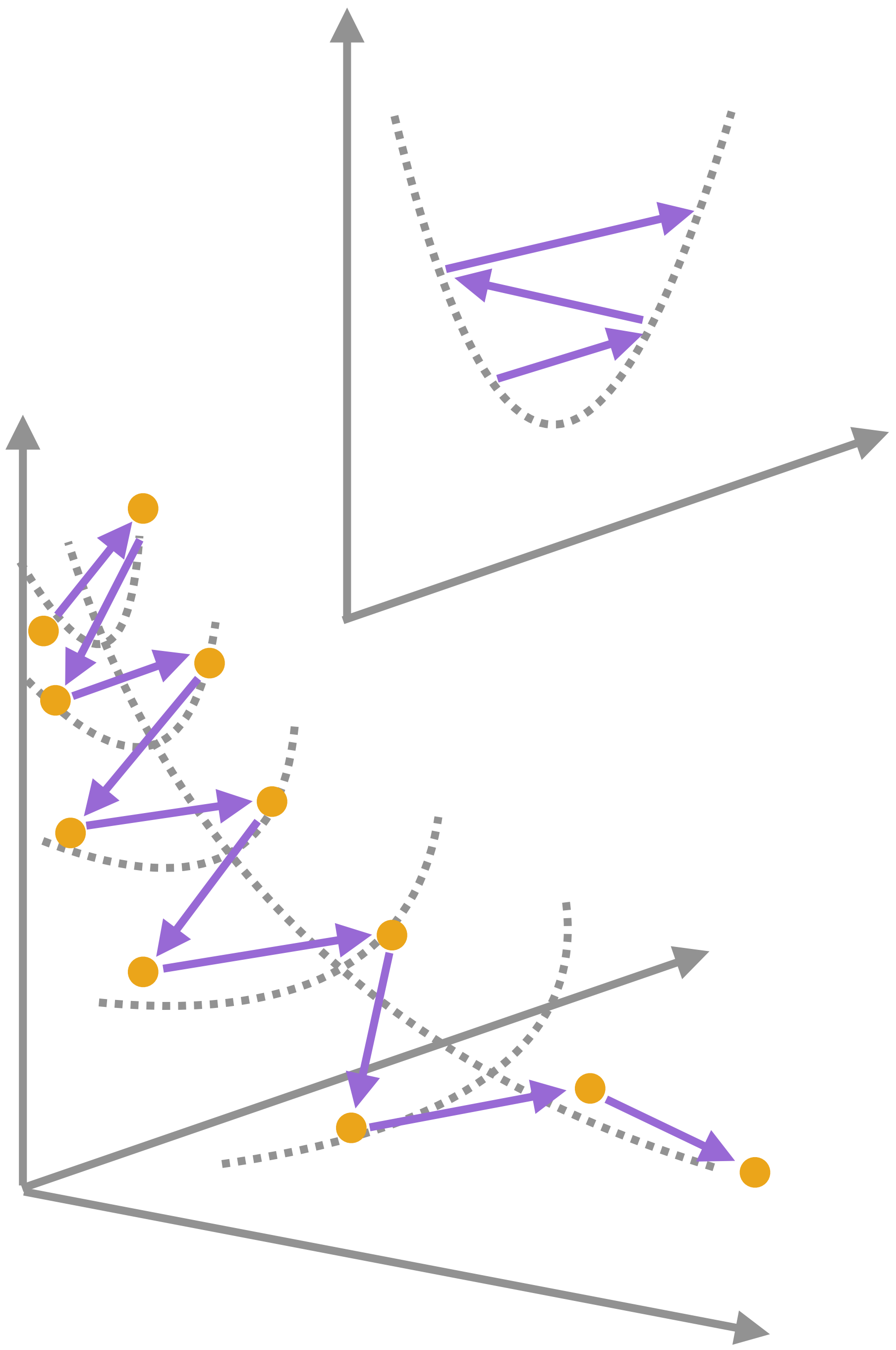

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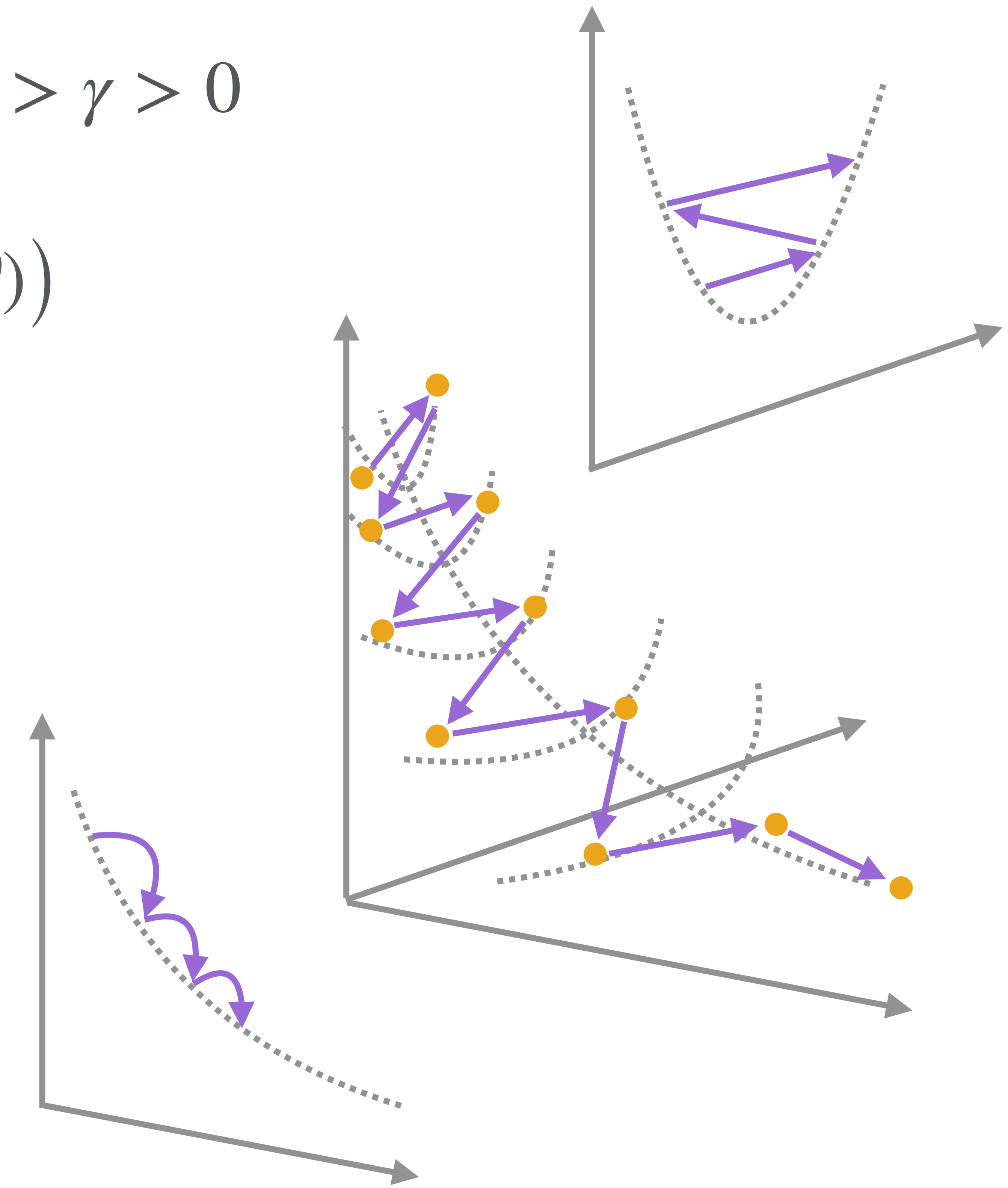

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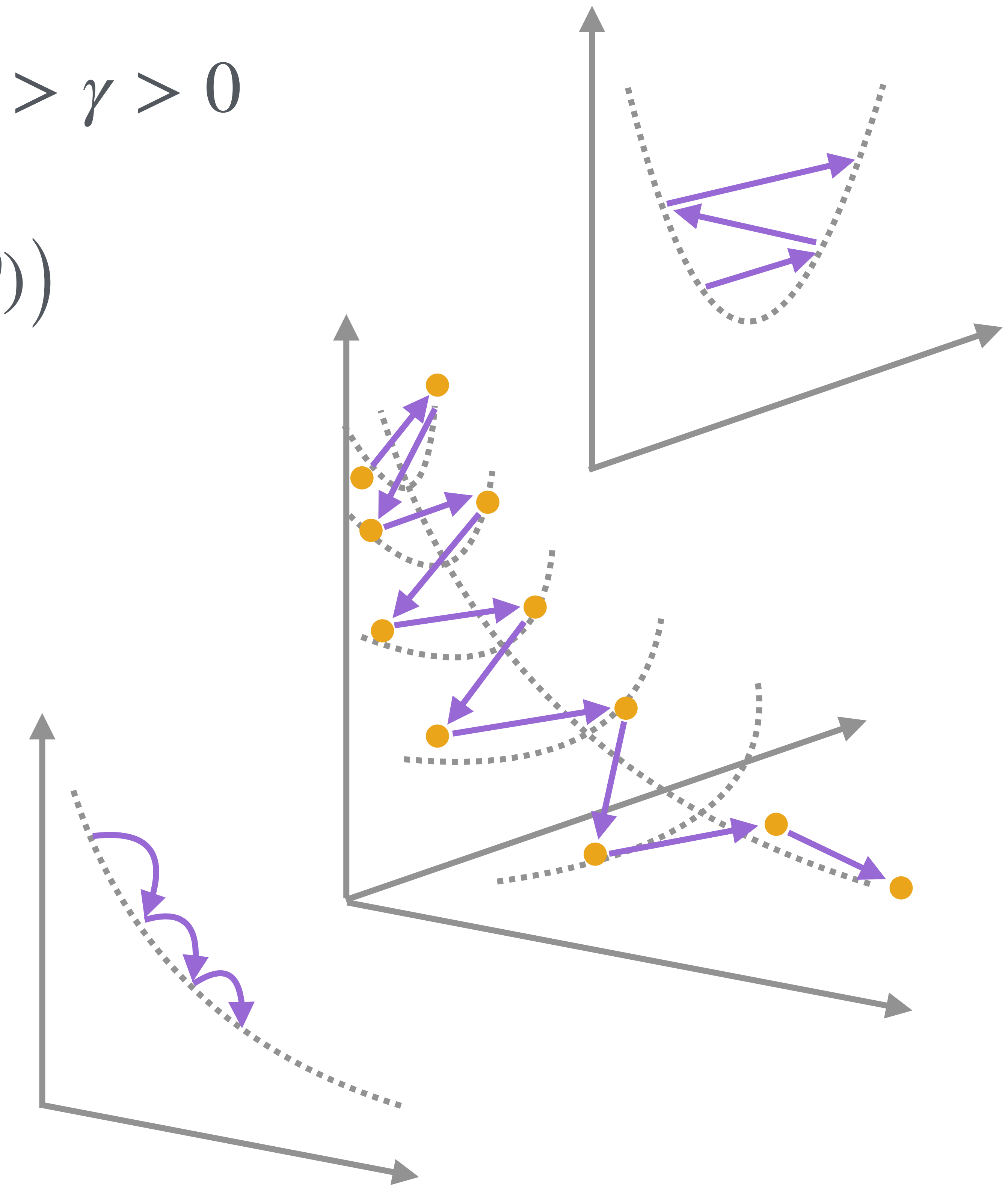
self-bounded

$\|\nabla^2 L\| \leq L$



Two extensions

minimizer at ∞

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finite minimizer

e.g. regularization

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enabling "tricks"

e.g. adaptive GD
[Ji & Telgarsky 2021]

Ji & Telgarsky. "Characterizing the implicit bias via a primal-dual analysis." ALT 2021.

