Towards a Less Conservative Theory of Machine Learning

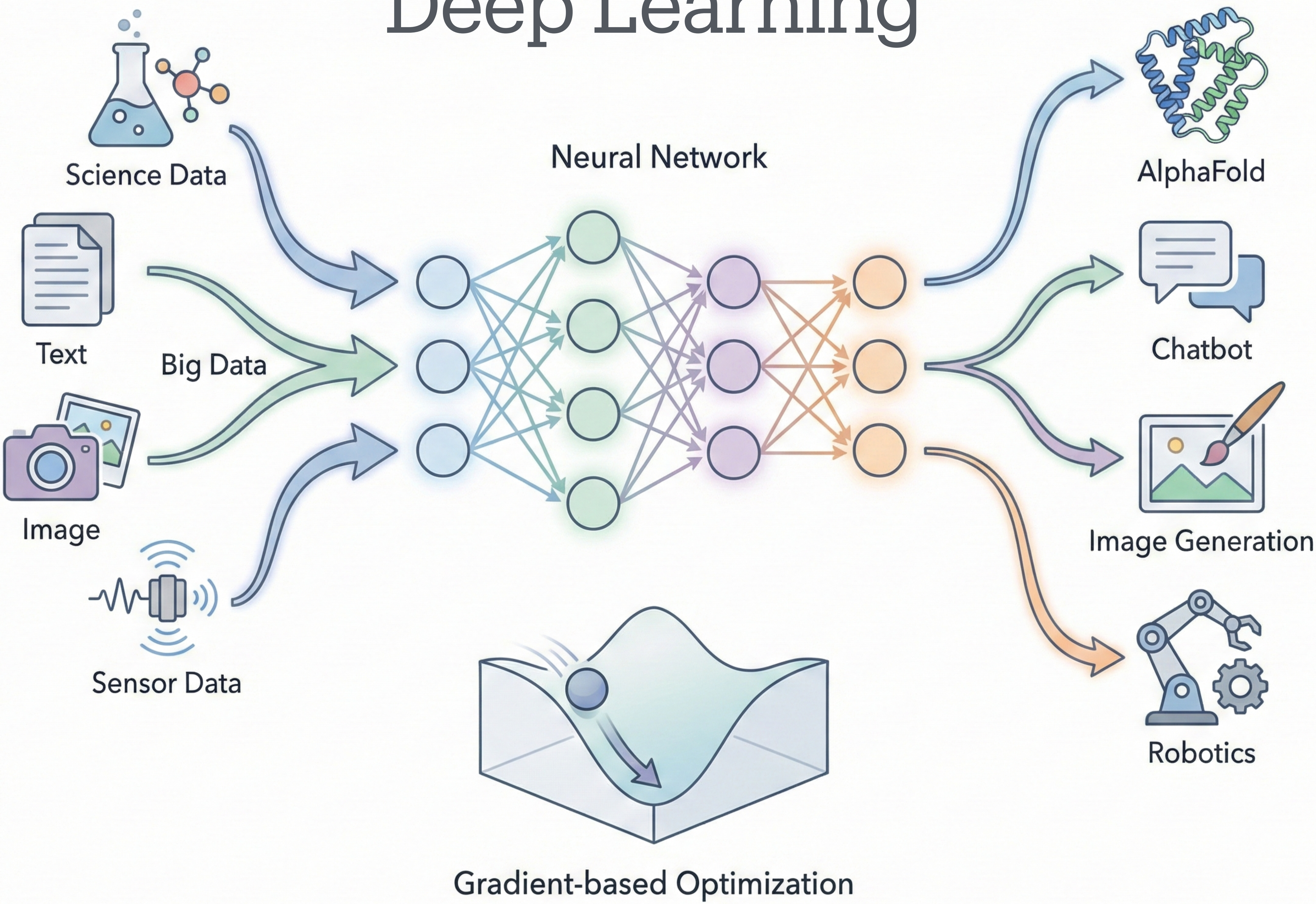
Unstable Optimization & Implicit Regularization

Jingfeng Wu

Simons Institute for the Theory of Computing

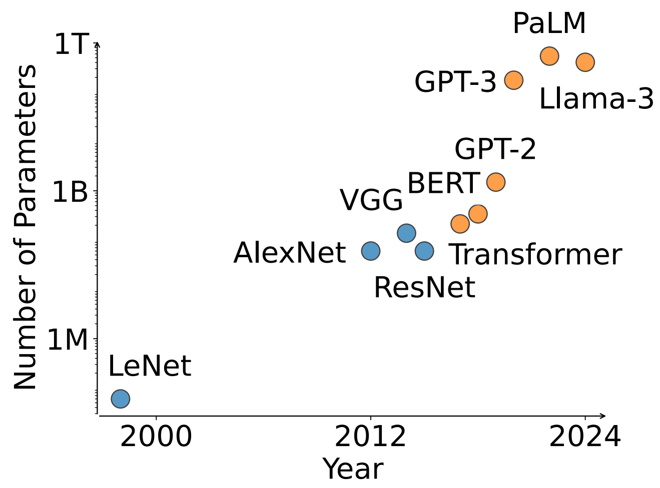
Berkeley University of California

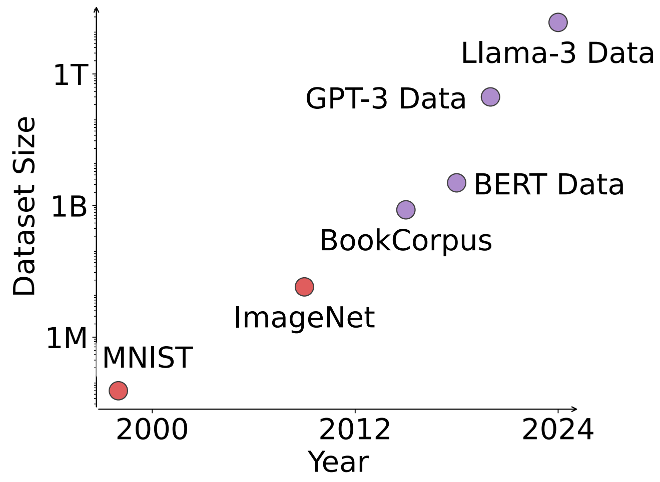
Deep Learning



What makes deep learning thrive?

scaling





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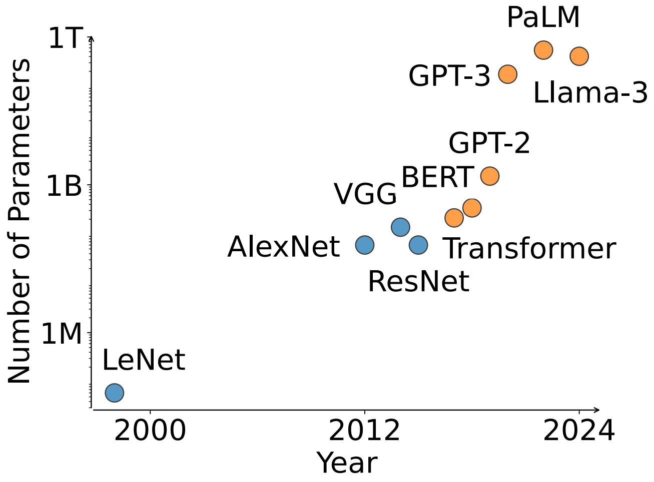
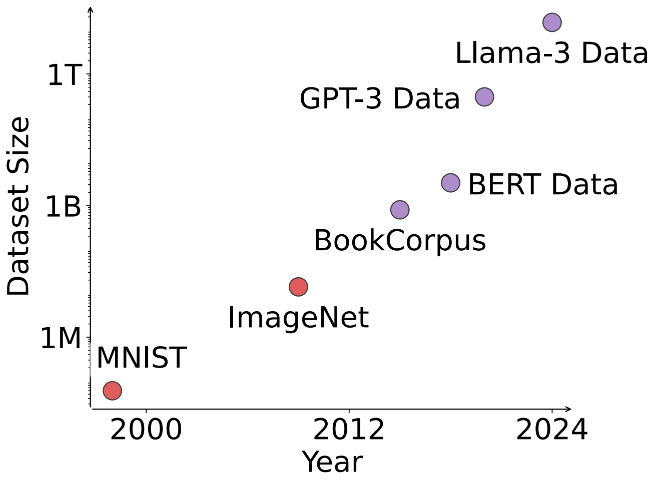
scaling	new mechanisms





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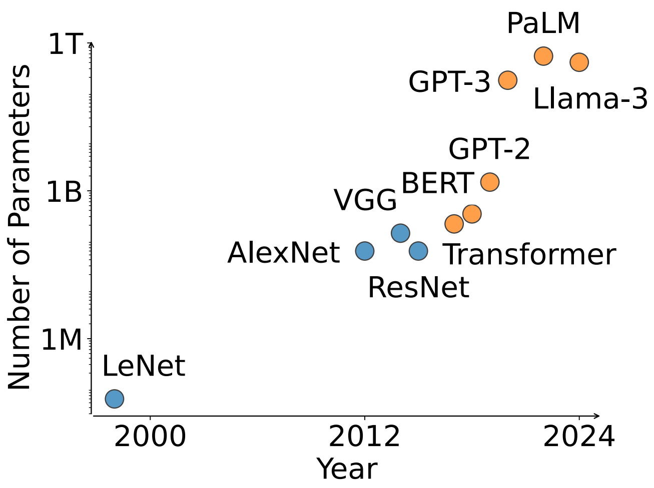
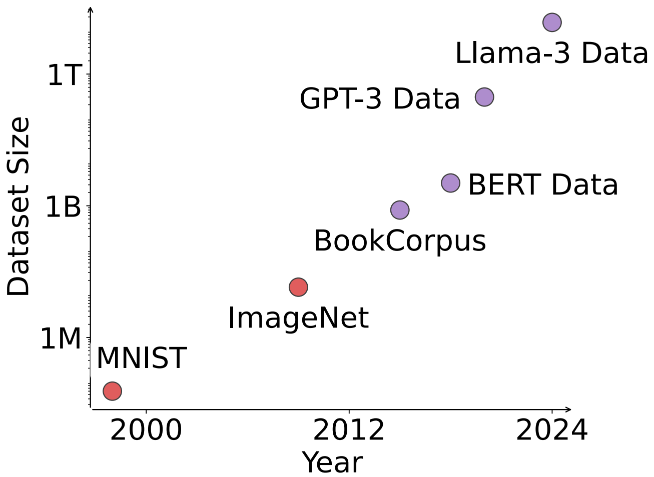
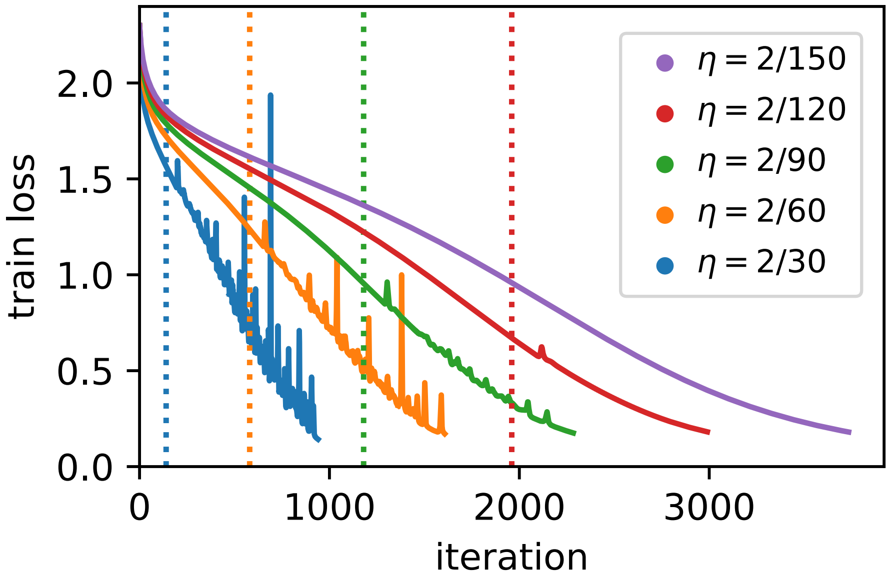




optimization



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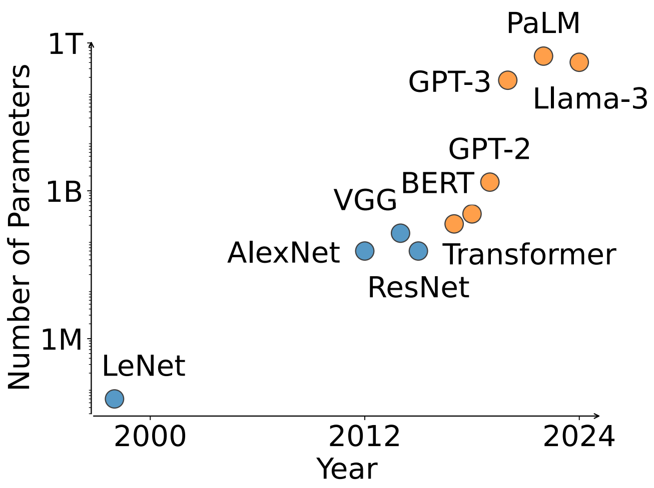
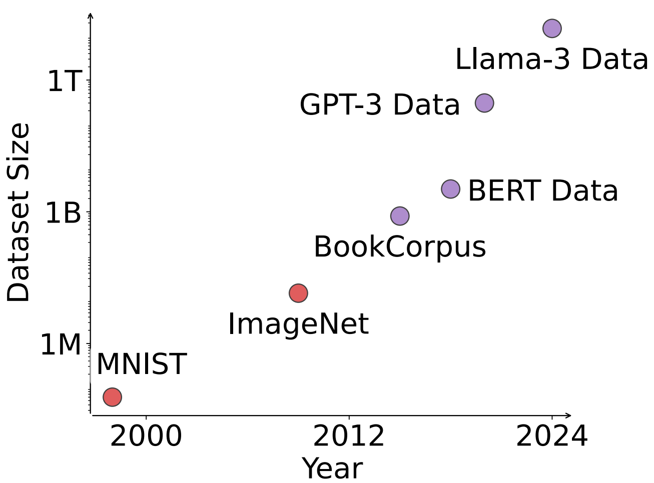
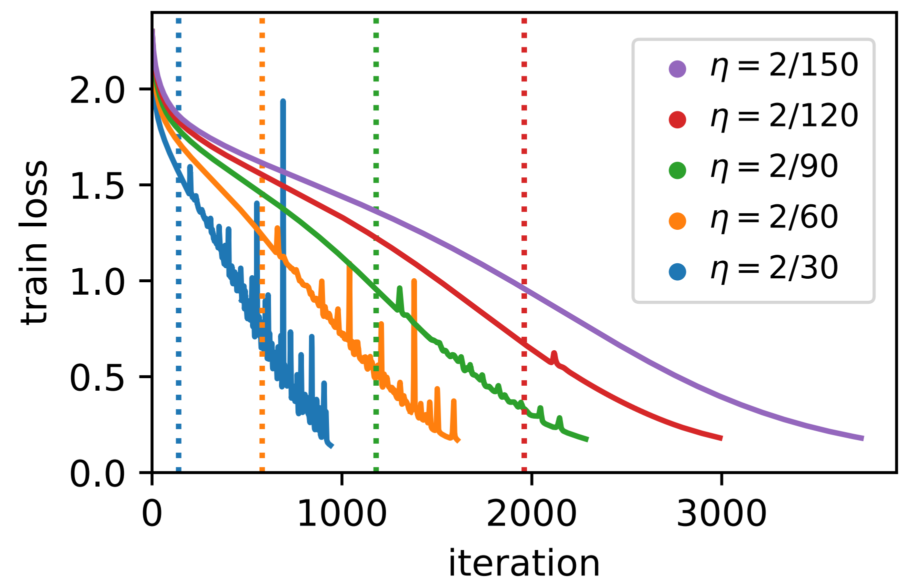




optimization

training instability



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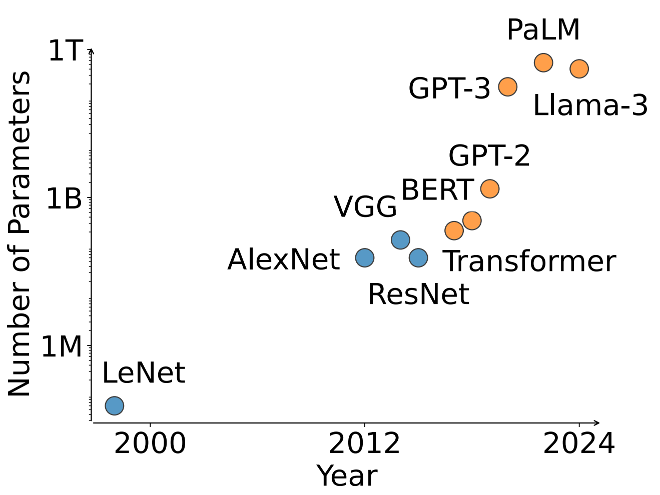

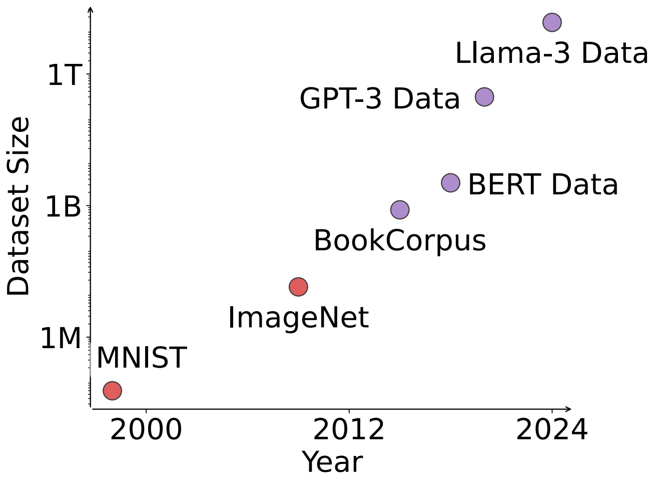

optimization

training instability

"edge of stability"

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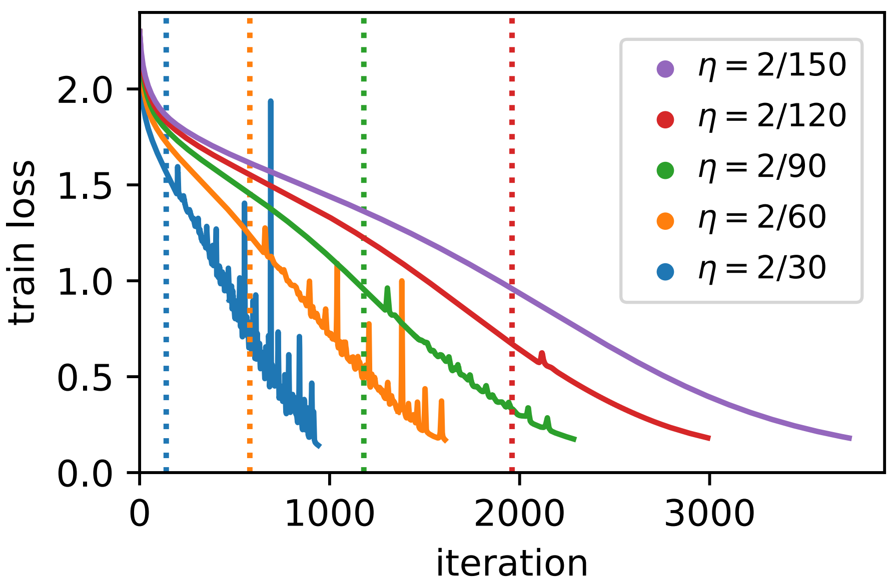

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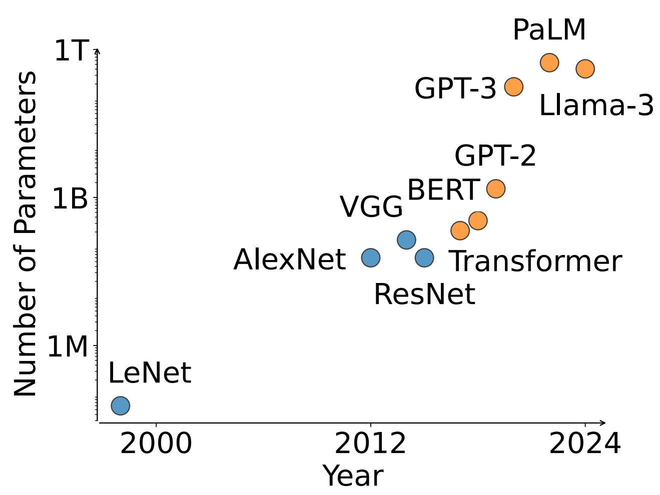

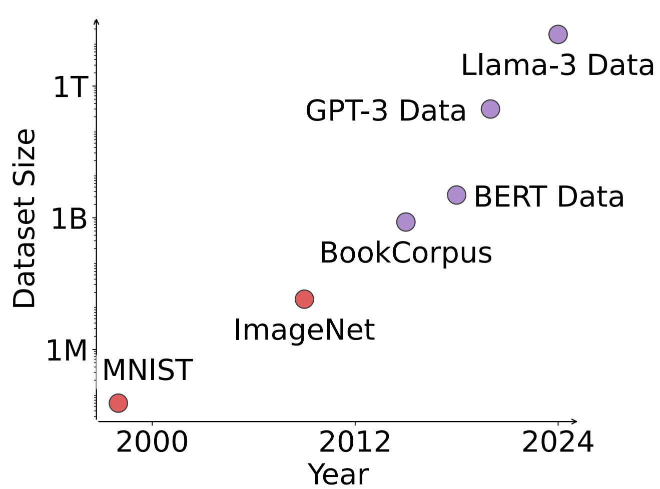

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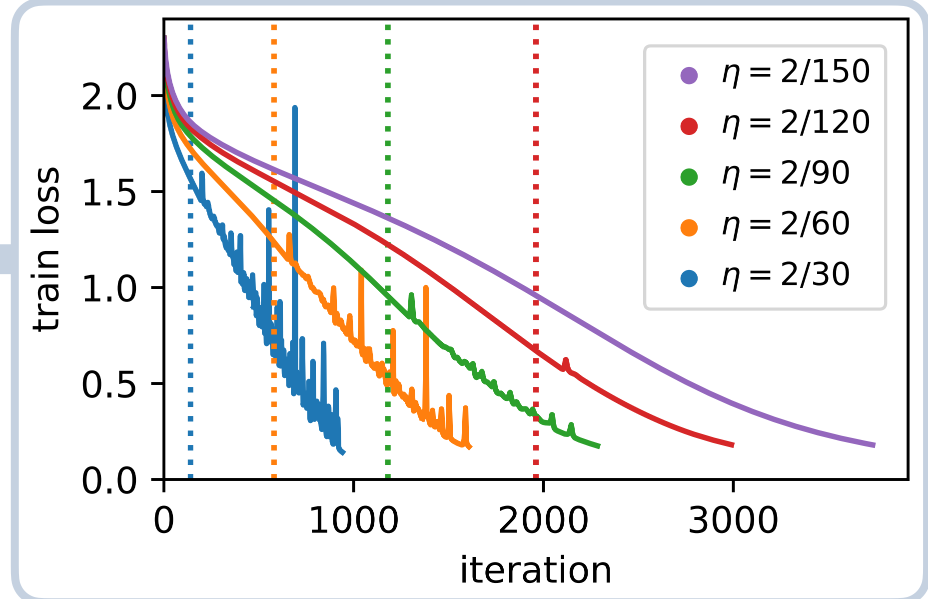

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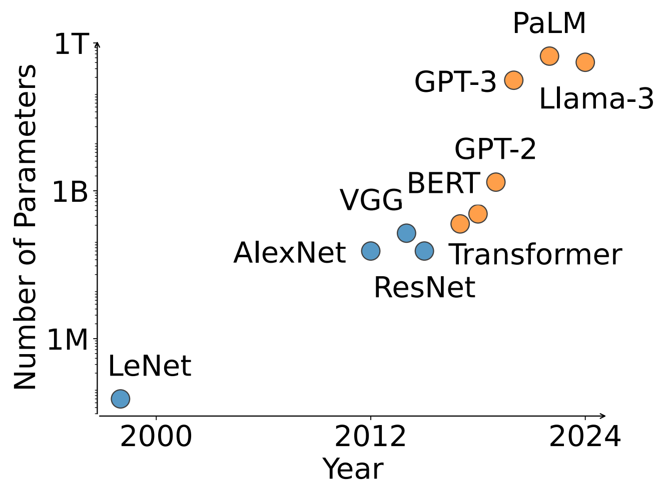

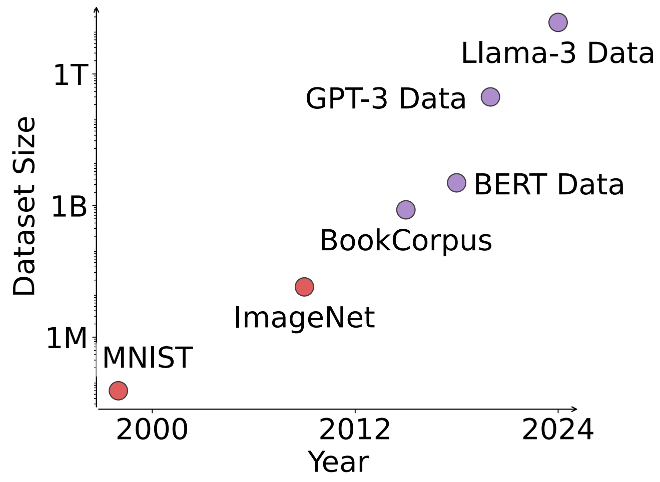

new mechanisms

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- training instability
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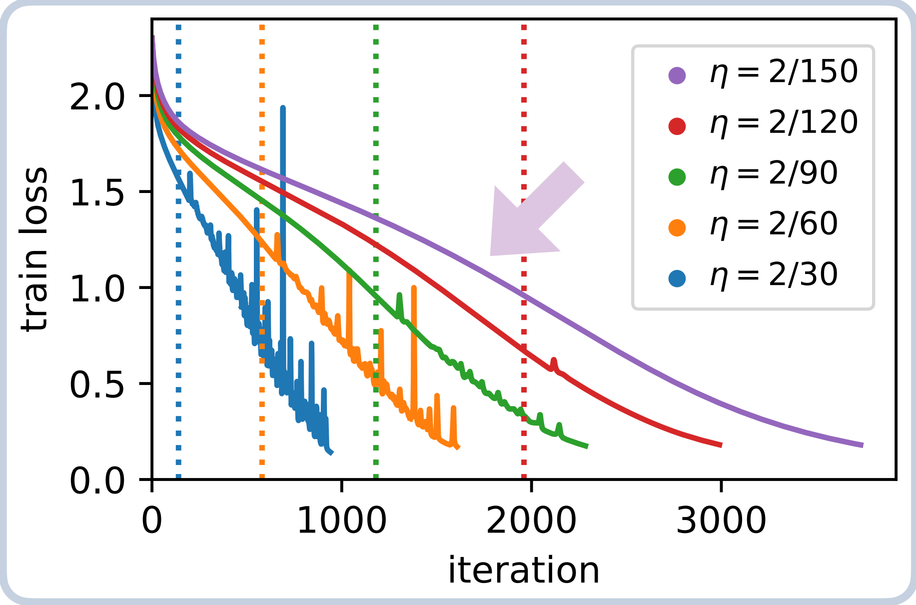

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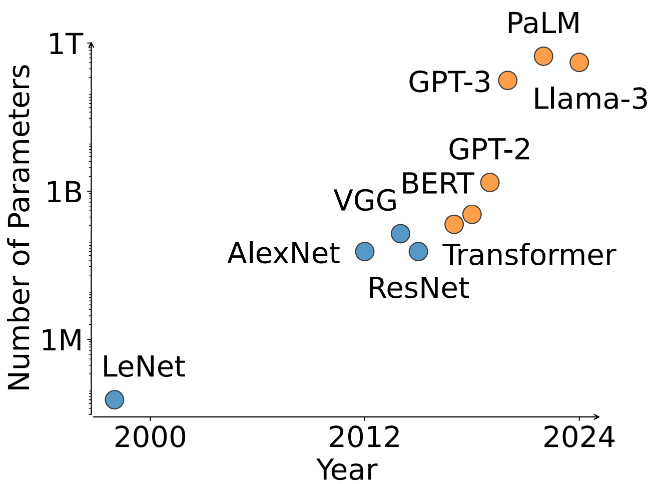

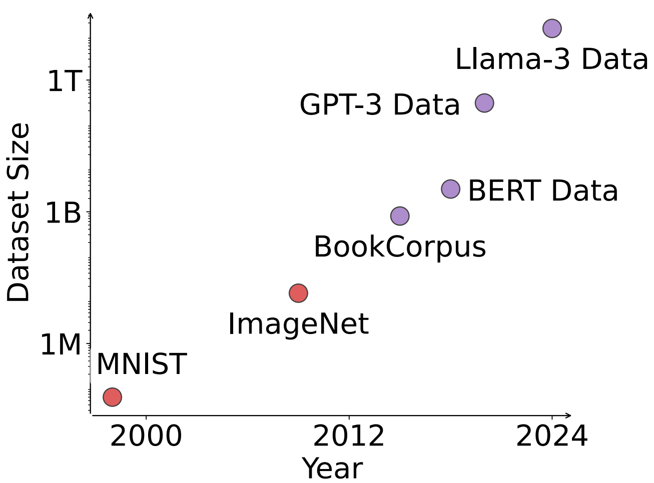

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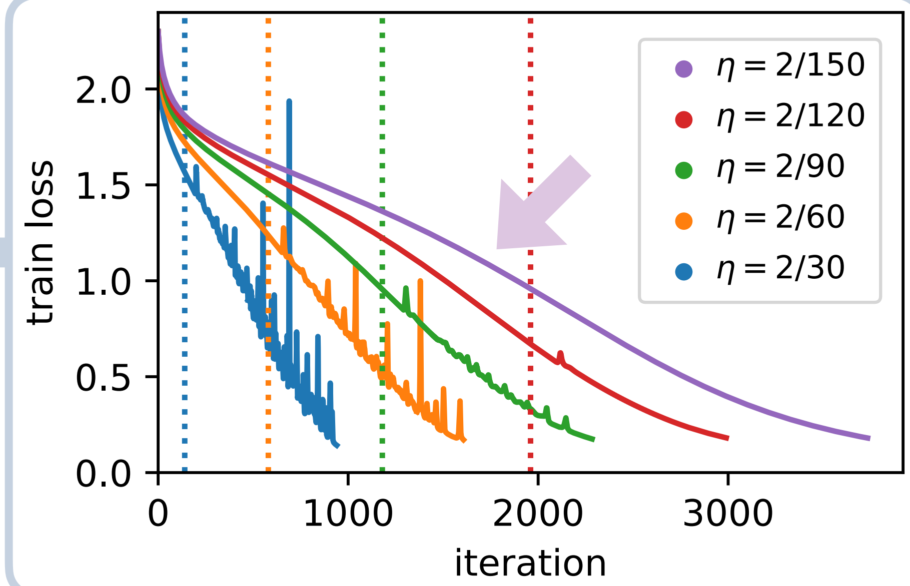
large stepsize

unstable optimization



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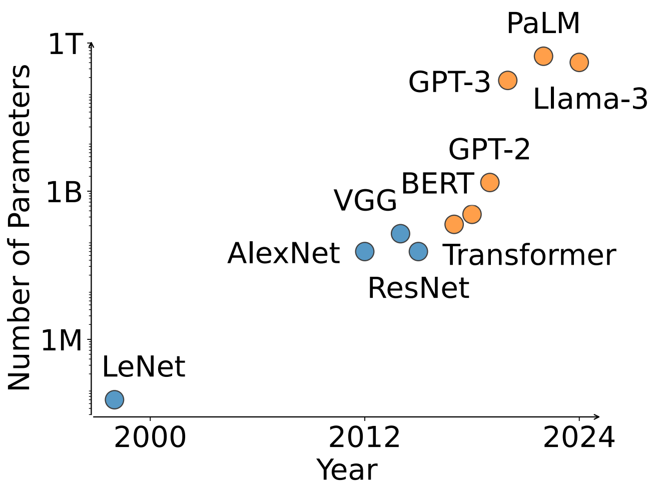