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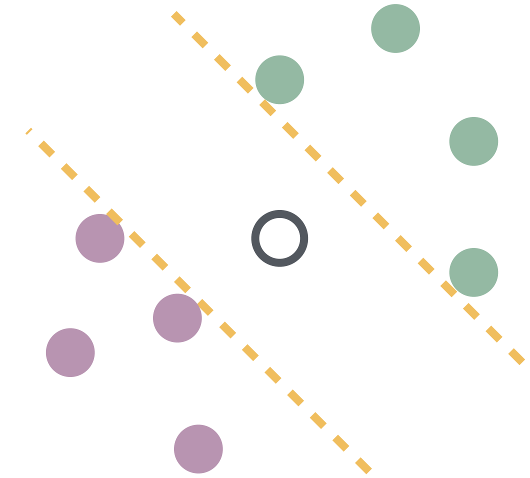
large stepsizes for GD variants

Ji & Telgarsky. "Characterizing the implicit bias via a primal-dual analysis." ALT 2021.

(2/3) Large, adaptive stepsize



$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i x_i^\top \theta) \qquad \ell(t) = \ln\big(1 + \exp(-t)\big)$$

$$\begin{aligned}\theta_{t+1} &= \theta_t - \eta\big((-\ell^{-1})' \circ L(\theta_t)\big)\,\nabla L(\theta_t) \\ &\approx \theta_t - \frac{\eta}{L(\theta_t)}\nabla L(\theta_t)\end{aligned}$$

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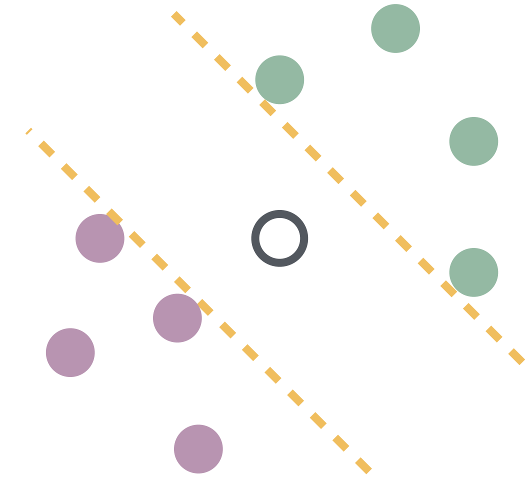

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adapt to curvature

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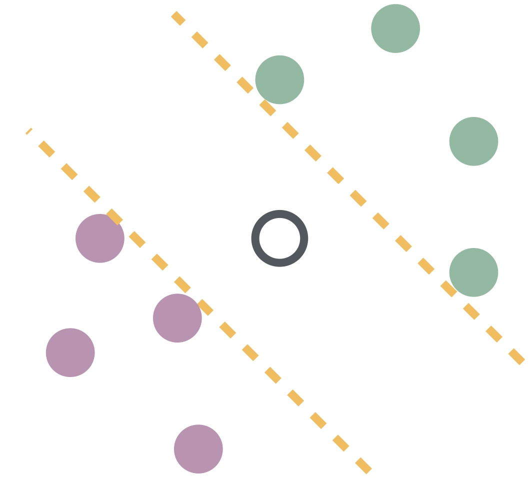

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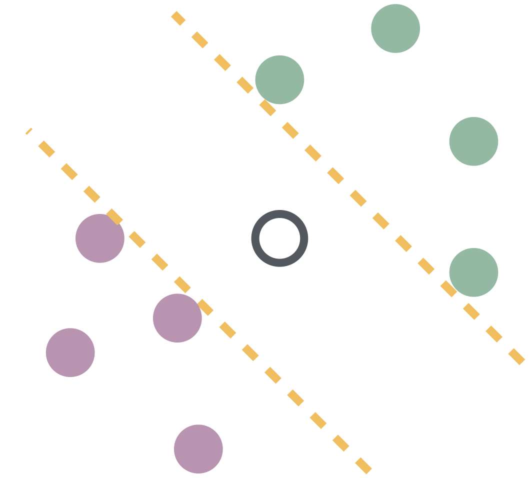

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[Ji & Telgarsky, 2021]

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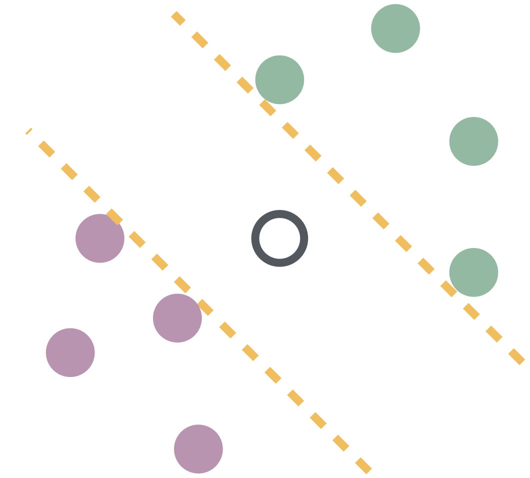

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[Ji & Telgarsky, 2021]

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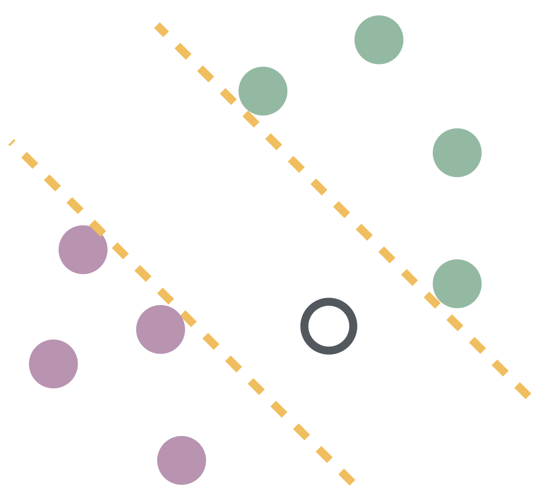
large stepsize makes adaptive GD even faster

(2/3) Theorem

Assume separability with margin γ. For $t \geq 1/\gamma^2$ and every η

$$L(\bar{\theta}_t) \leq \exp\Big(- \Theta(\gamma^2 \eta t)\Big), \quad \text{where } \bar{\theta}_t = \frac{1}{t} \sum_{k=1}^{t} \theta_k$$



Zhang, **Wu**, Lin, Bartlett. "Minimax optimal convergence of gradient descent in logistic regression via large and adaptive stepsizes." ICML 2025

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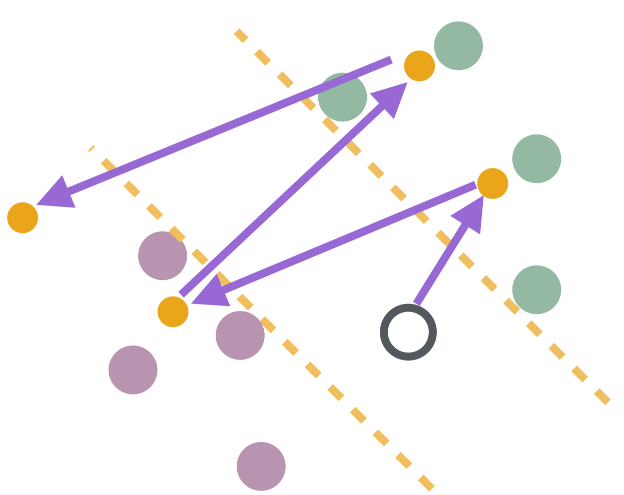

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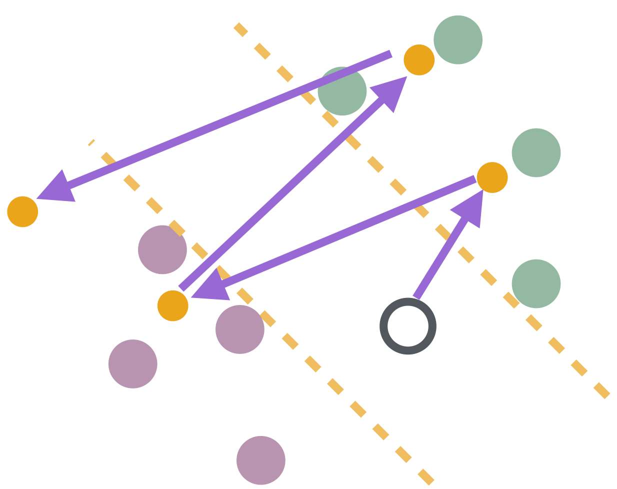

arbitrarily small error in $1/\gamma^2$ steps

$$\lim_{\eta \to \infty} L(\bar{\theta}_t) = 0 \quad \text{for} \quad t = 1/\gamma^2$$

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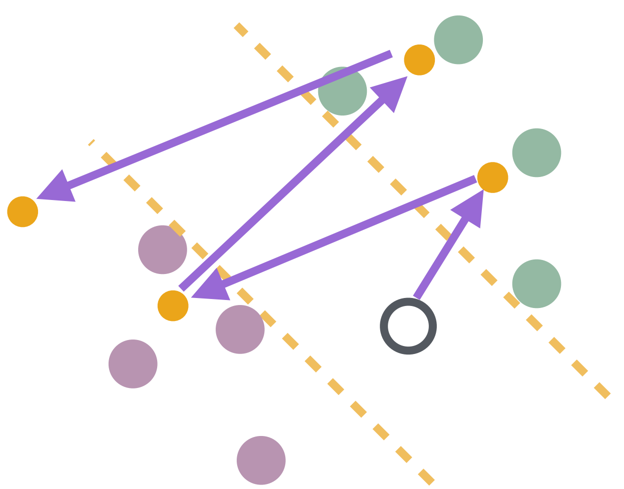

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matching "Perceptron"
[Novikoff, 1962, or earlier]

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(2/3) Theorem (lower bound)

$\forall \theta_0$, $\exists\ (x_i, y_i)_{i=1}^n$ with margin γ such that: for any first-order batch method

$$\min_i y_i x_i^\top \theta_t > 0 \ \Rightarrow\ t \geq \Omega(1/\gamma^2)$$

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first-order batch method:

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where $L(\theta) = \hat{\mathbb{E}} \ell(y x^\top \theta)$ for any ℓ

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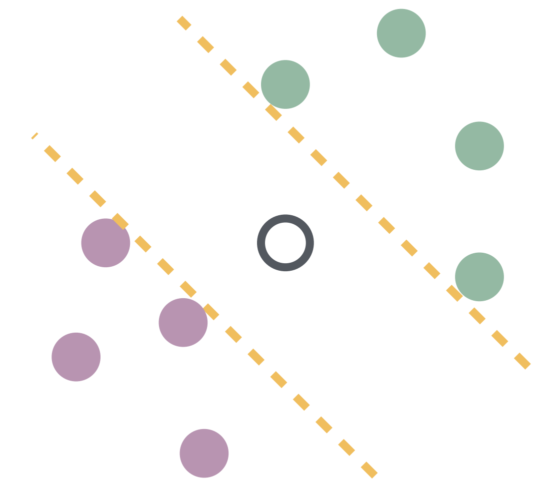
large, adaptive stepsizes = minimax optimal