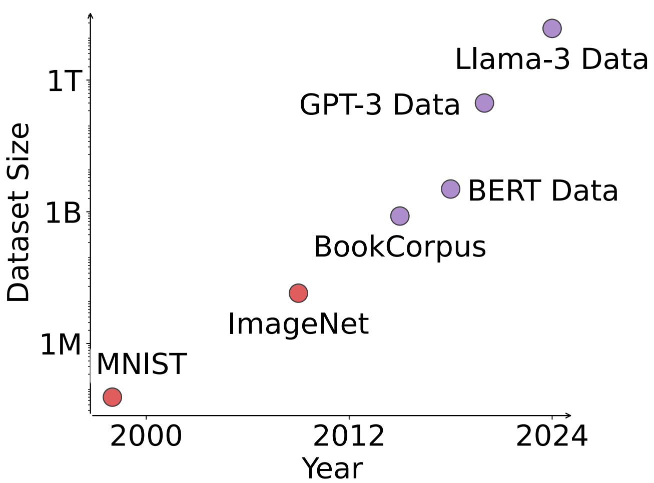

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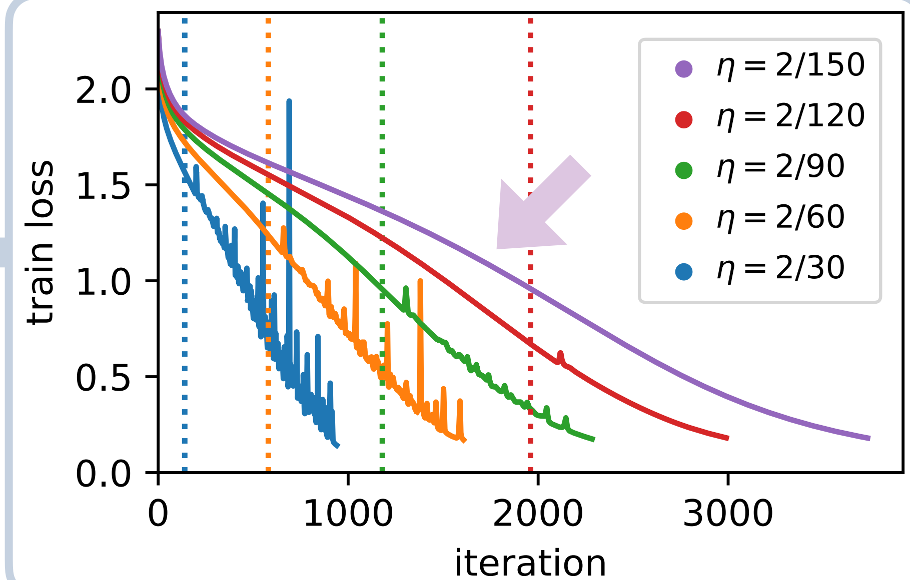
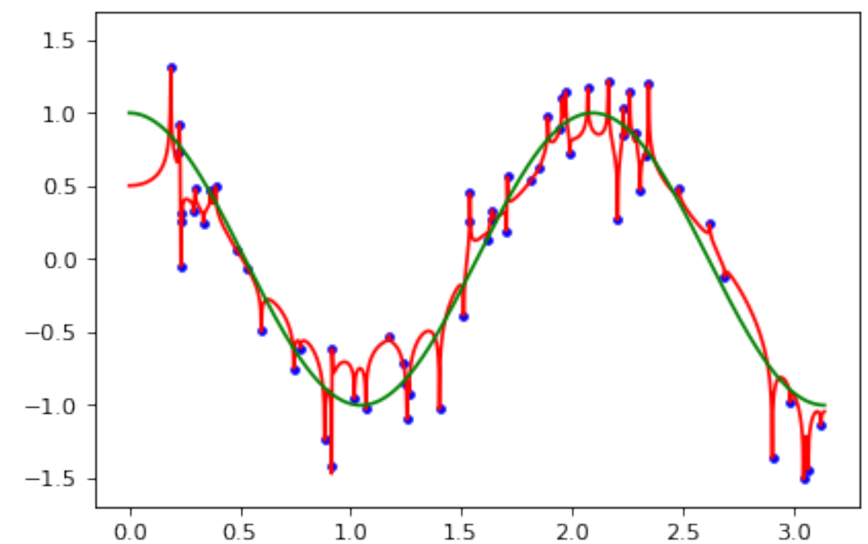


generalization



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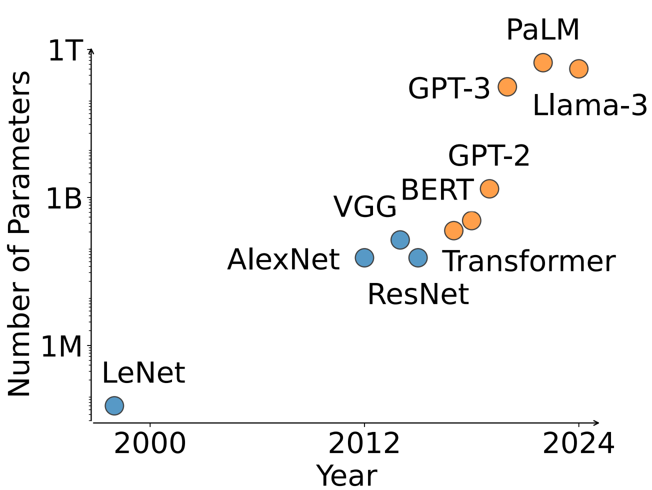

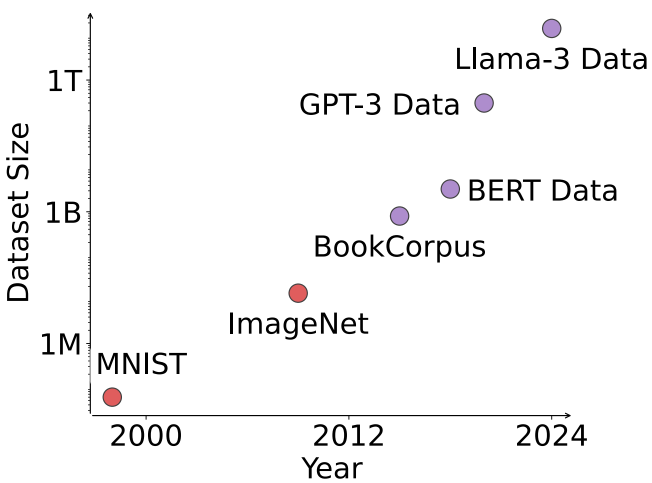

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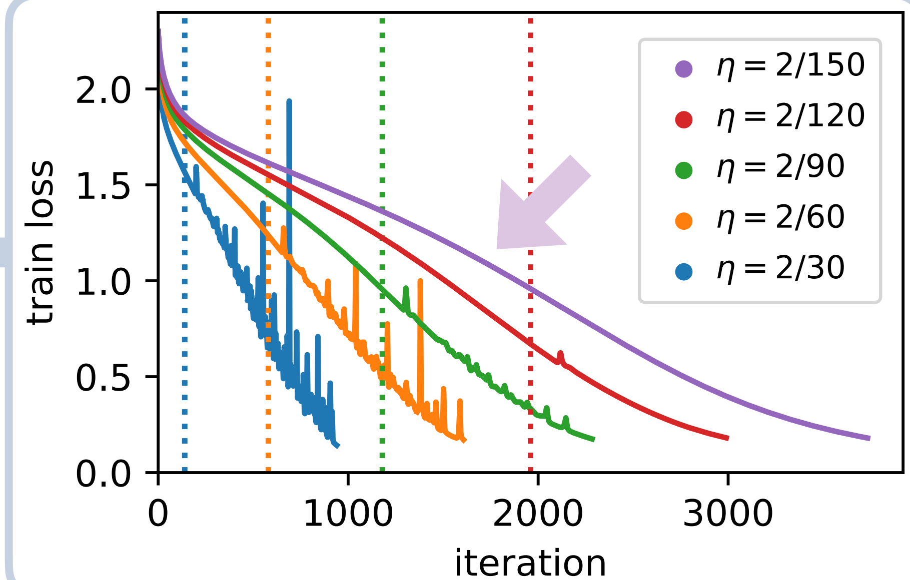
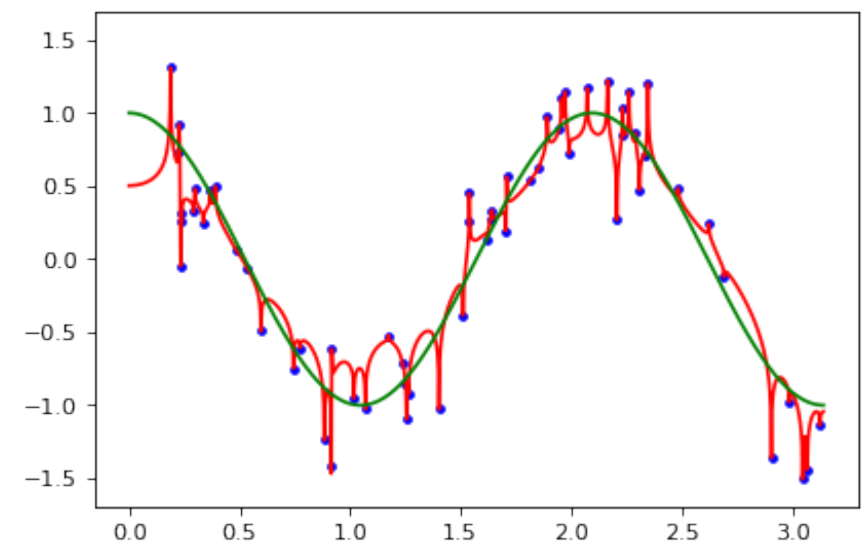


generalization

overparameterization



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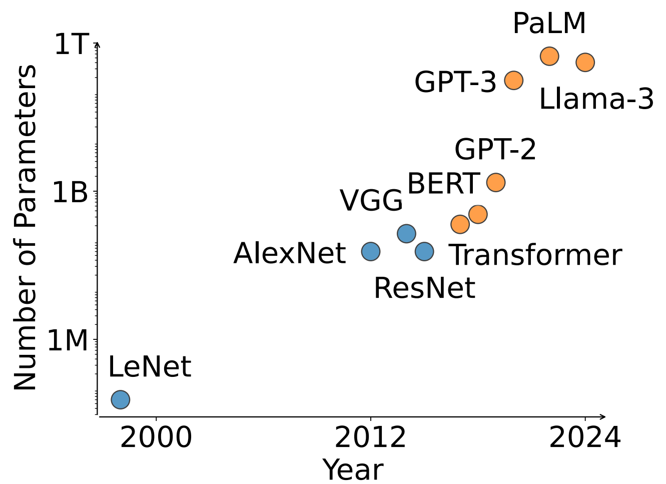

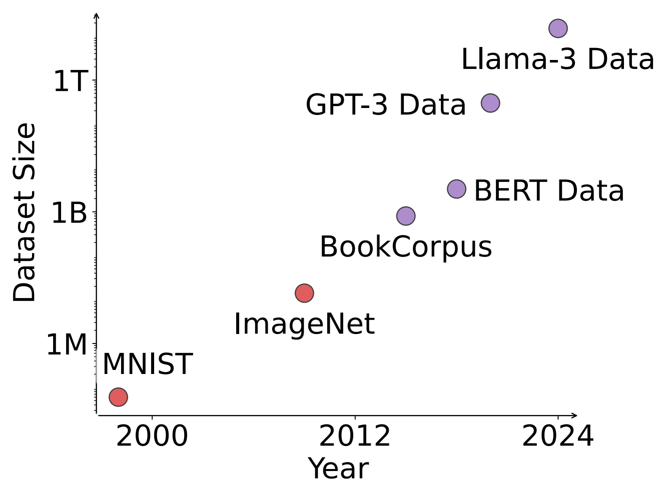

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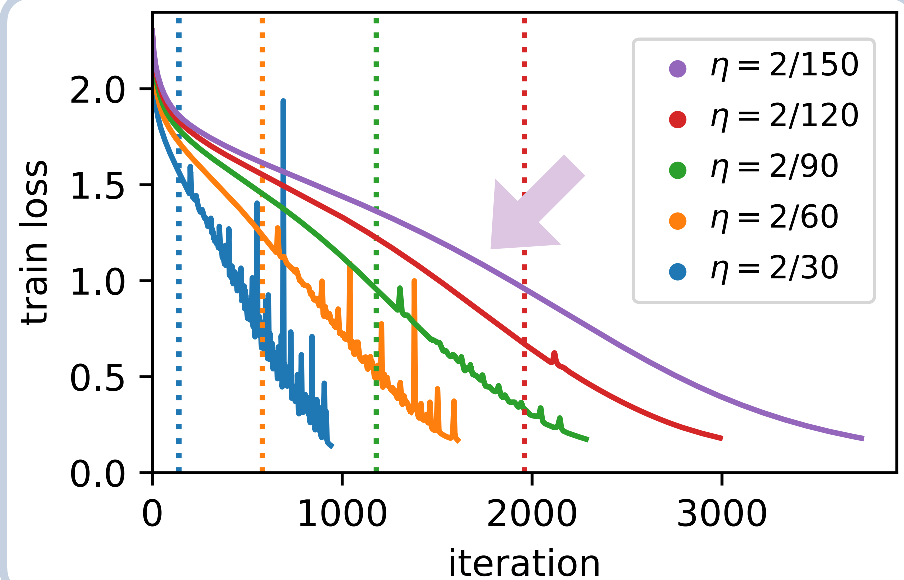

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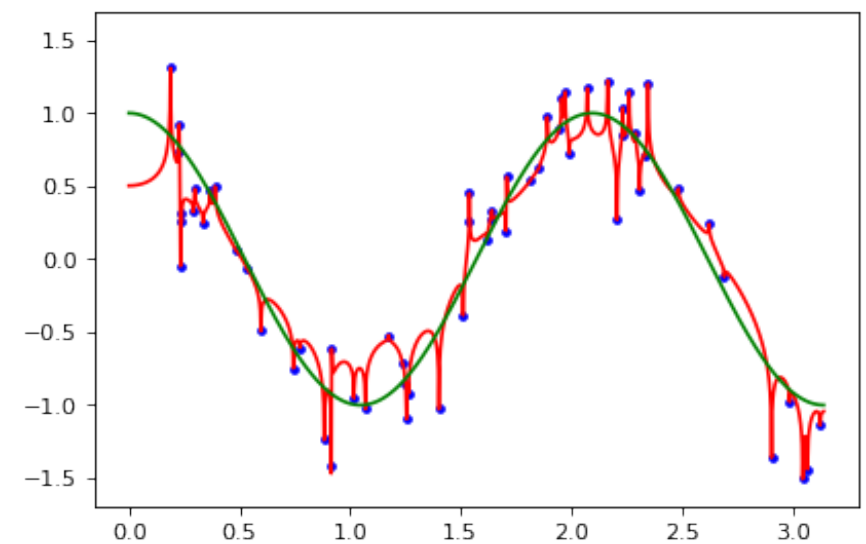

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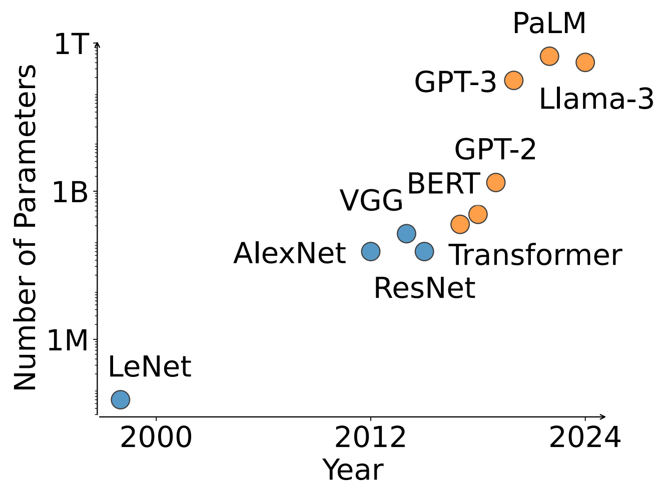

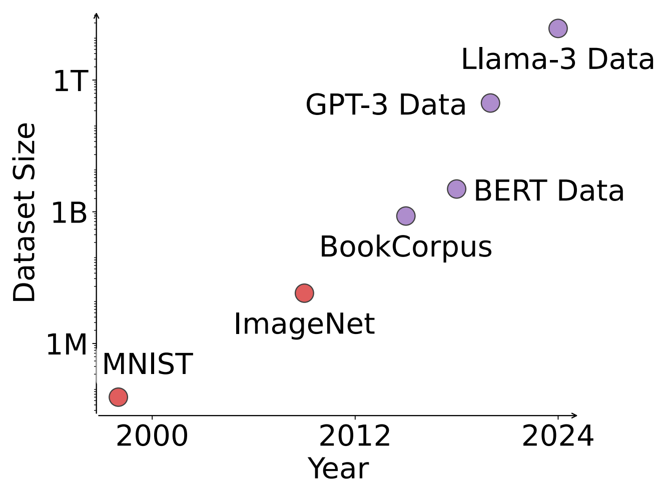

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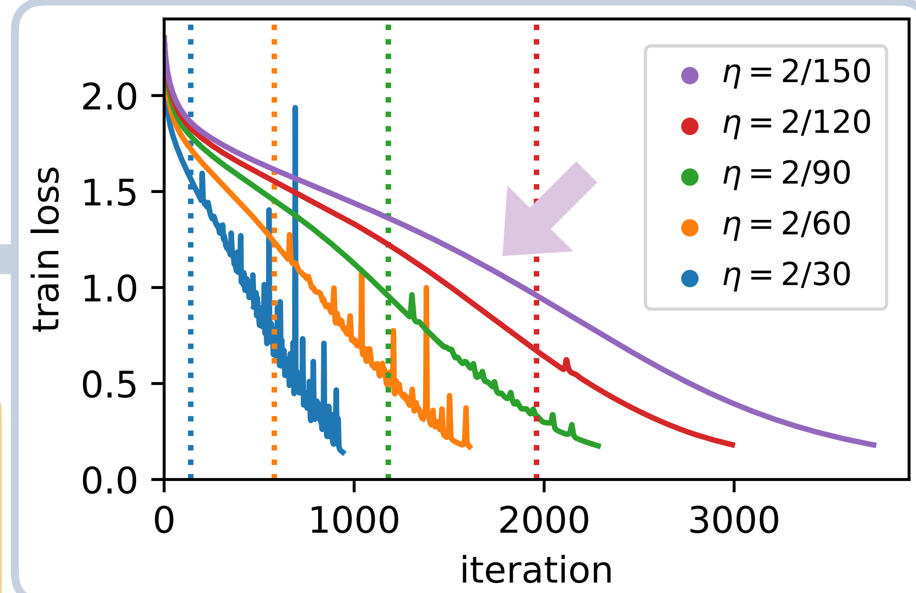

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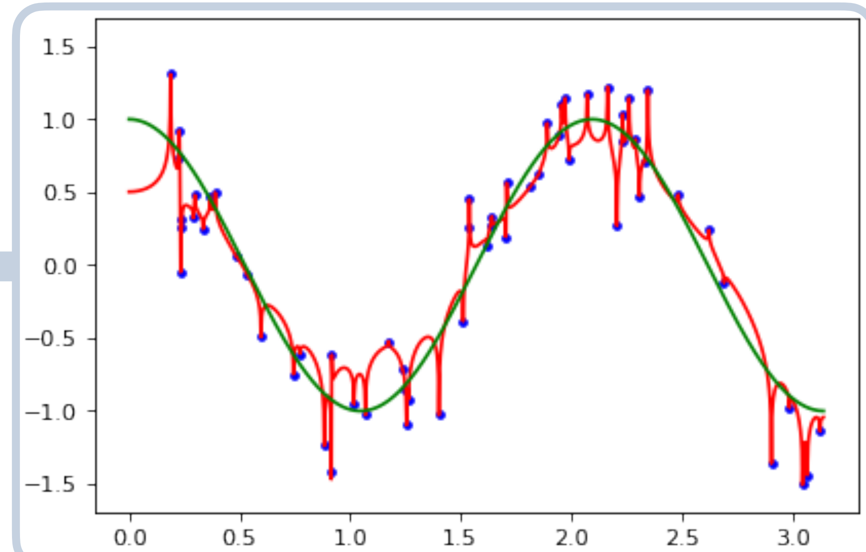

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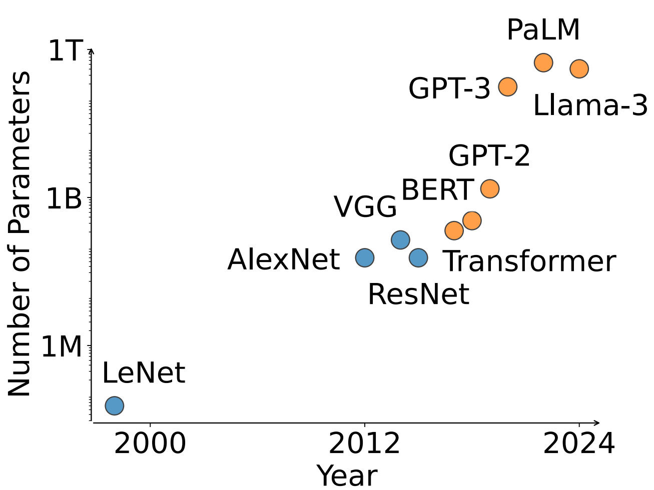

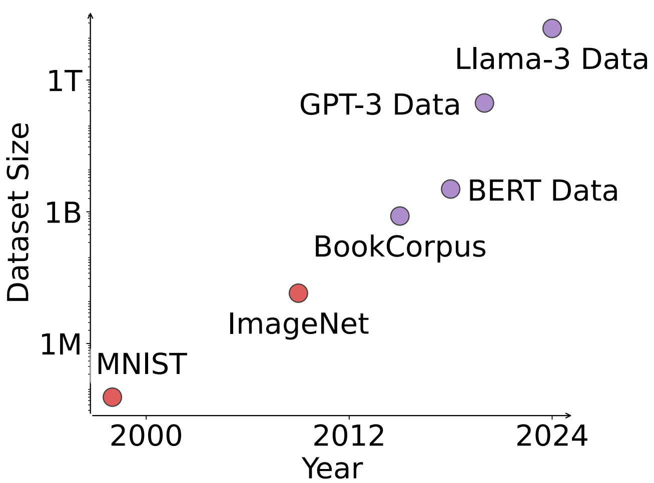

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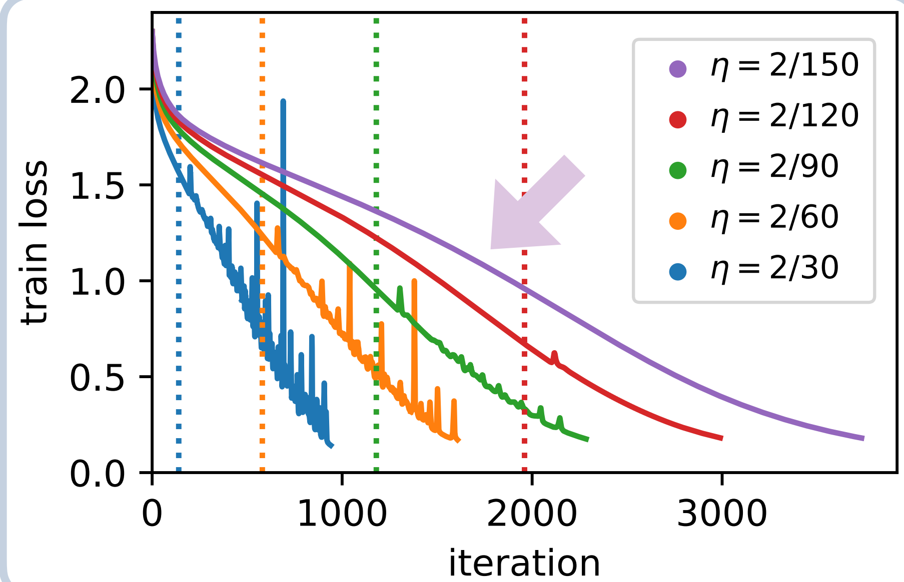

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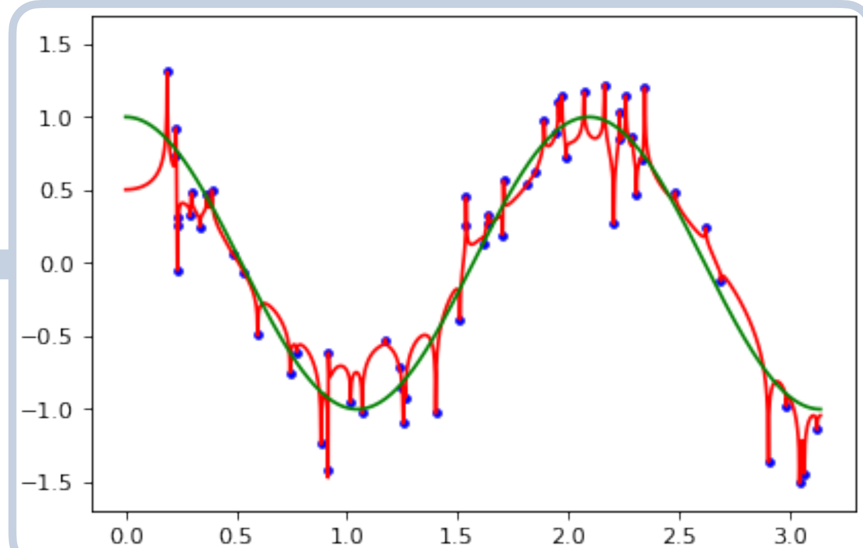
optimization path

implicit regularization



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My research

deep learning = scaling + new mechanisms

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My research

not covered by classical theory

deep learning = scaling + new mechanisms

My research

💡💡💡

not covered by classical theory

deep learning = scaling + new mechanisms

My research

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not covered by classical theory

deep learning = scaling + **new mechanisms**

not specific to deep learning

My research

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deep learning = scaling + new mechanisms

ML fields
(beyond DL)

not specific to
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✨✨✨

My research

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Approach. Demystify new mechanisms in **sandboxes**

My research

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Approach. Demystify new mechanisms in **sandboxes**

simple

My research

💡 💡 💡

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✨✨✨

Approach. Demystify new mechanisms in **sandboxes**

simple

meaningful

Contribution 1: unstable optimization

large stepsize accelerates gradient descent in logistic regression

Contribution 2: implicit regularization

gradient descent dominates ridge regression in linear regression

Contribution 3: from theory to practice

principled parallelization method for training language models

Contribution 1: unstable optimization

large stepsize accelerates gradient descent in logistic regression

- "Large stepsize gradient descent for logistic loss: non-monotonicity of the loss improves optimization efficiency"
  W, Peter Bartlett, Matus Telgarsky, Bin Yu
  COLT 2024

- "Large stepsizes accelerate gradient descent for regularized logistic regression"
  W*, Pierre Marion*, Peter Bartlett
  NeurIPS 2025

Unstable optimization

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

Unstable optimization

how to choose η?

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classical theory:

small stepsize for stability

$L(\theta_t) \downarrow$

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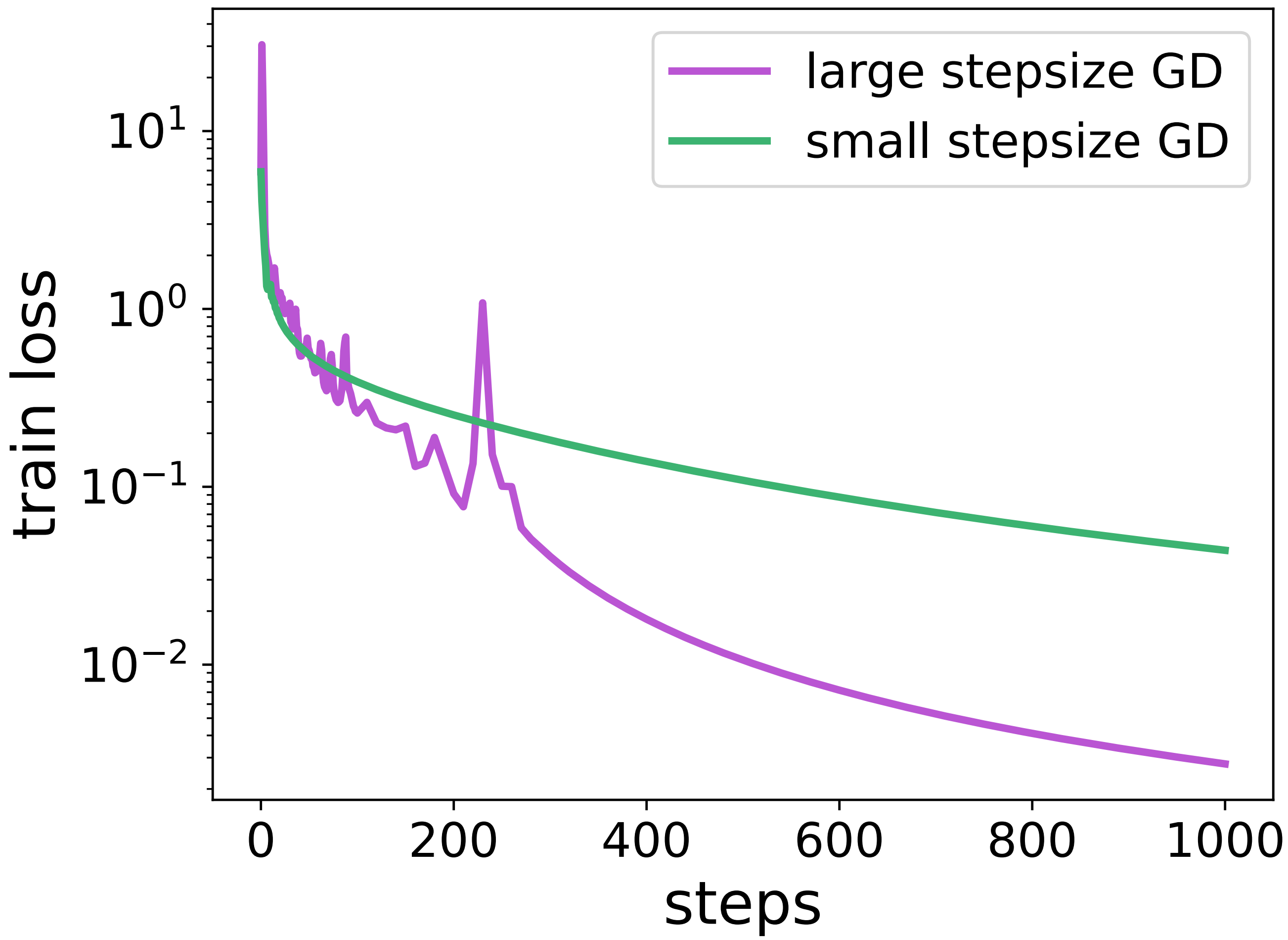