Zhang, **Wu**, Lin, Bartlett. "Minimax optimal convergence of gradient descent in logistic regression via large and adaptive stepsizes." ICML 2025

(3/3) ℓ_2-regularization



$$\tilde{L}(\theta) = L(\theta) + \frac{\lambda}{2}\|\theta\|^2 \qquad L(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ln\left(1 + \exp(-y_i x_i^\top \theta)\right)$$

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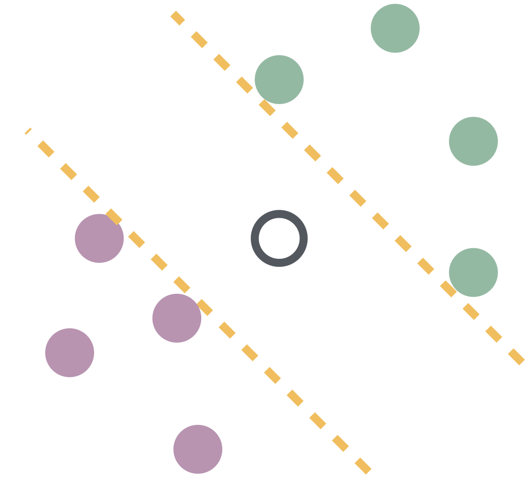

$\Theta(1)$-smooth, λ-strongly convex

condition number $\kappa = \Theta(1/\lambda)$

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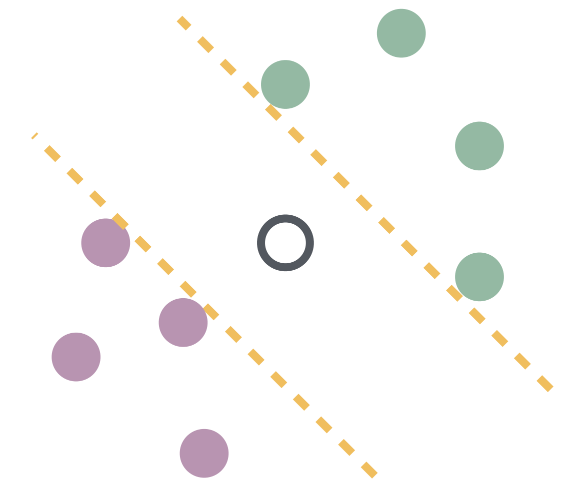

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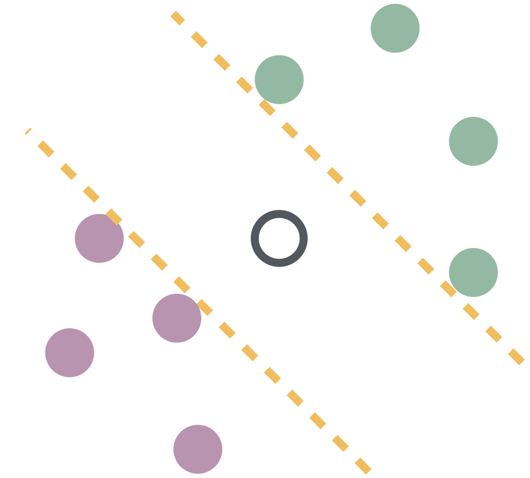
finite minimizer $\tilde{\theta}$ with norm $||\tilde{\theta}|| = O(\ln \kappa)$

(3/3) ℓ_2-regularization



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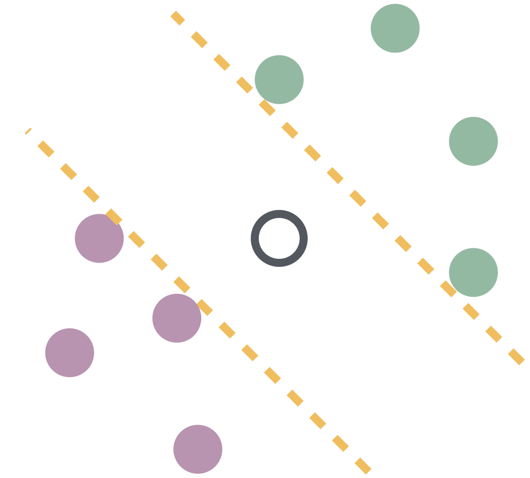
GD $\quad \theta_{t+1} = \theta_t - \eta \nabla \tilde{L}(\theta_t)$

(3/3) ℓ_2-regularization



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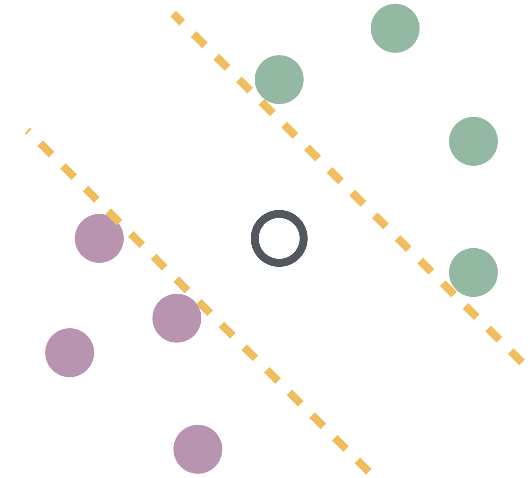
GD $\quad \theta_{t+1} = \theta_t - \eta \nabla \tilde{L}(\theta_t)$

Classical theory

For $\eta = \Theta(1)$, $\tilde{L}(\theta_t) \downarrow$ and $\tilde{L}(\theta_t) - \min \tilde{L} \le \epsilon$ for $t = O(\kappa \ln(1/\epsilon))$

(3/3) ℓ_2-regularization



$\Theta(1)$-smooth, λ-strongly convex

condition number $\kappa = \Theta(1/\lambda)$

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improved to $\tilde{O}(\sqrt{\kappa})$ by Nesterov

(3/3) Theorem

Let $\kappa = 1/\lambda$. Assume separability and

$$\lambda \leq \Theta\left(\frac{1}{n \ln n}\right) \qquad \eta \leq \Theta\big(\min\{\sqrt{\kappa}, \kappa/n\}\big)$$

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from $\tilde{O}(\kappa)$ to $\tilde{O}(\sqrt{\kappa})$: acceleration via large stepsize

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(3/3) Theorem

for $\lambda \le \Theta(1)$, improvement is $\tilde{O}(\kappa^{2/3})$

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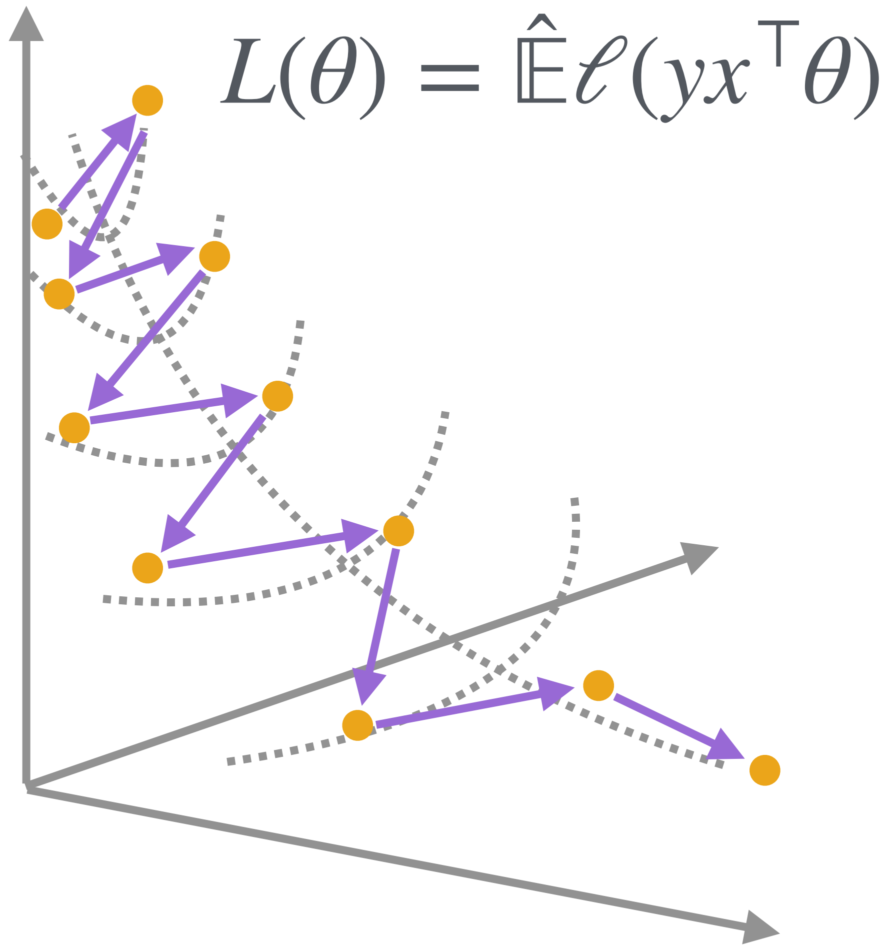
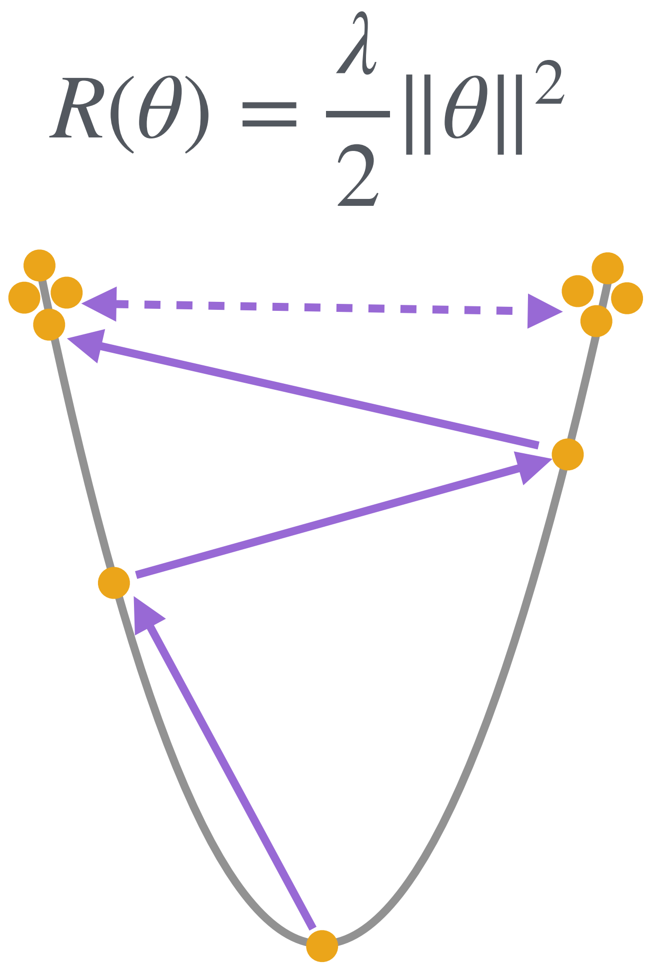
(3/3) Picture: valley + basin