MLP, GD, classification task

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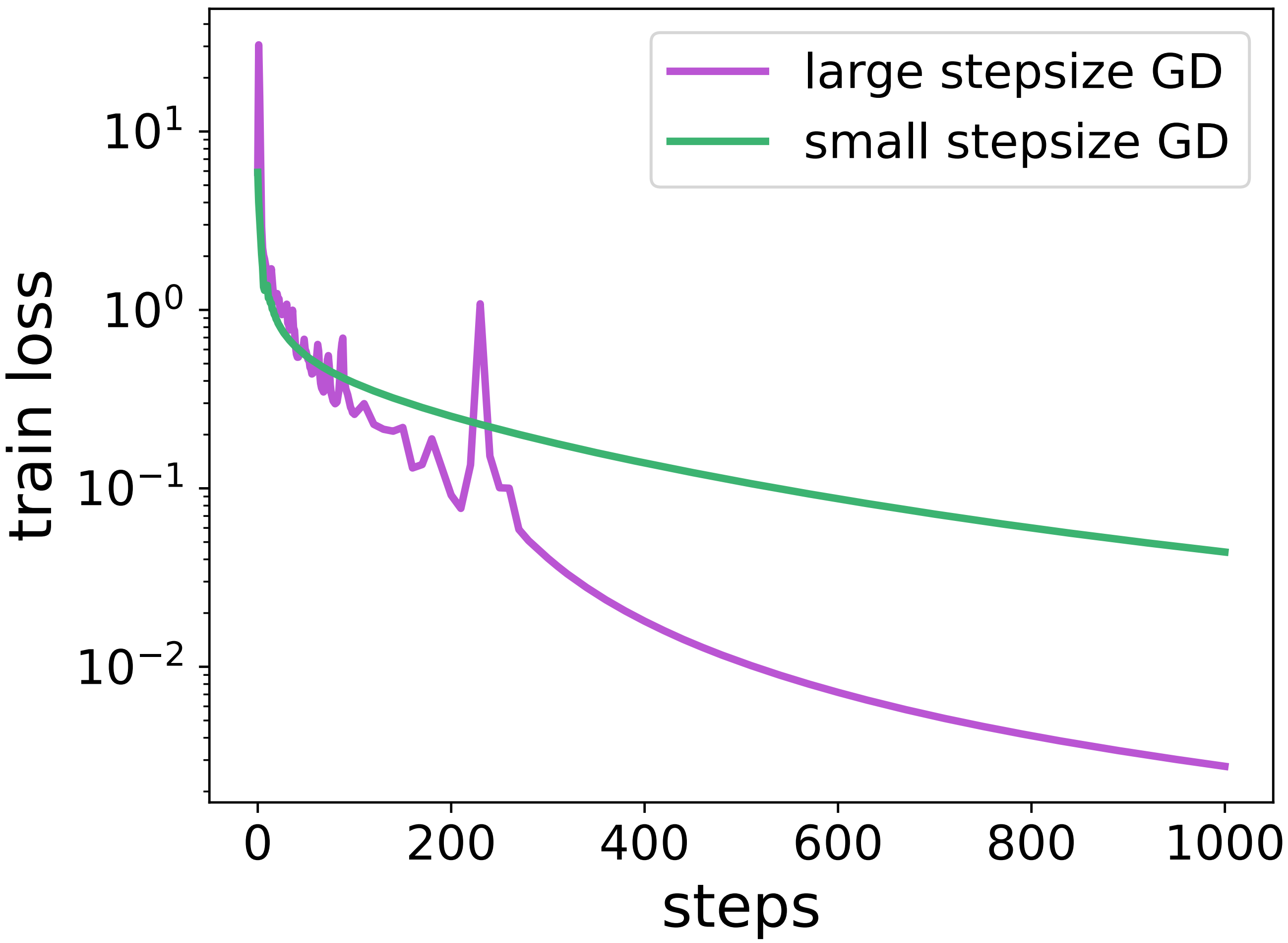

classical theory:
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practice:
best stepsize is large
oscillatory loss

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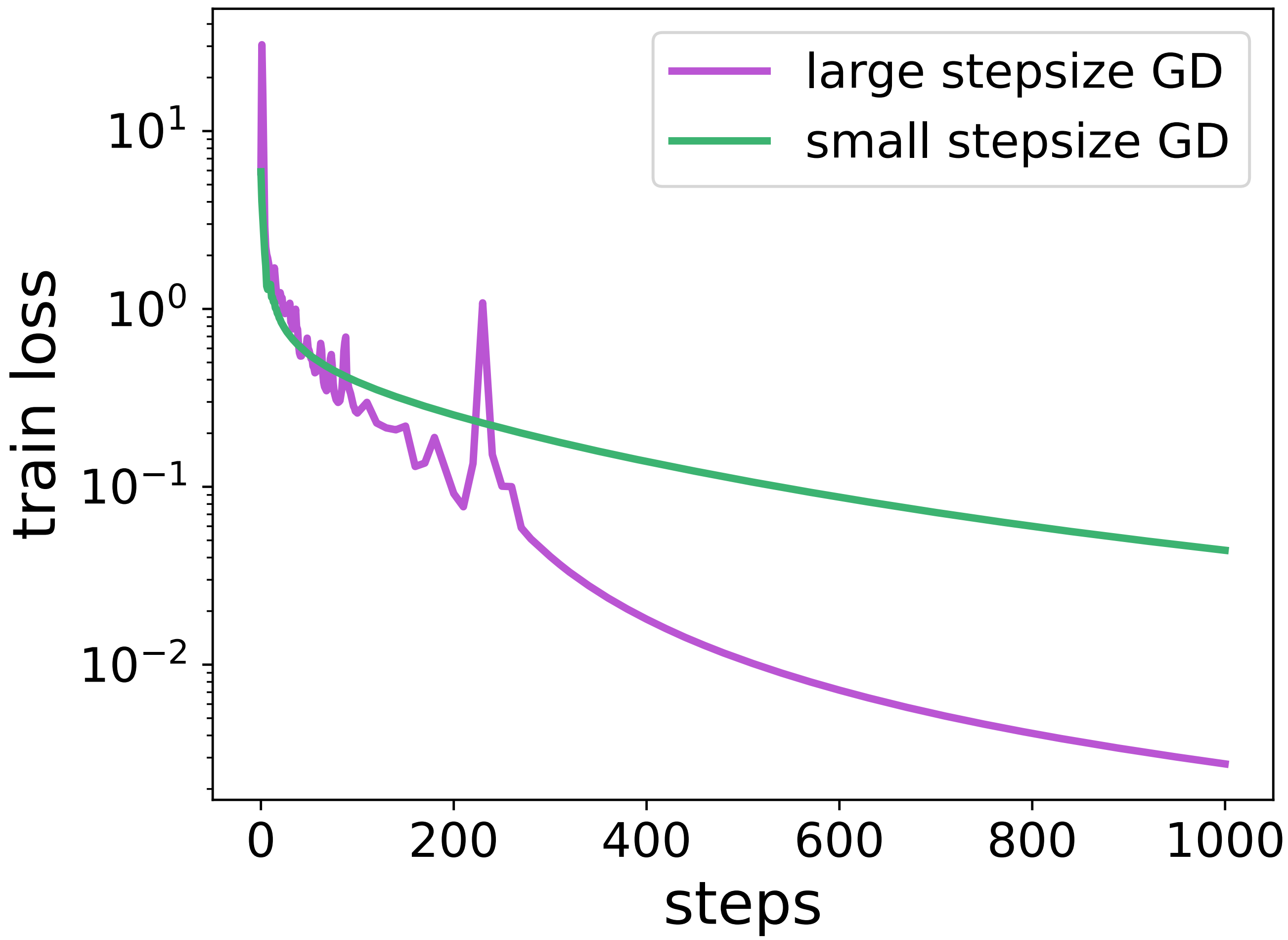

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classical theory fails to predict best stepsize

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Classical theory

Let L be 1-smooth ($\|\nabla^2 L\| \leq 1$) with finite minimizer

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Descent lemma.

- **small stepsize** $\eta < 2 \Rightarrow L(\theta_t) \downarrow$
- **large stepsize** $\eta > 2 \Rightarrow L(\theta_t) \uparrow \infty$ for quadratics

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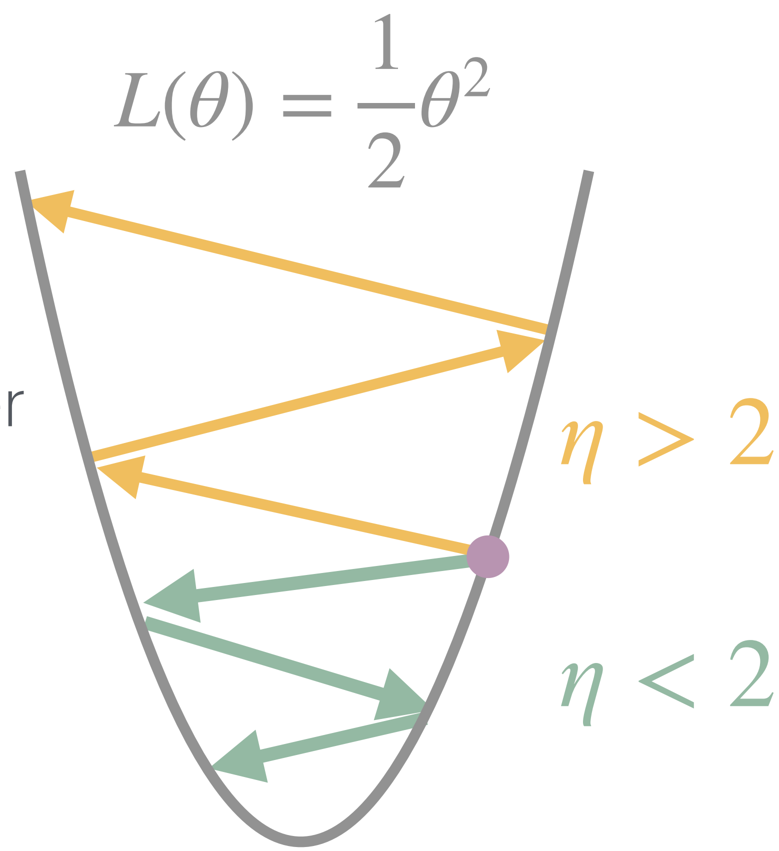

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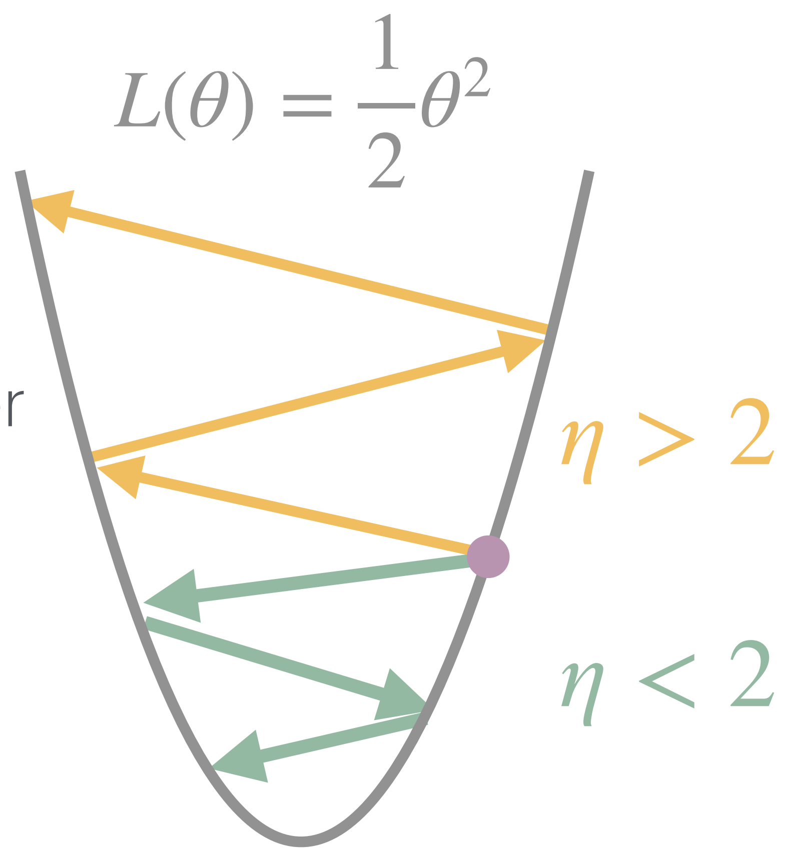

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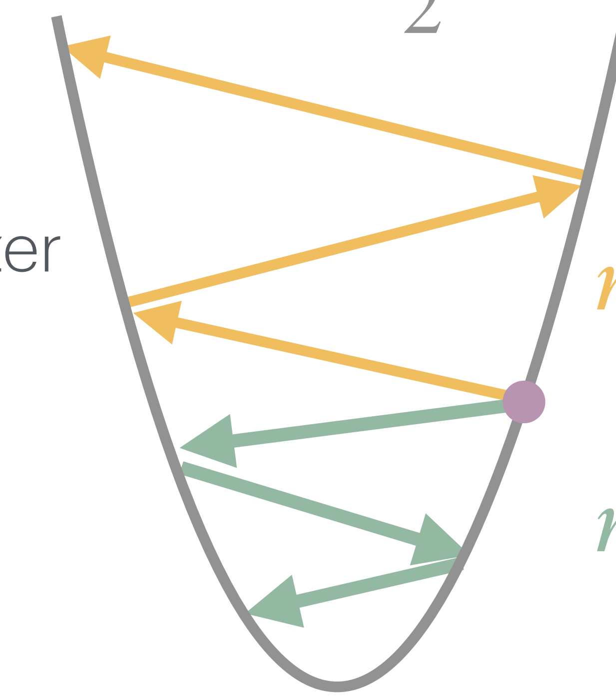

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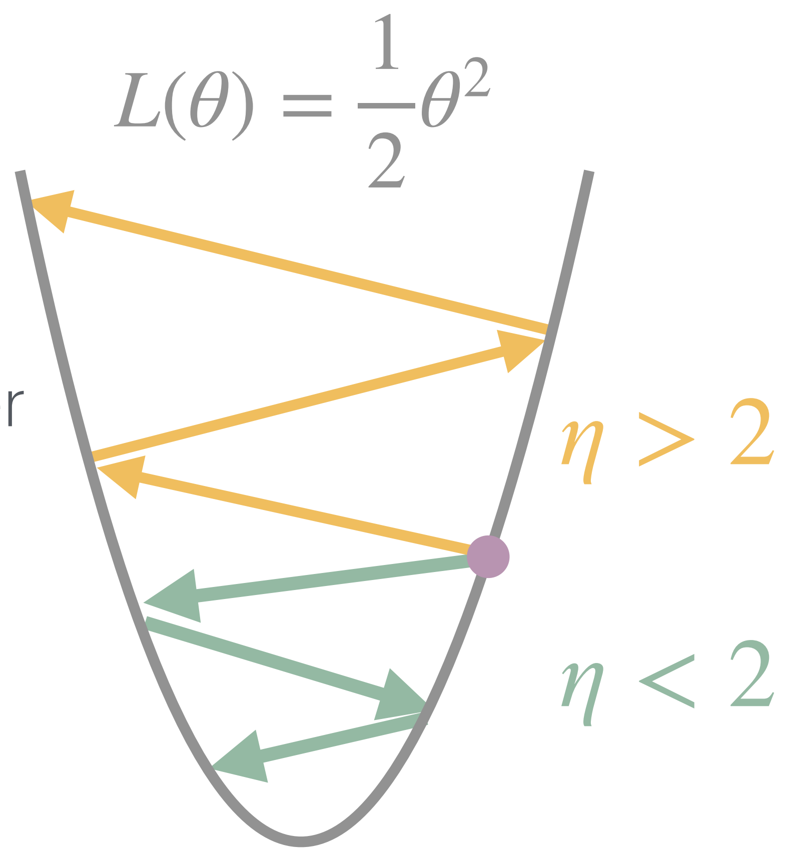
Rates. GD with $\eta = 1$ achieves

- **convexity** $L(\theta_t) - \min L \leq O(1/t)$
- λ**-strong convexity** $L(\theta_t) - \min L \leq \epsilon$ for $t = O\big(\kappa \ln(1/\epsilon)\big)$

Classical theory



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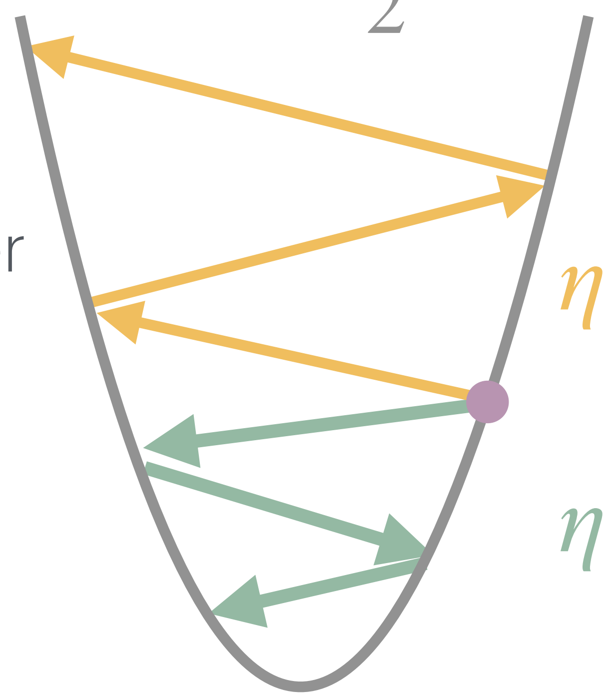

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Descent lemma.

- **small stepsize** $\eta < 2 \Rightarrow L(\theta_t) \downarrow$
- **large stepsize** $\eta > 2 \Rightarrow L(\theta_t) \uparrow \infty$ for quadratics

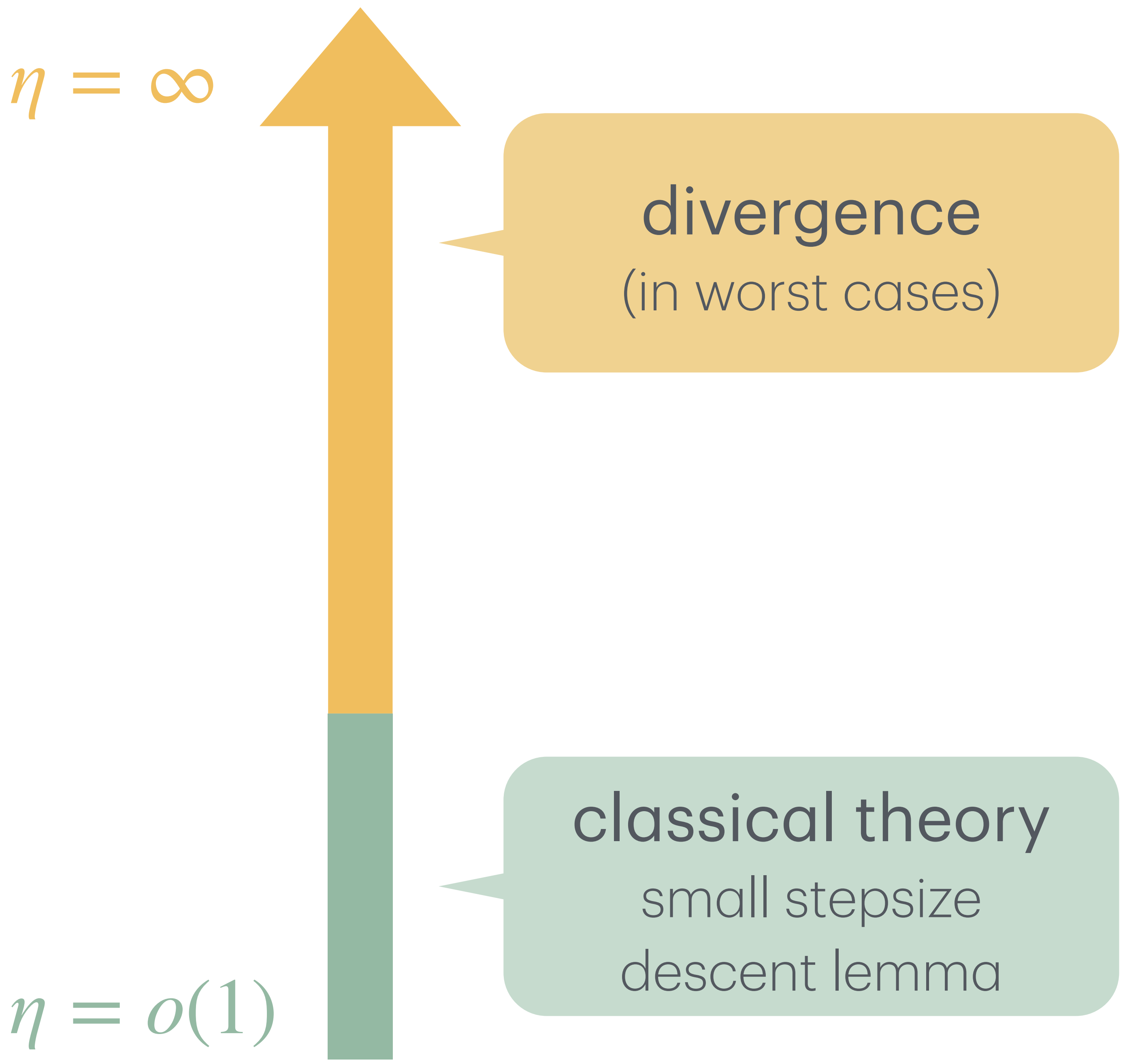
Rates. GD with $\eta = 1$ achieves

- **convexity** $L(\theta_t) - \min L \leq O(1/t)$
- **λ-strong convexity** $L(\theta_t) - \min L \leq \epsilon$ for $t = O\big(\kappa \ln(1/\epsilon)\big)$

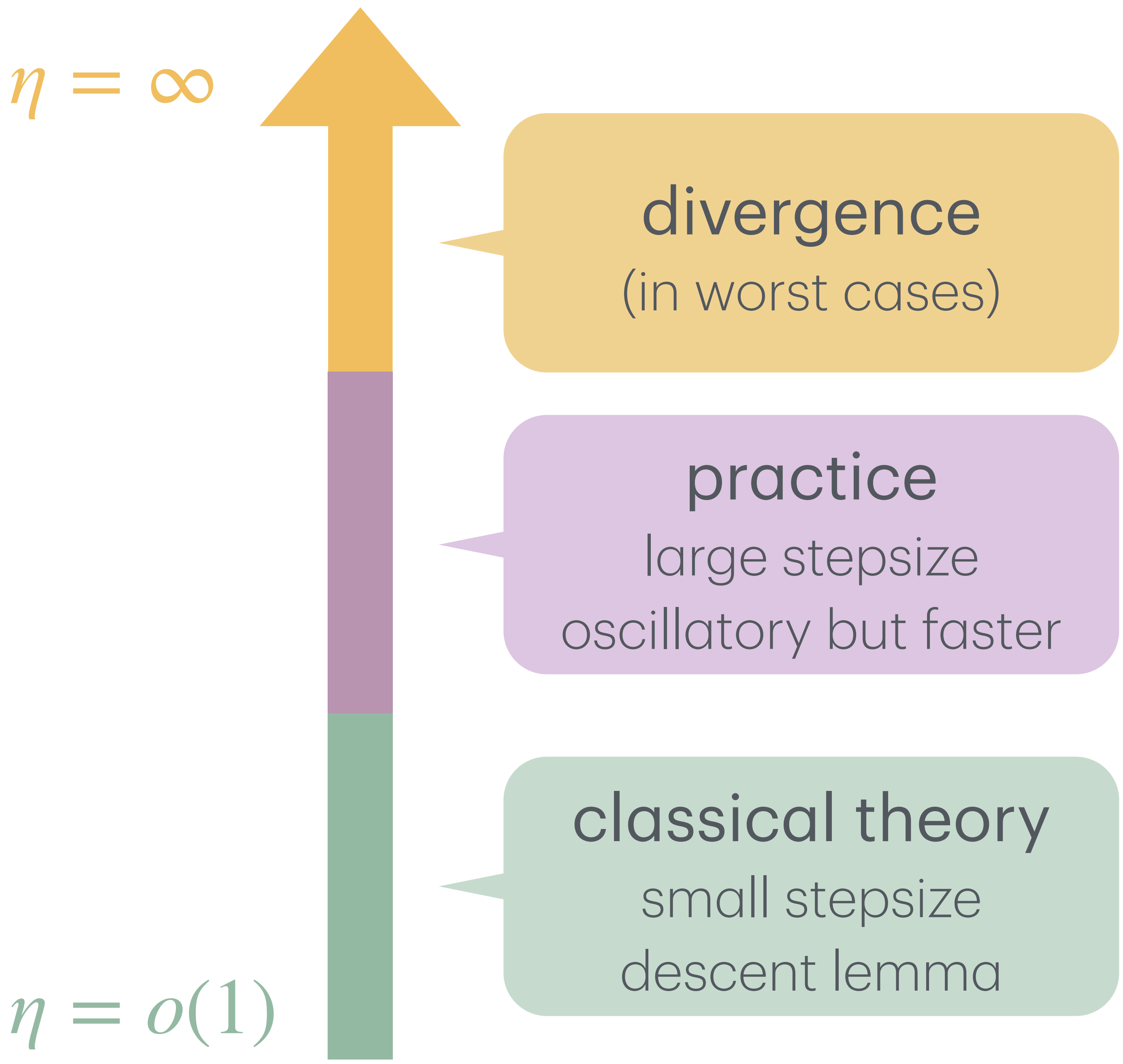
condition number
$\kappa = 1/\lambda \gg 1$

acceleration by Nesterov's momentum:
$O\big(1/t^2\big)$ & $O\big(\sqrt{\kappa}\ln(1/\epsilon)\big)$

Stepsize


$\eta = \infty$
divergence
(in worst cases)
classical theory
small stepsize
descent lemma
$\eta = o(1)$