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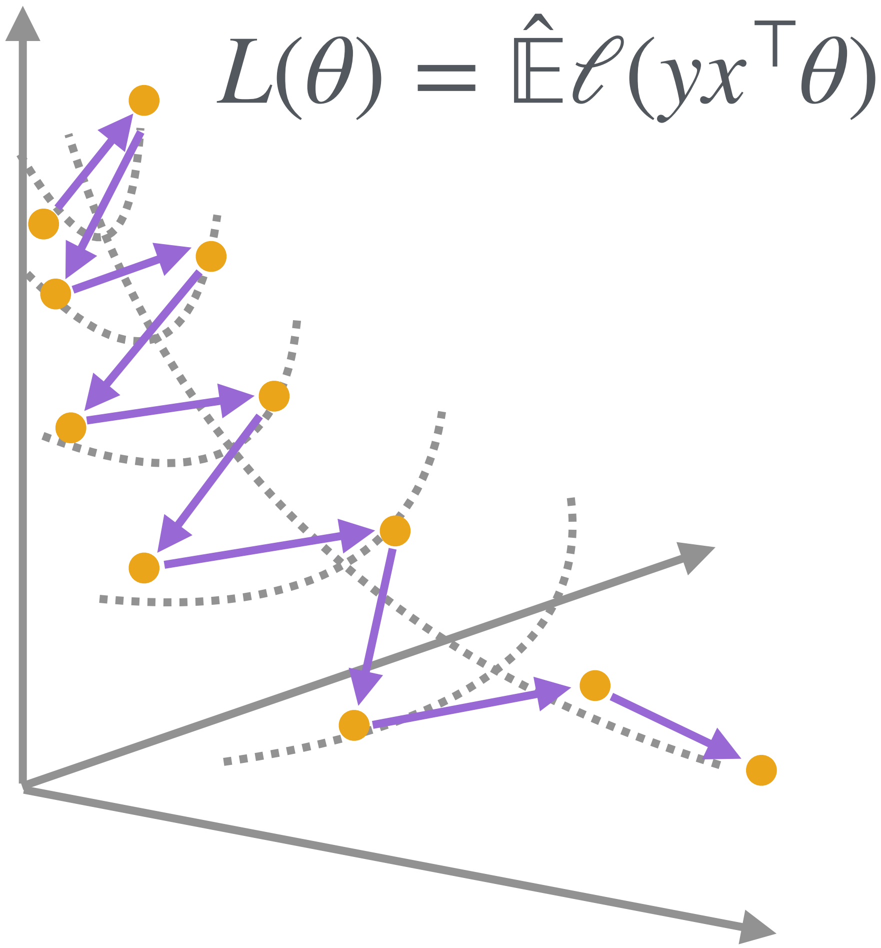

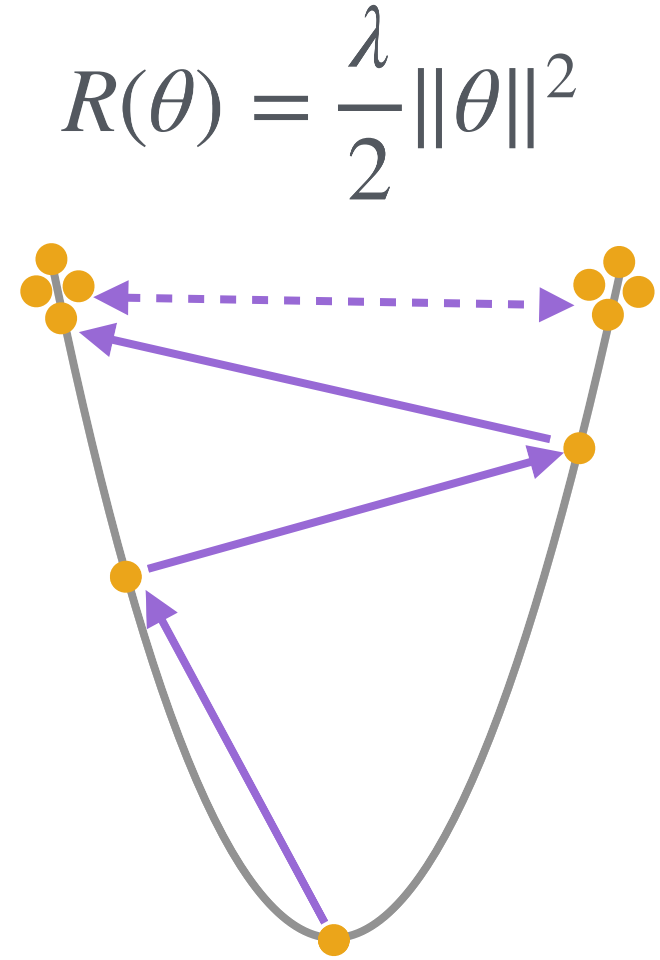

Unstable. $\tilde{L} \approx L$, $R \leq \Theta(1)$, "overshoot"

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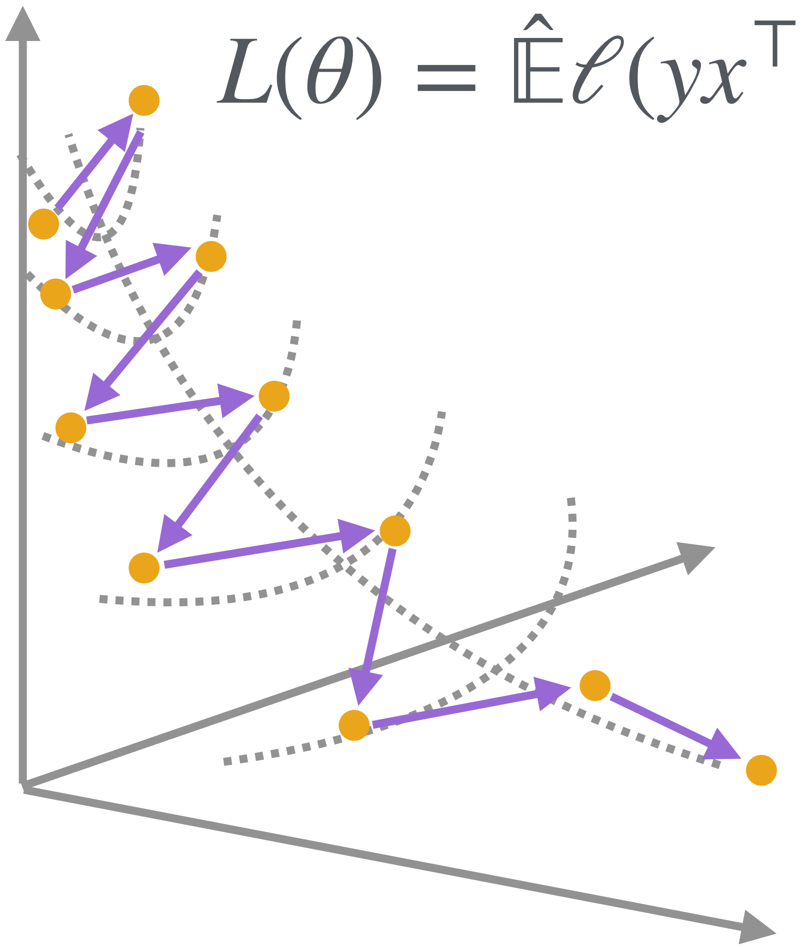
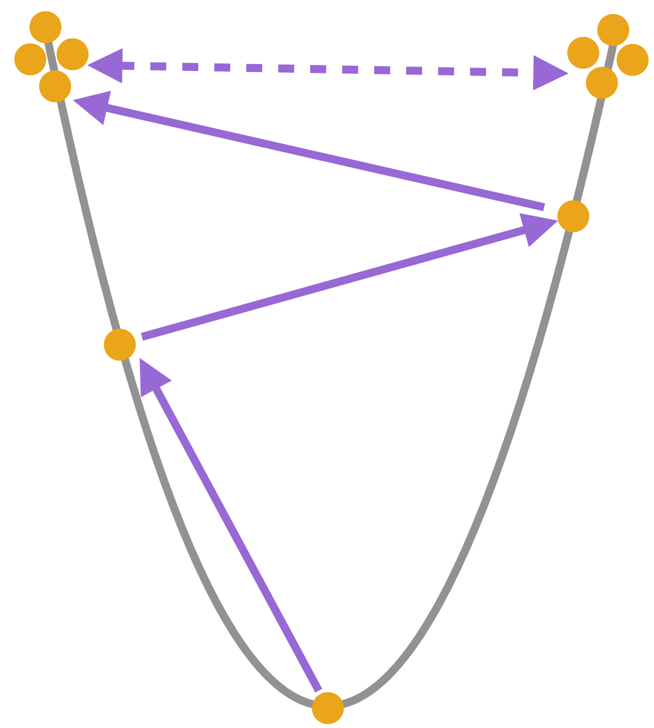
$$L(\theta) = \hat{\mathbb{E}}\ell(yx^\top\theta)$$



$$R(\theta) = \frac{\lambda}{2}\|\theta\|^2$$



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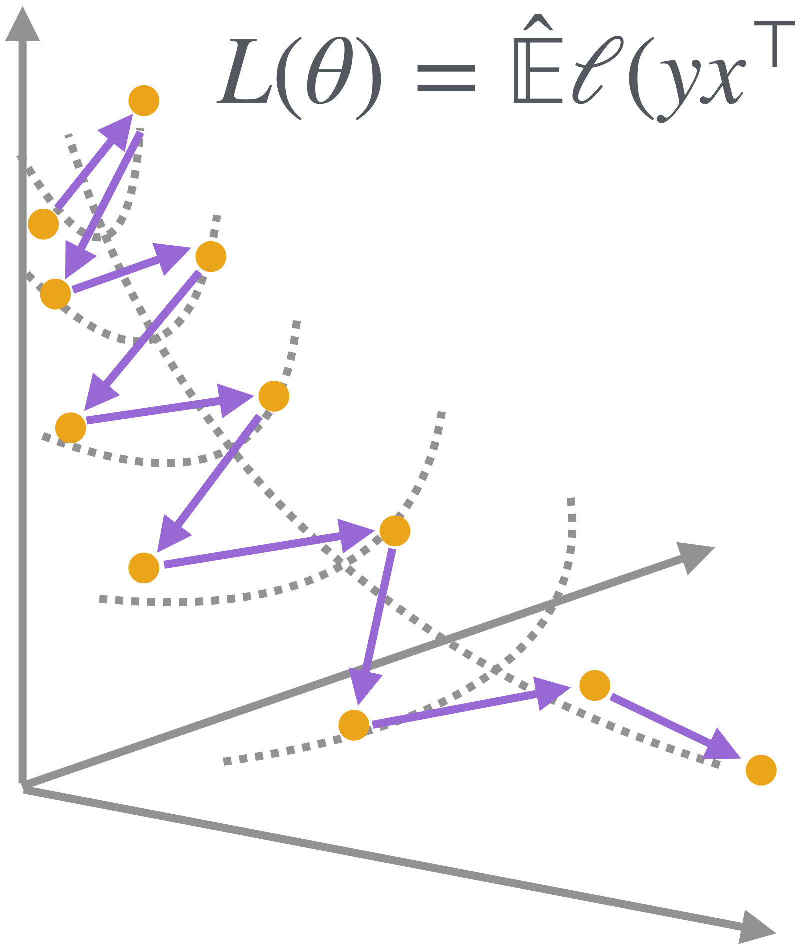

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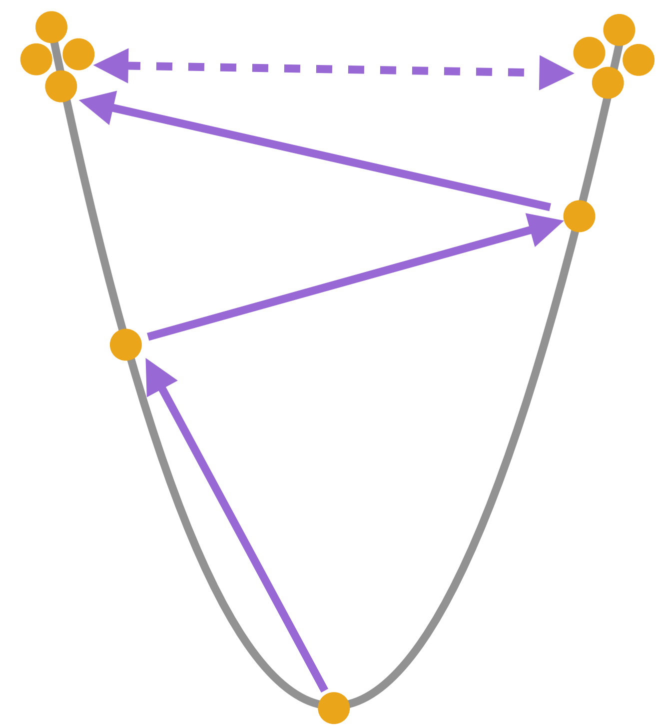

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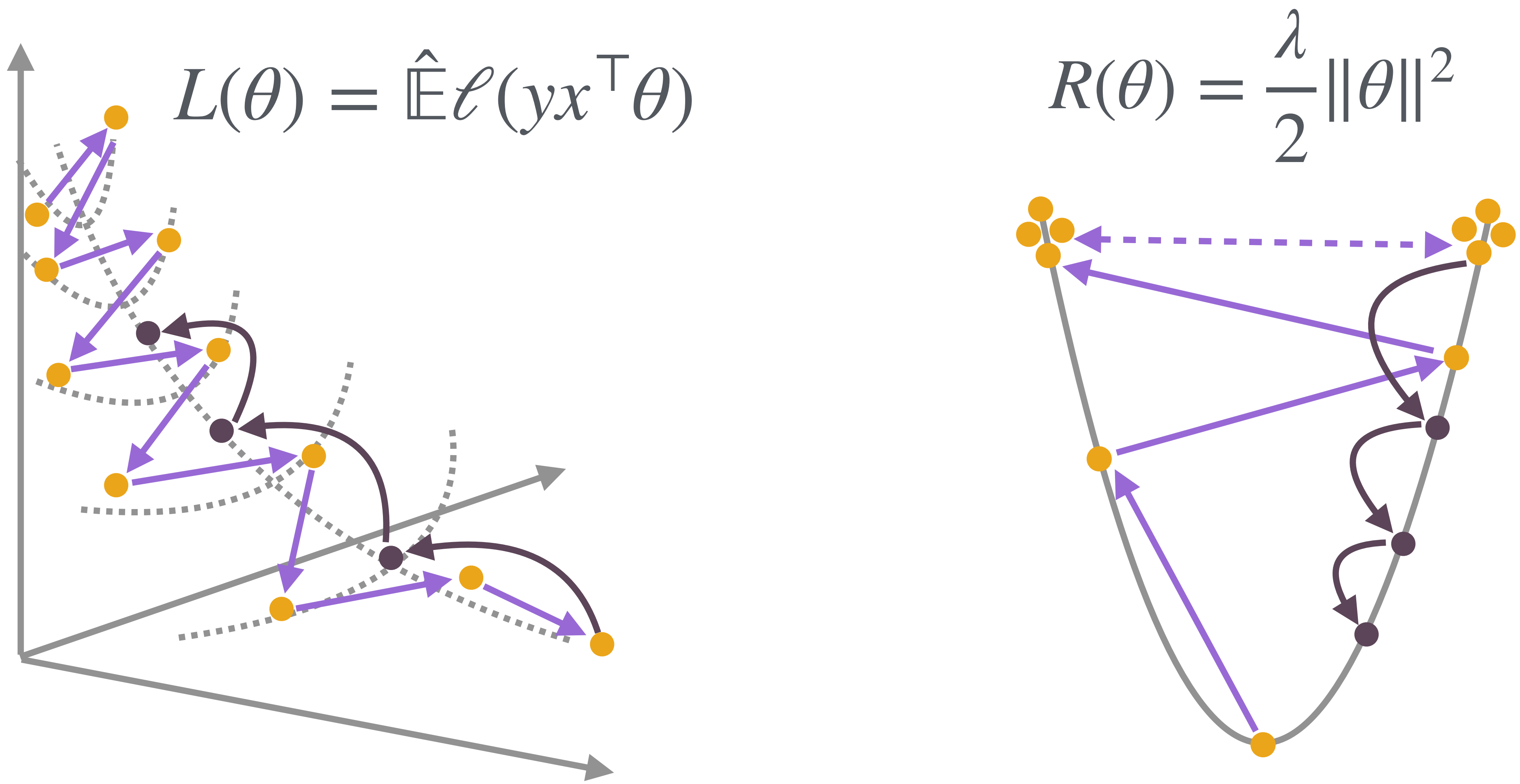

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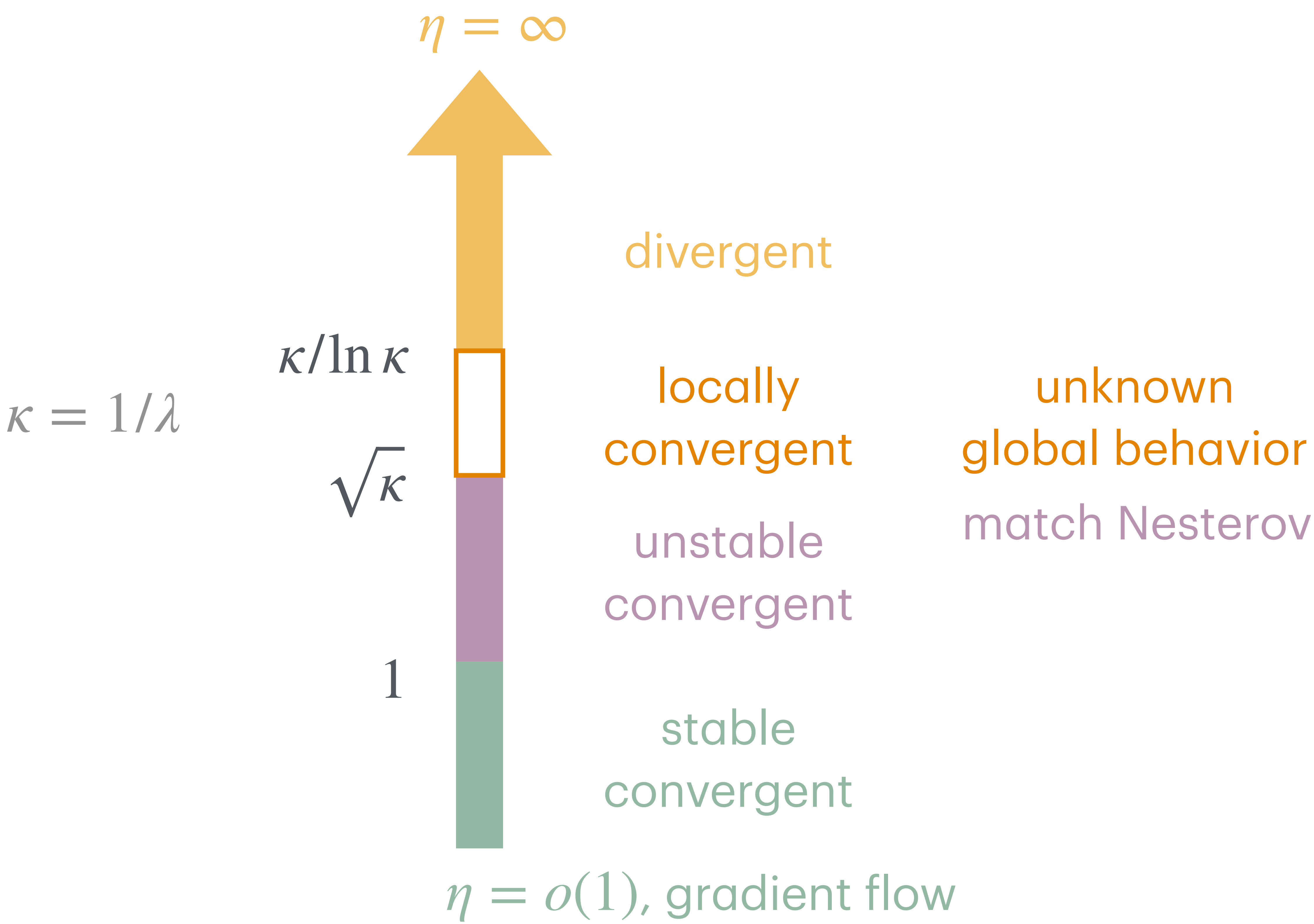
Stable. “move back” $\qquad \sup \|\theta_t\| = \Theta(\eta) = \mathrm{poly}(\kappa)$

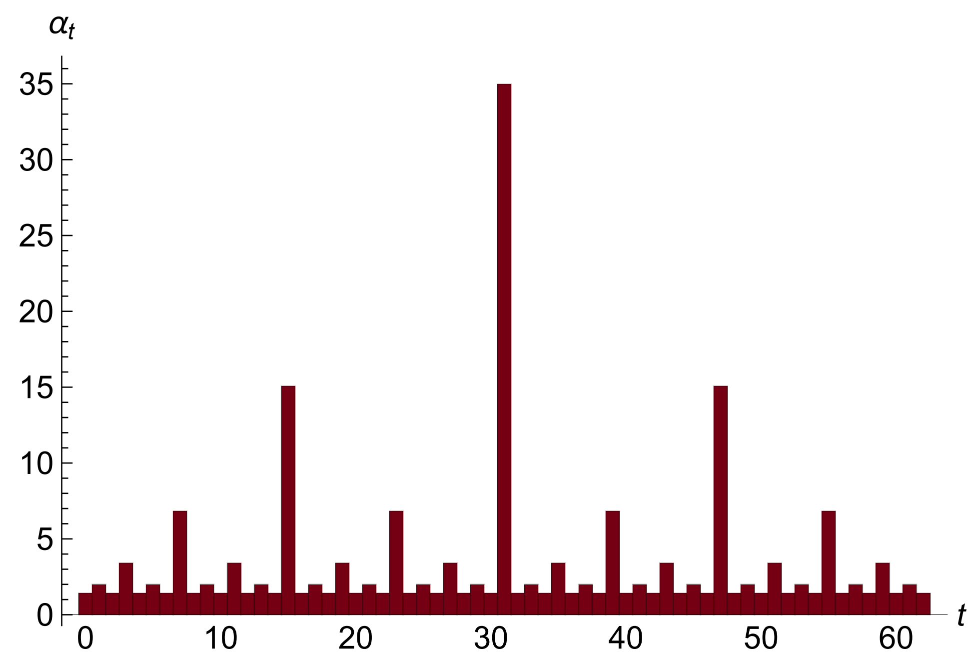
(3/3) Stepsize diagram



Related: long steps

Theorem. Let L be convex and smooth. For GD with *silver stepsize scheduler* $(\alpha_s)_{s\geq 0}$ and $t = 2^k - 1$, we have