Stepsize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oscillatory but faster
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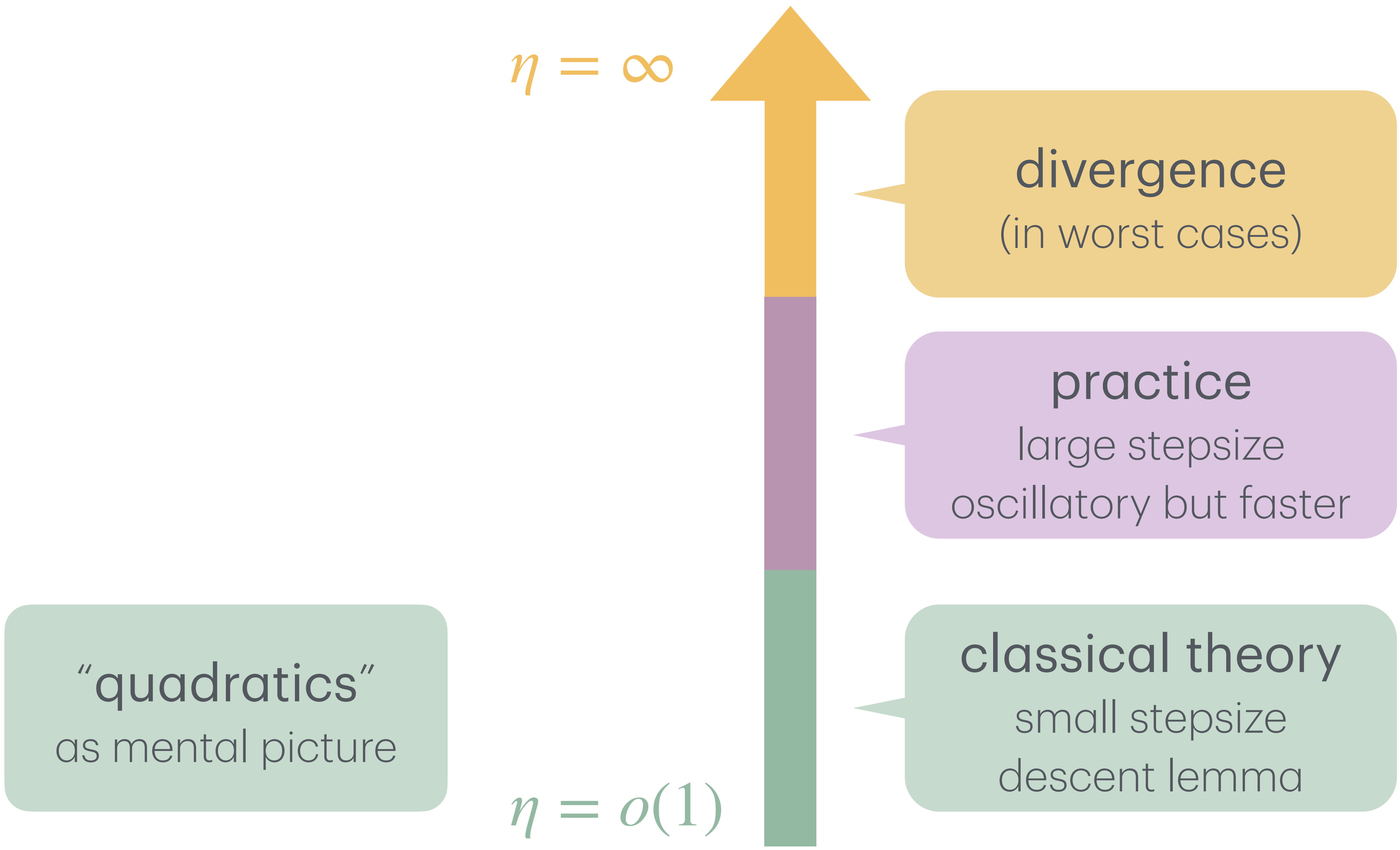
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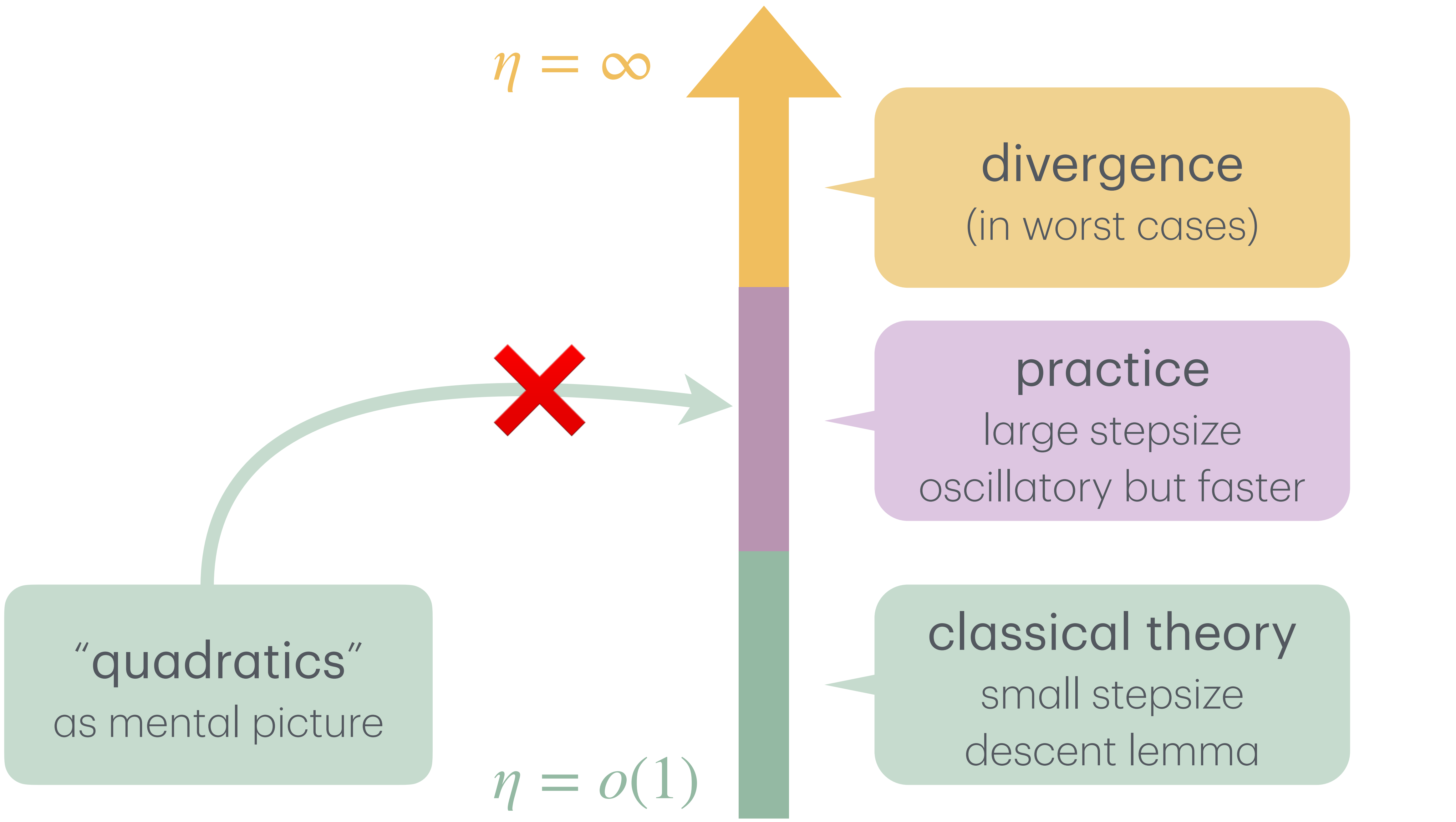
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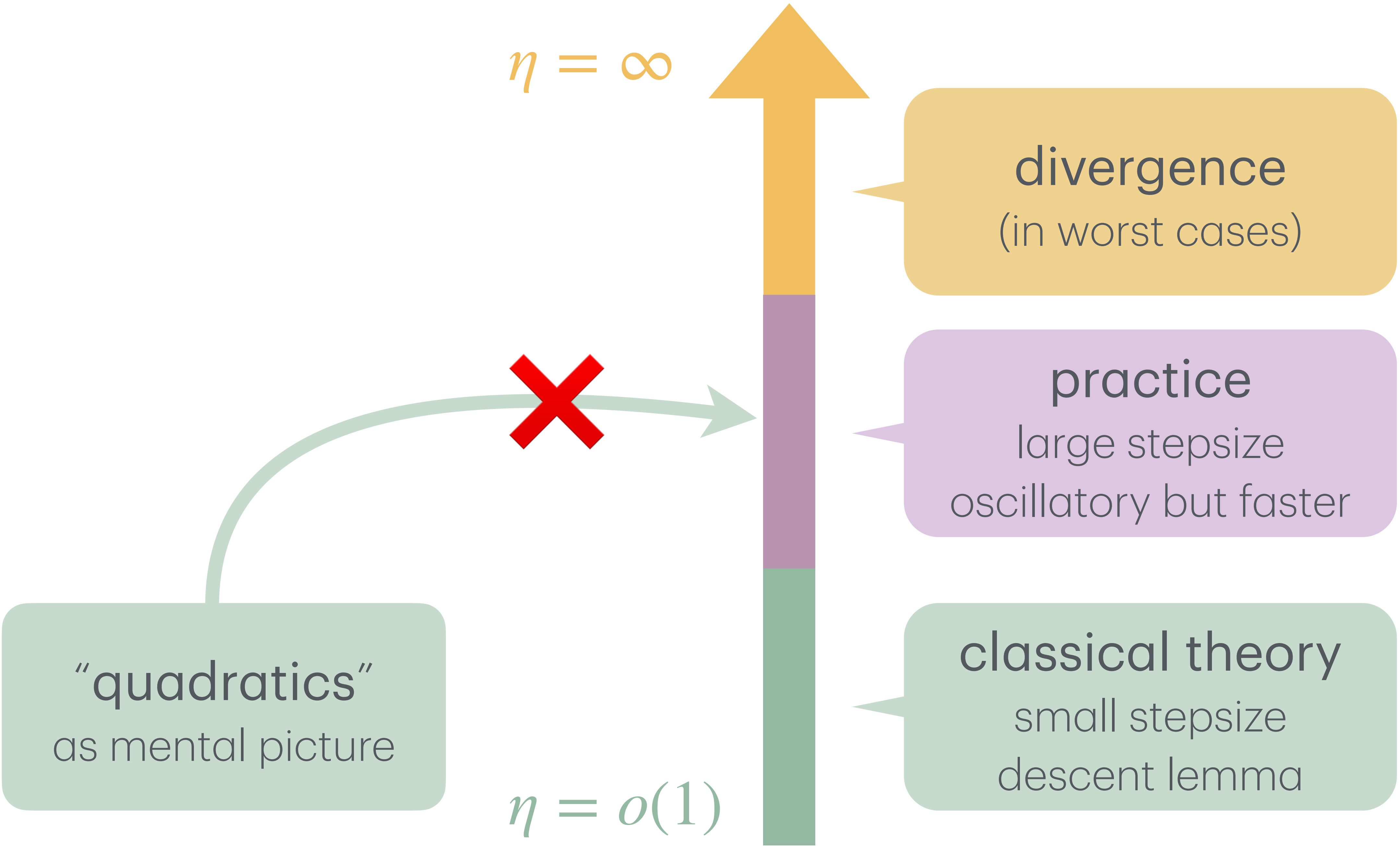

Related works

- Altschuler, Parrilo. "Acceleration by stepsize hedging I: multi-step descent and the silver stepsize schedule." Journal of the ACM 2024
- Grimmer, Shu, Wang. "Composing optimized stepsize schedules for gradient descent." Mathematics of Operations Research 2025

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Seeking simplest sandbox

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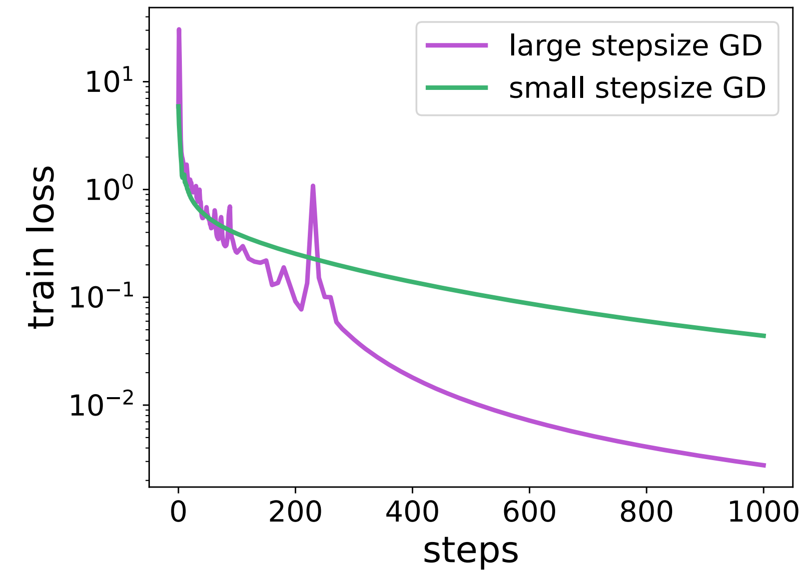
deep learning

unstable optimization observed

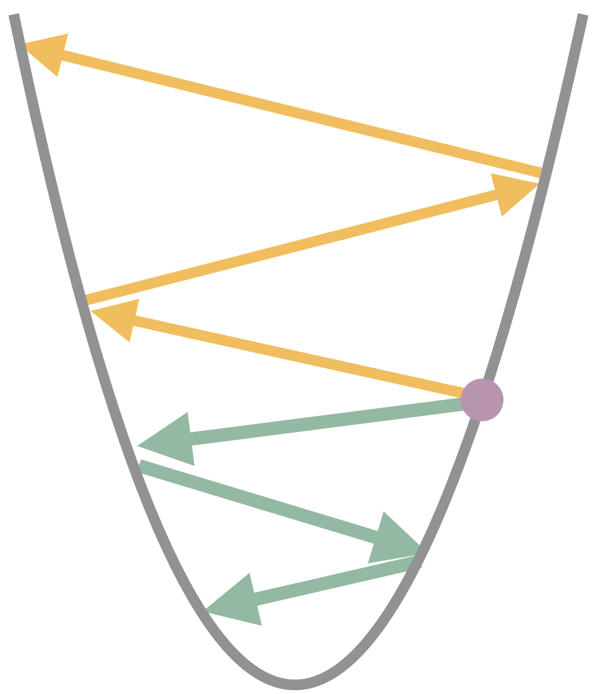


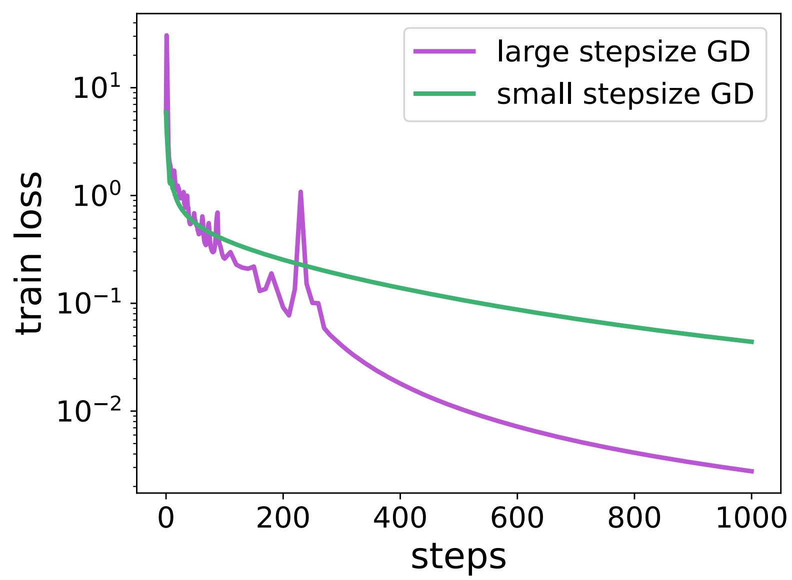
Seeking simplest sandbox

linear regression ...... deep learning

unstable optimization impossible

unstable optimization observed





Seeking simplest sandbox

linear regression

logistic regression

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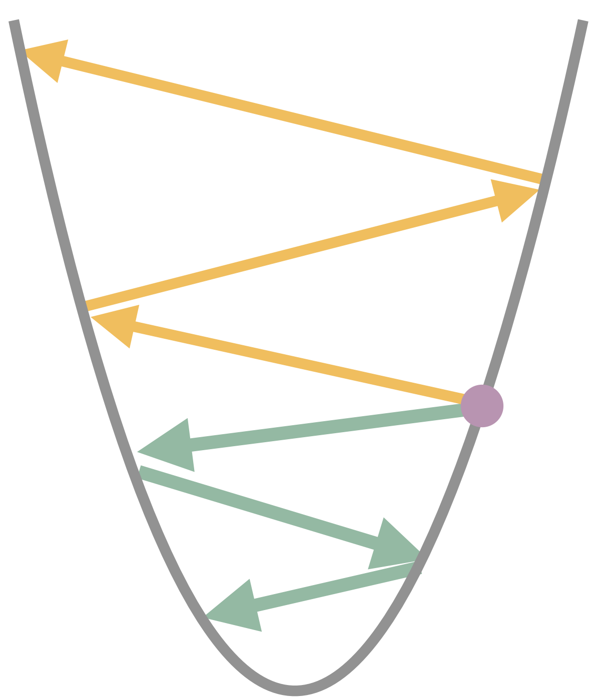
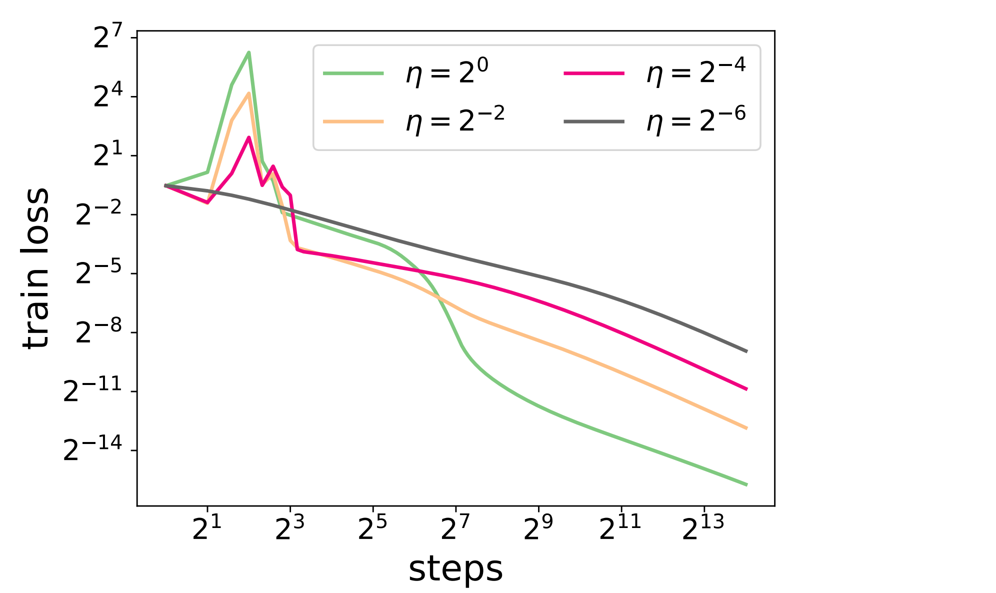
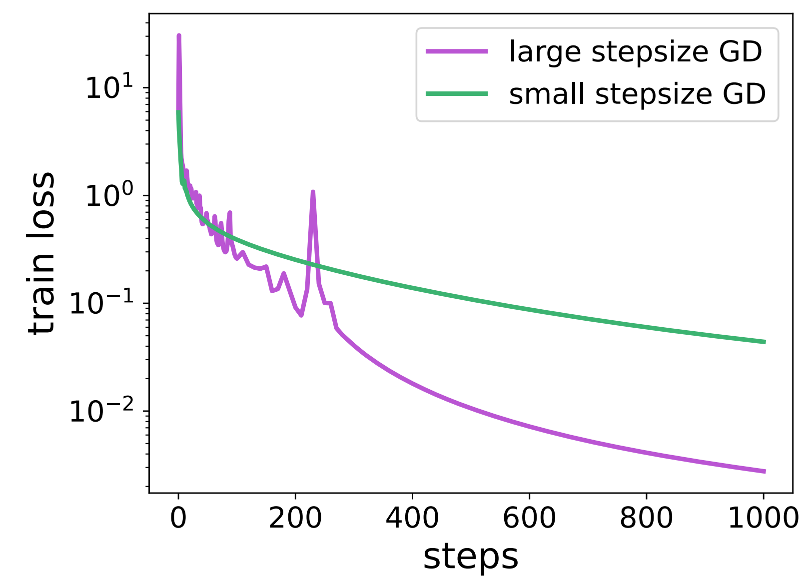
observable & provable