$$L(\theta_t) - \min L = O(1/t^{1.27})$$



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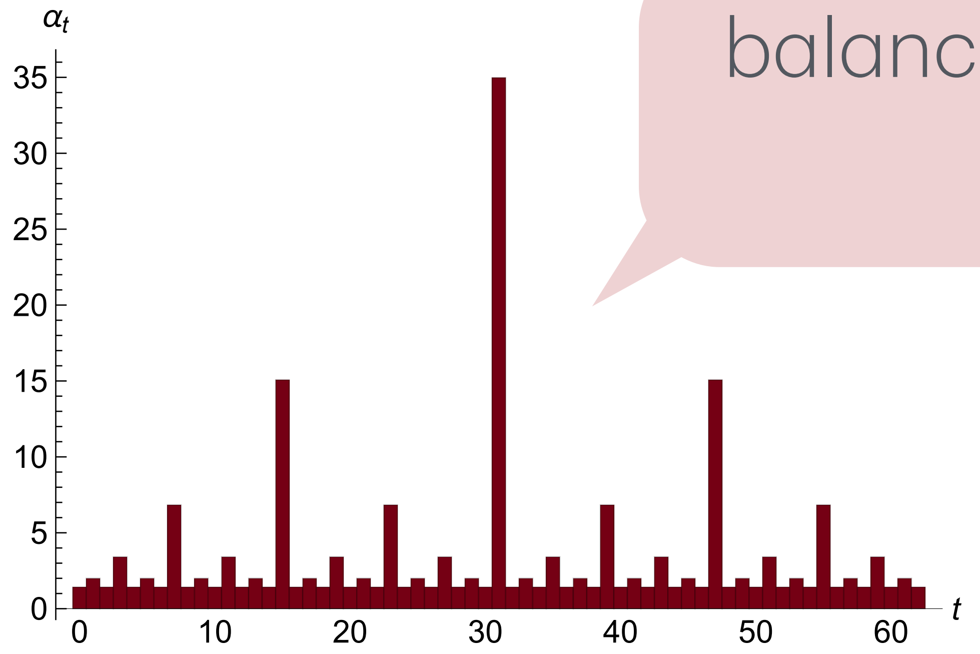

balance performance in high/low curvatures:
$0.5\theta^2$ vs Huber function

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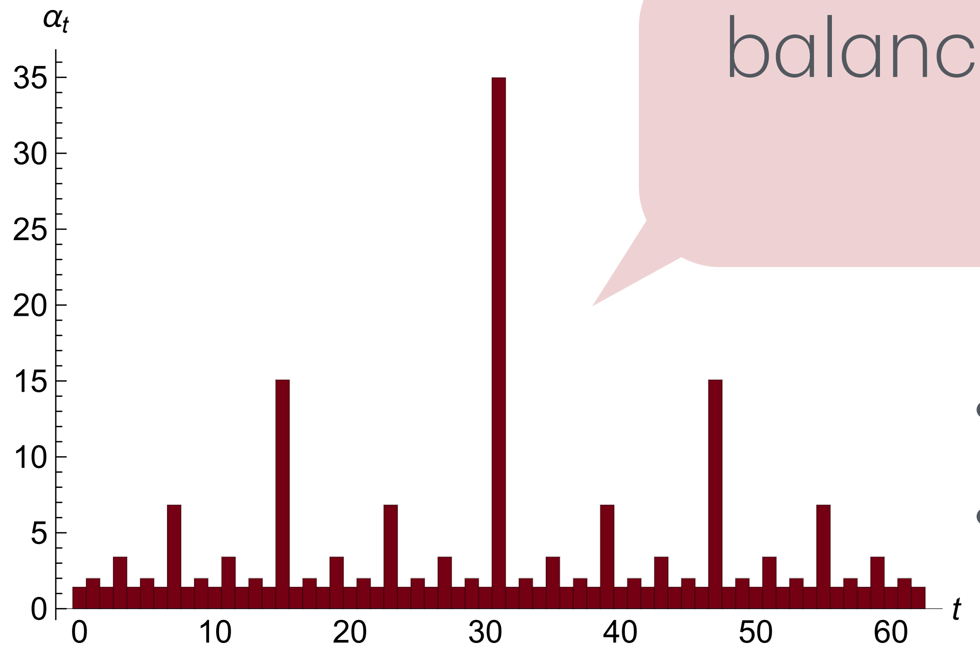

balance performance in high/low curvatures:
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- cover more problems, e.g., quadratics
- less practical stepsize scheduler

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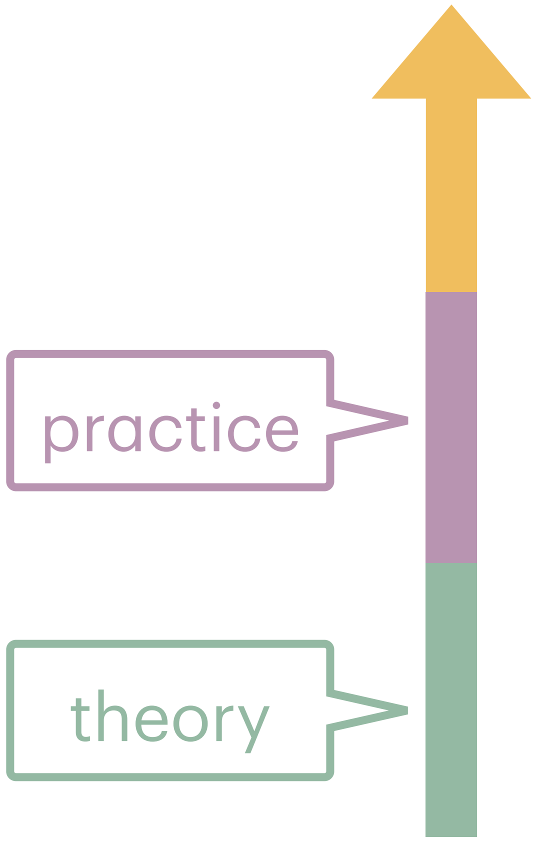
training instability caused by large stepsize



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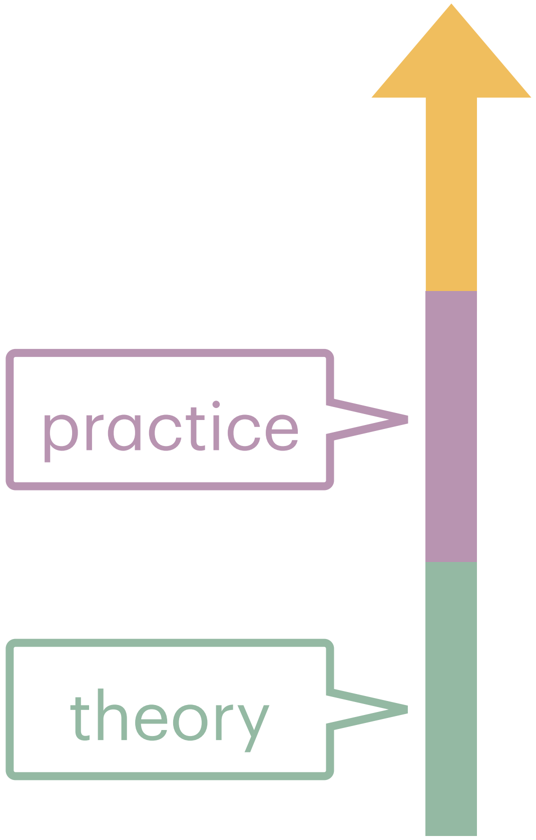

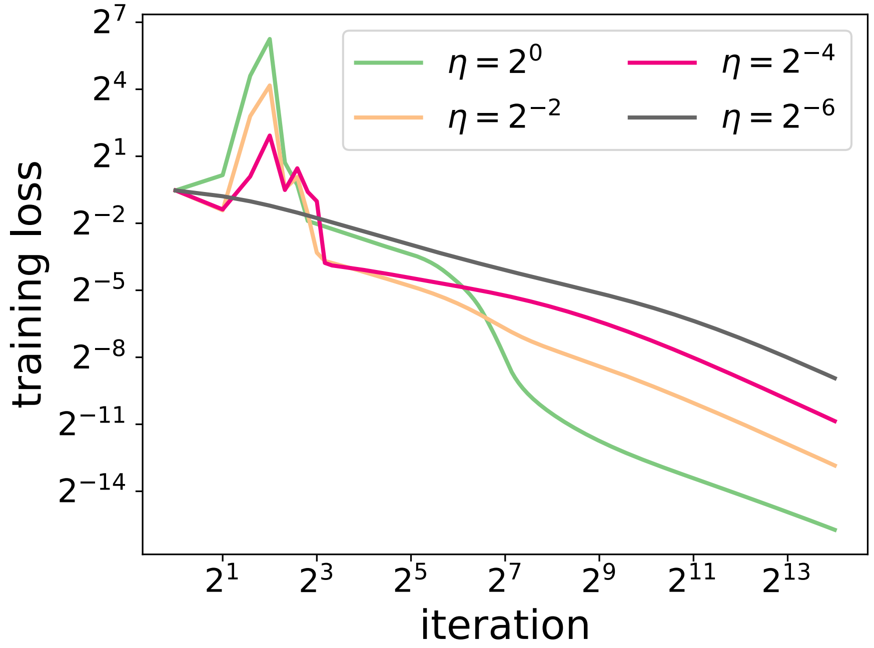

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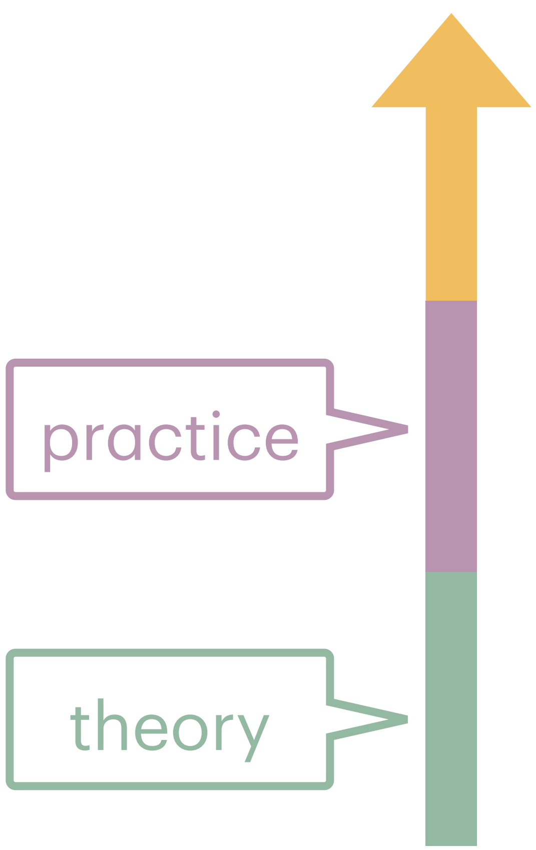

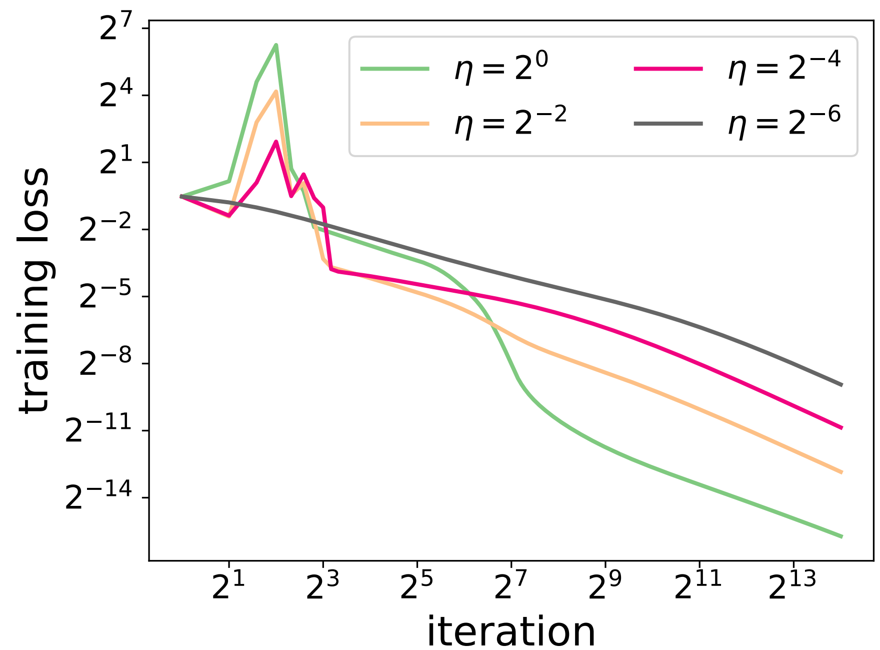

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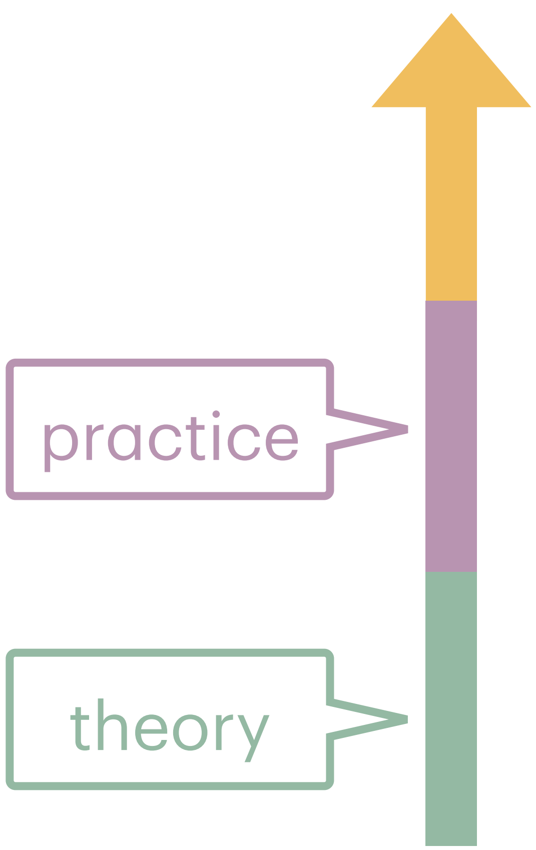

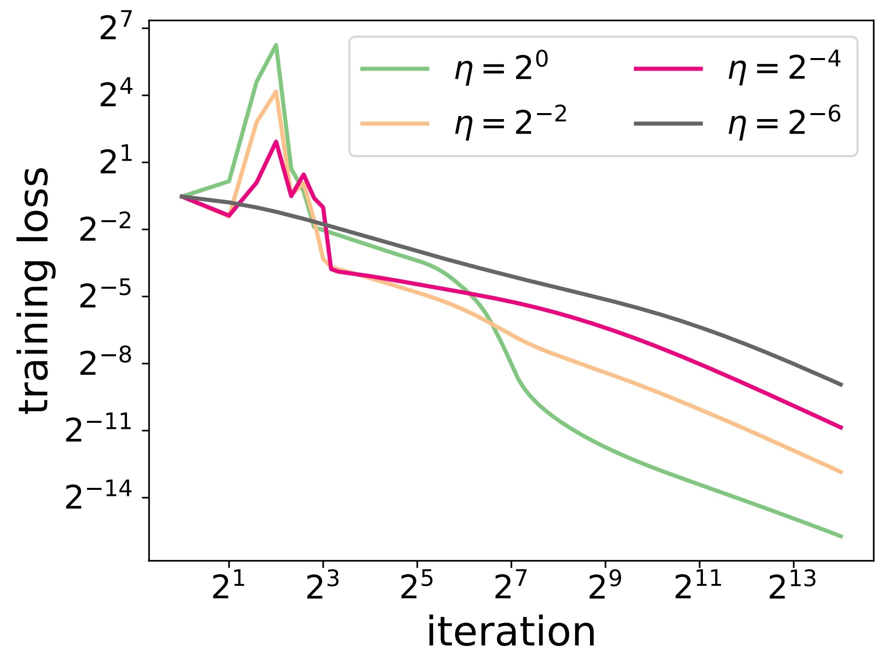

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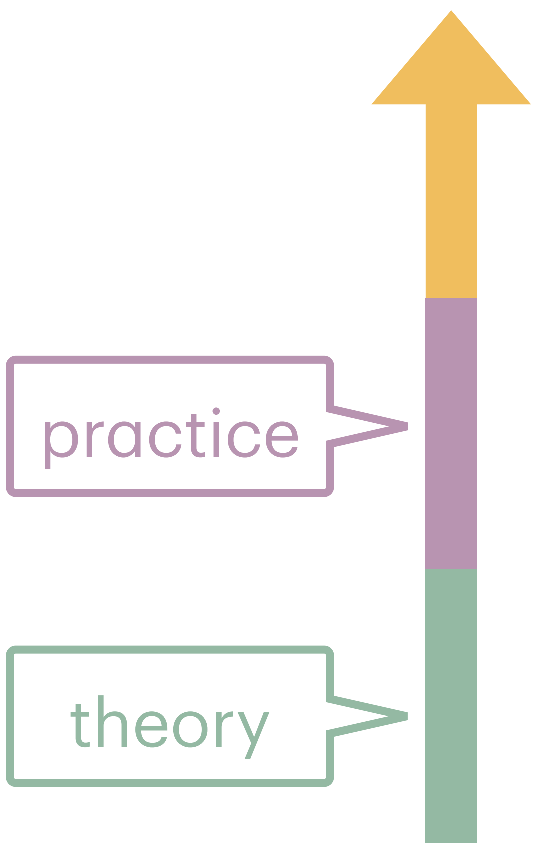

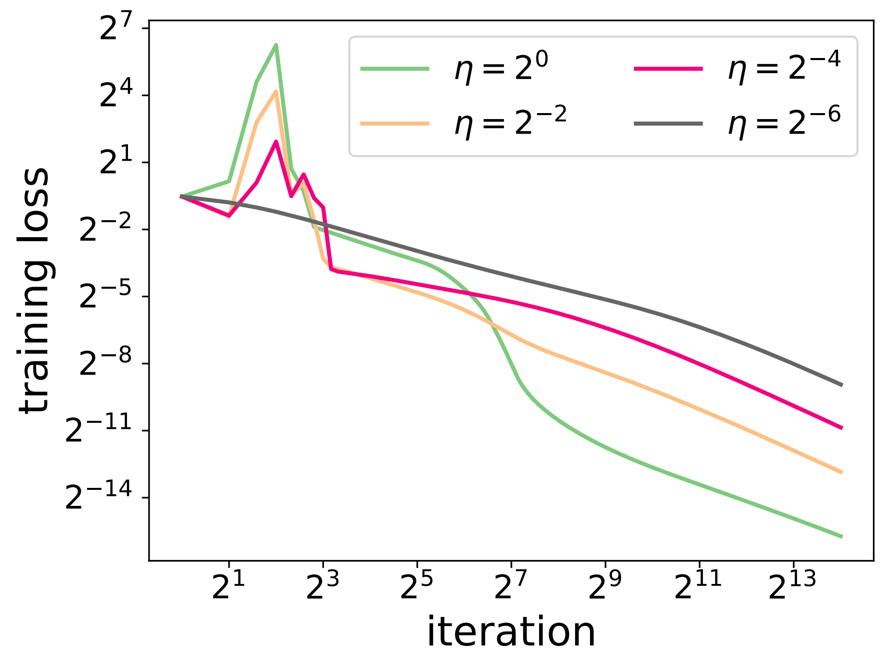

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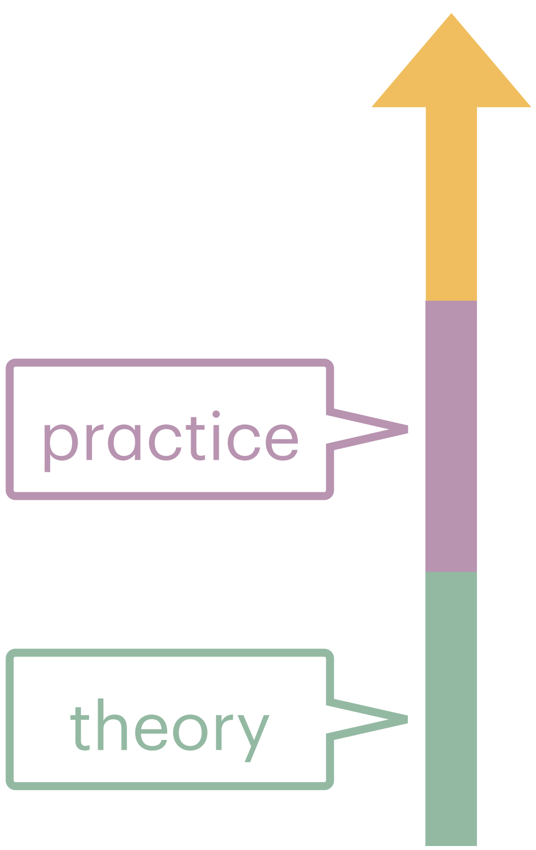

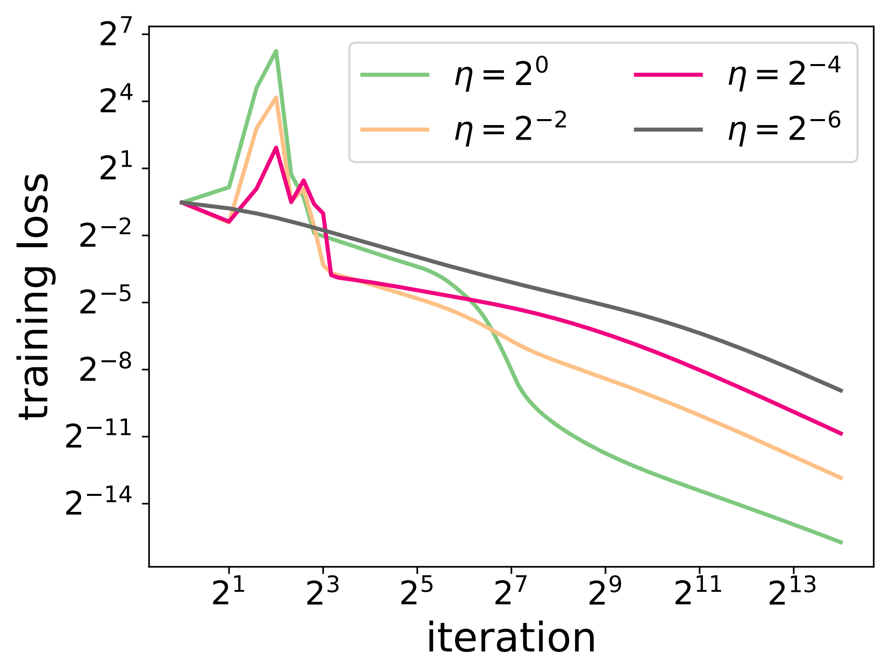

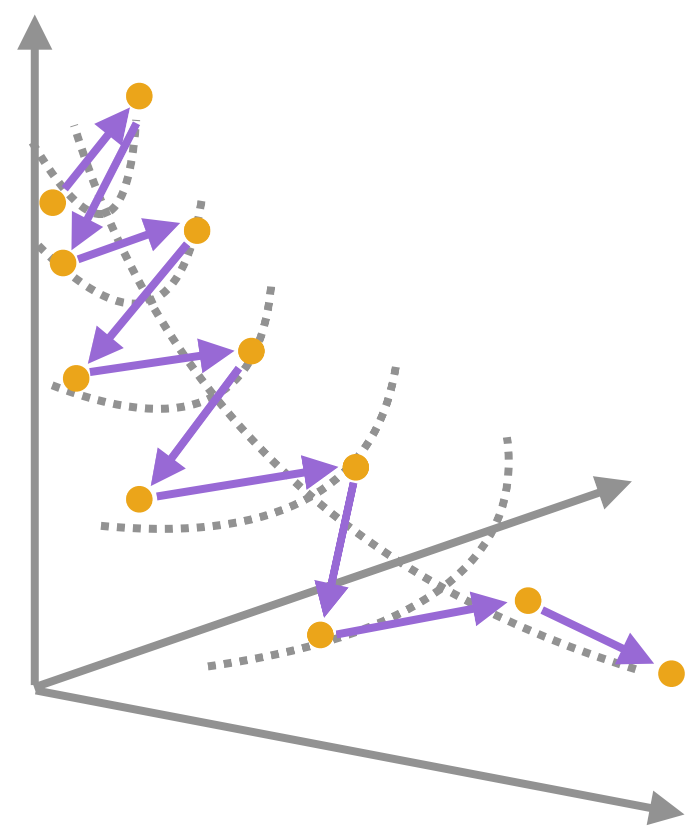

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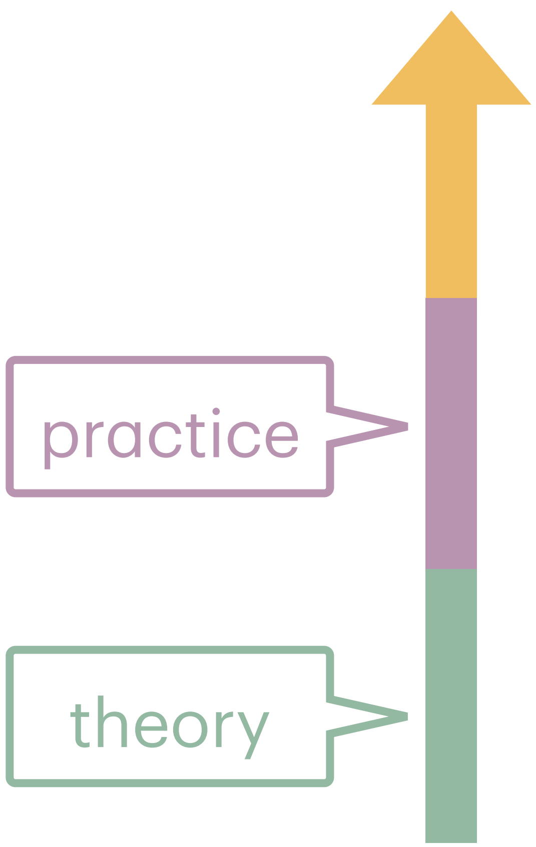
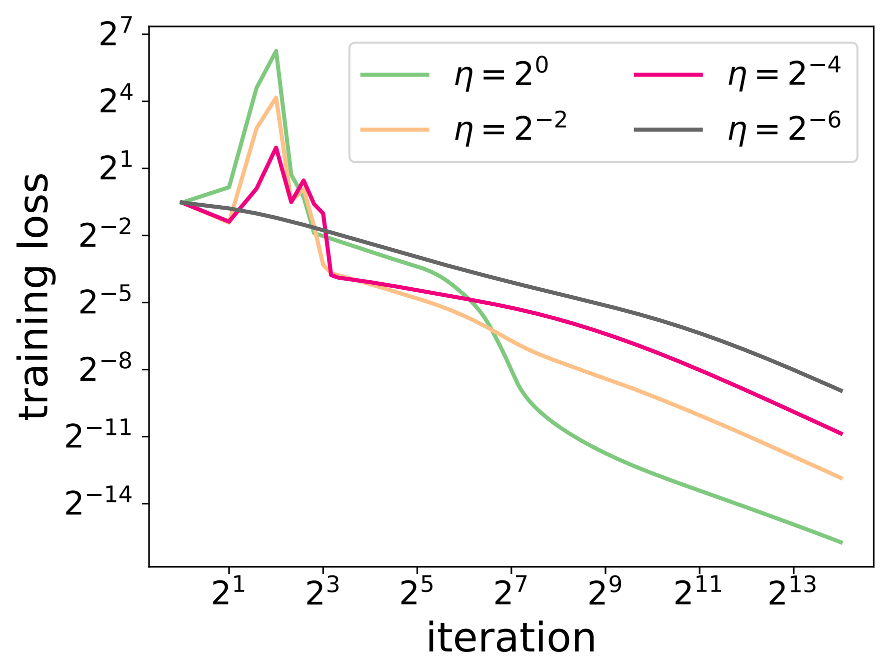
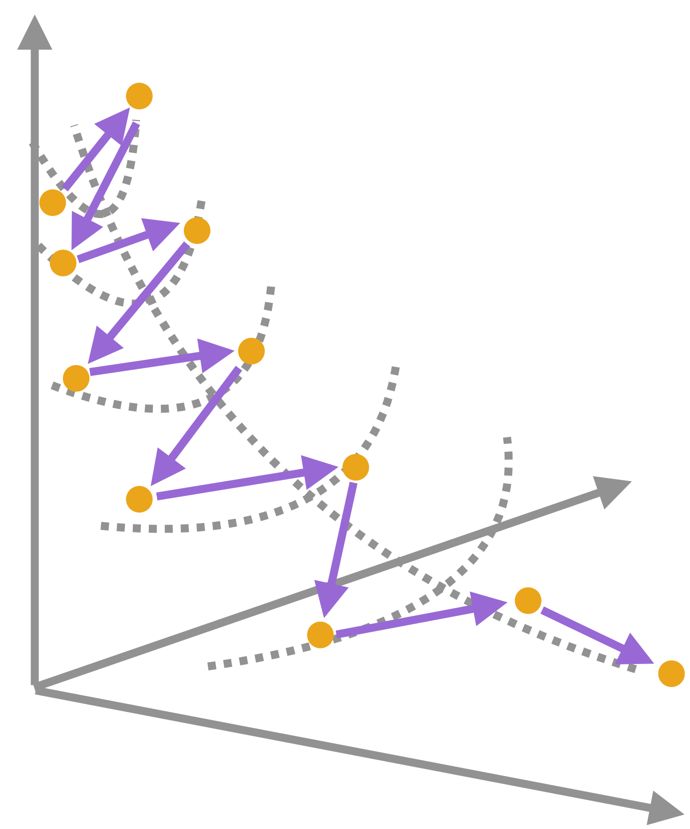
cross entropy, attention, ...







Open problems (set 1/2)

Call for clear, rigorous understanding on

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🤔 large stepsize for other optimizers, e.g., SGD, Adam?

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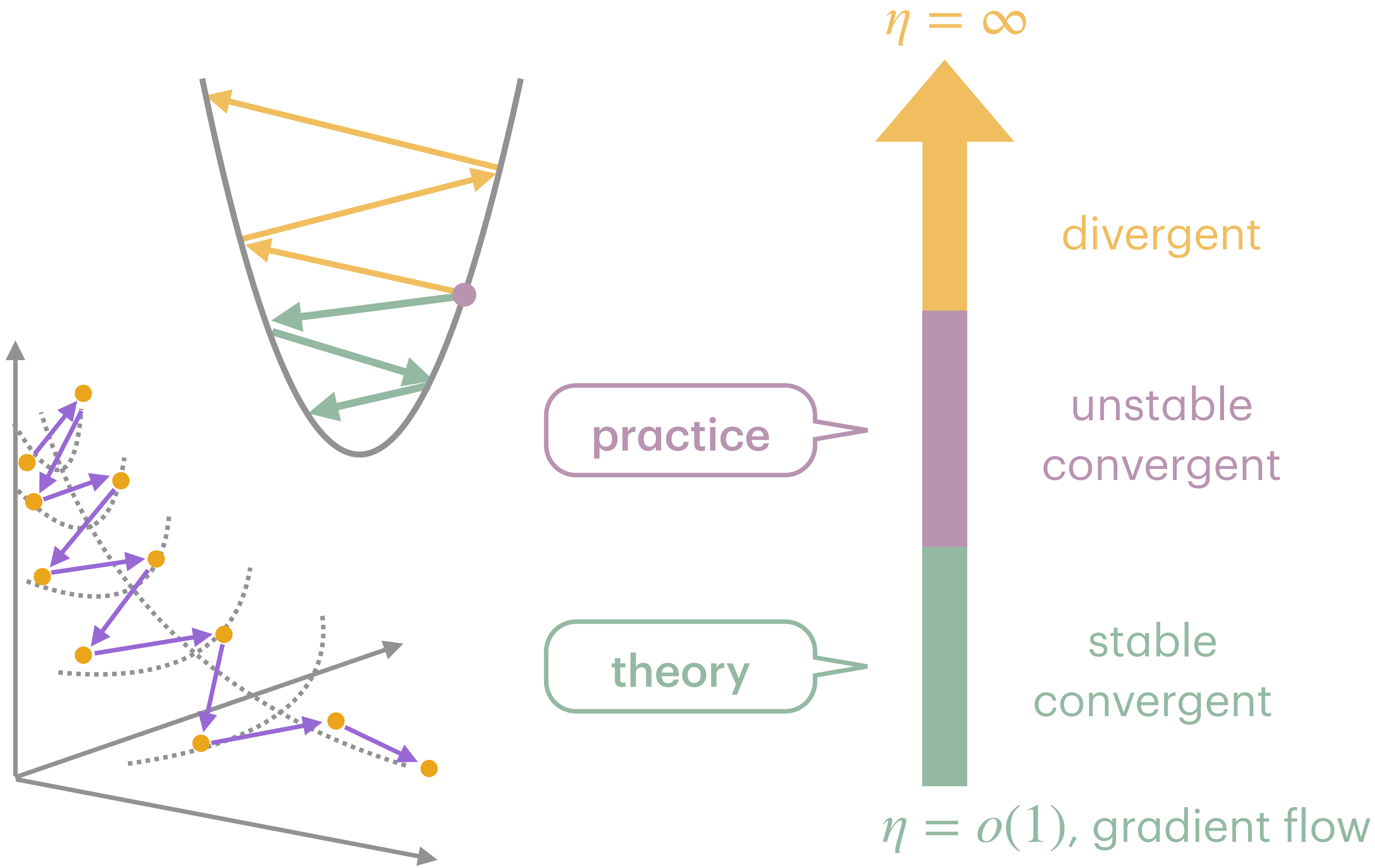
- 💡 better stepsize schedulers, e.g., warmup, stepsize decaying?
- 💡 better optimizer, e.g., preconditioning, normalization?
- 💡 interplay between stepsize vs structure, e.g., attention, depth?
- 💡 how to understand other instabilities, e.g., data, precision?

Q & A



$\eta = \infty$
divergent
unstable convergent
stable convergent
practice
theory
$\eta = o(1)$, gradient flow