unstable optimization observed







Logistic regression

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

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

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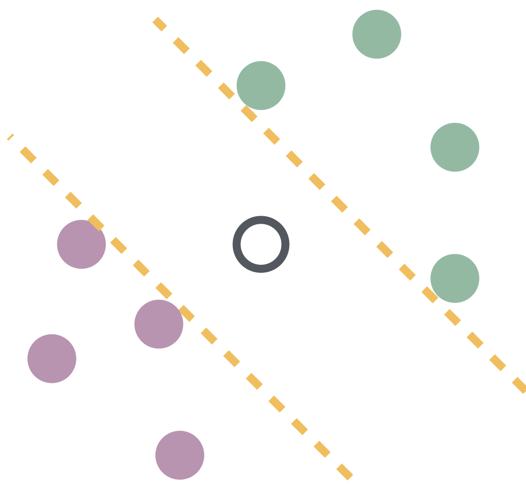

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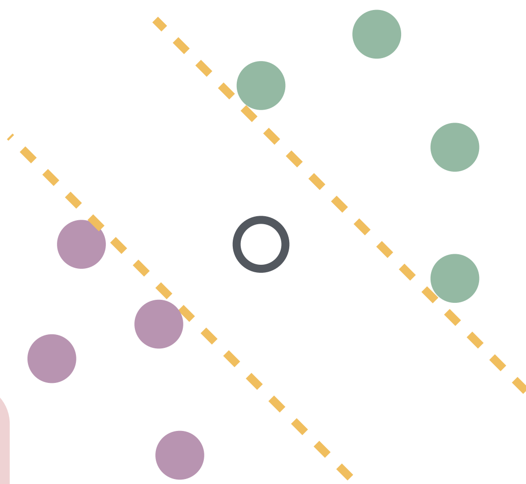
implied by overparameterization



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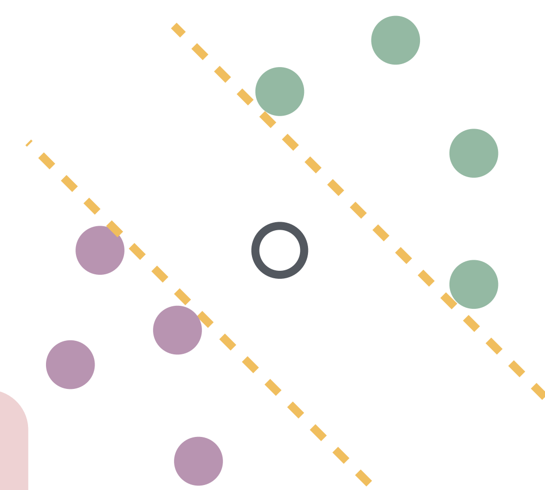

Logistic regression

smooth, convex
non-strongly convex

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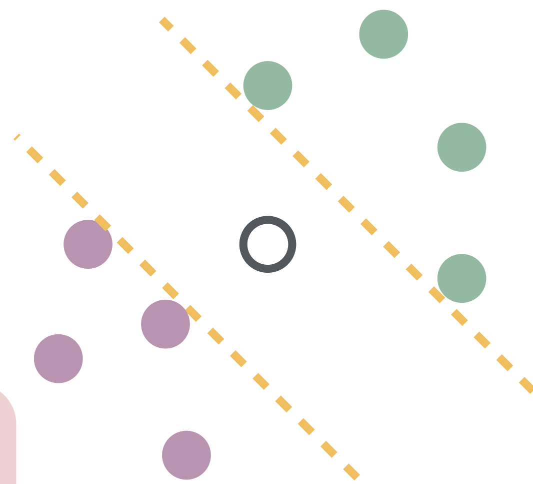

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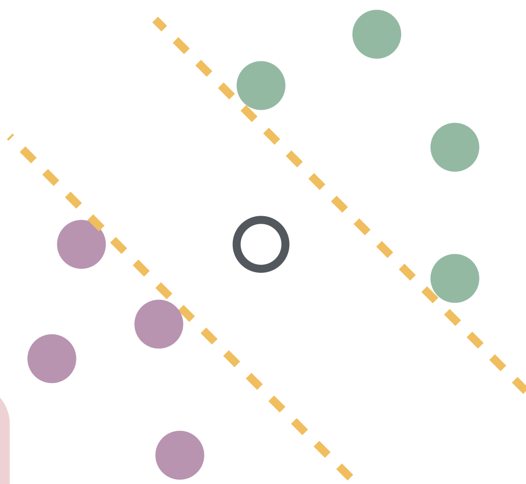

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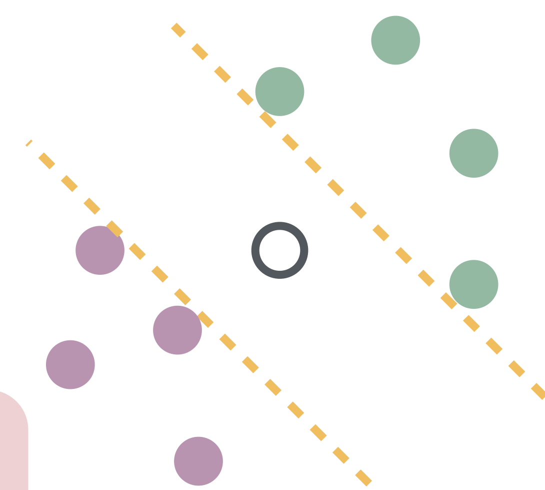

Classical theory. For $\eta = \Theta(1)$, $L(\theta_t) \downarrow$ and $L(\theta_t) = \tilde{O}(1/t)$

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

Large stepsize accelerates GD

Theorem. Let #steps be $T \geq \Theta(1)$. For some $\eta = \Theta(T)$, we have

$$L(\theta_T) = \tilde{O}(1/T^2)$$

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

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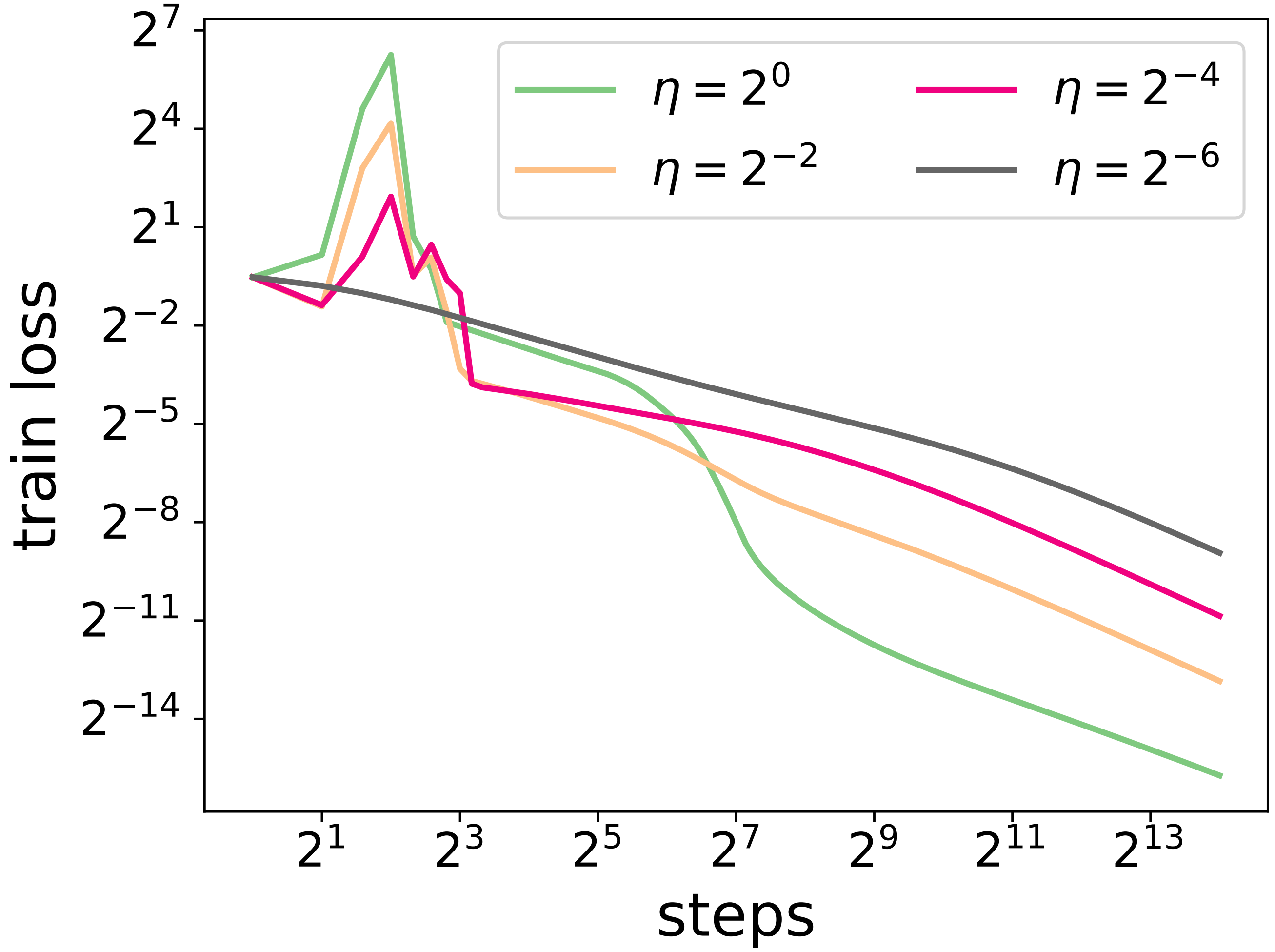

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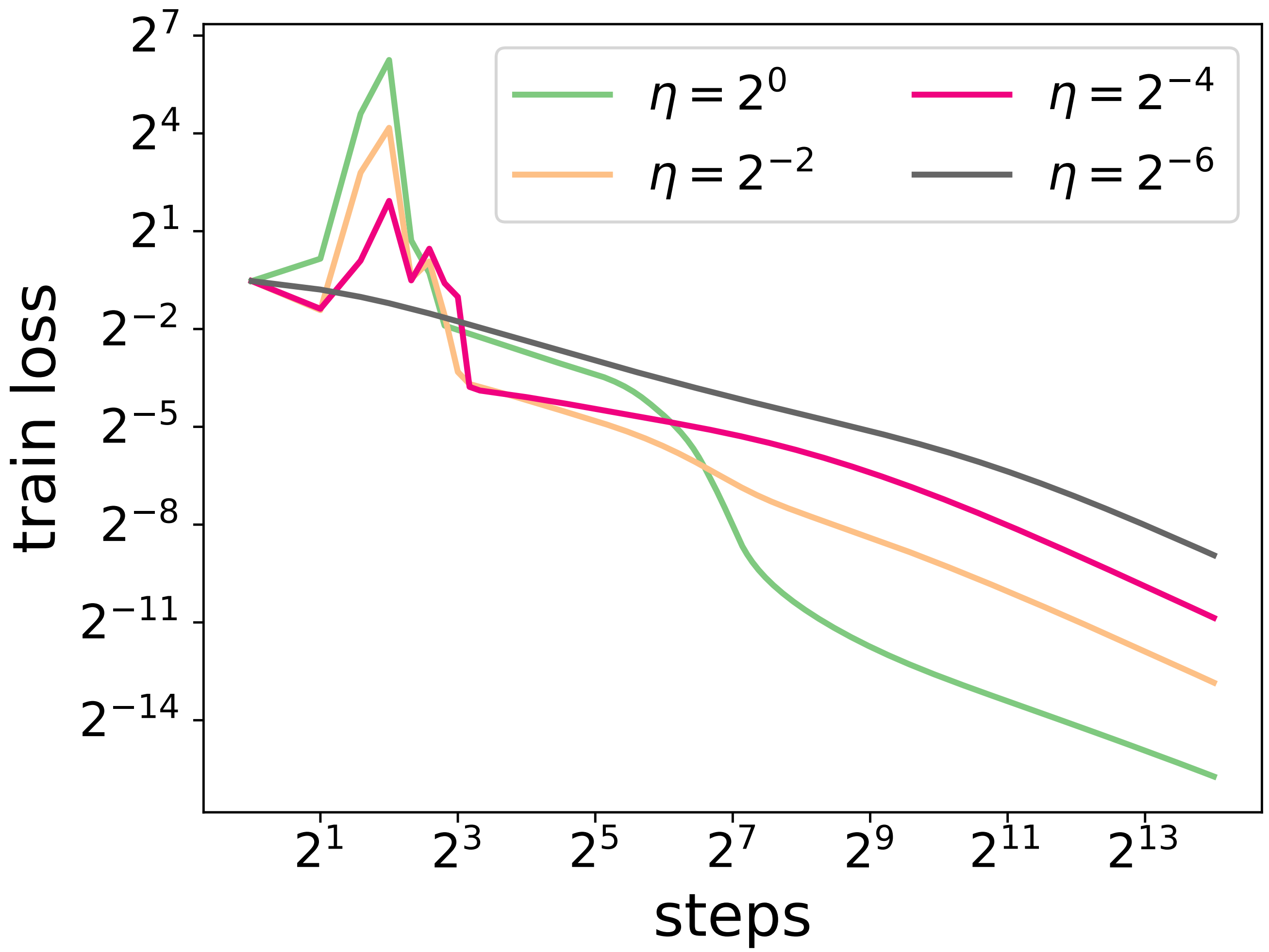

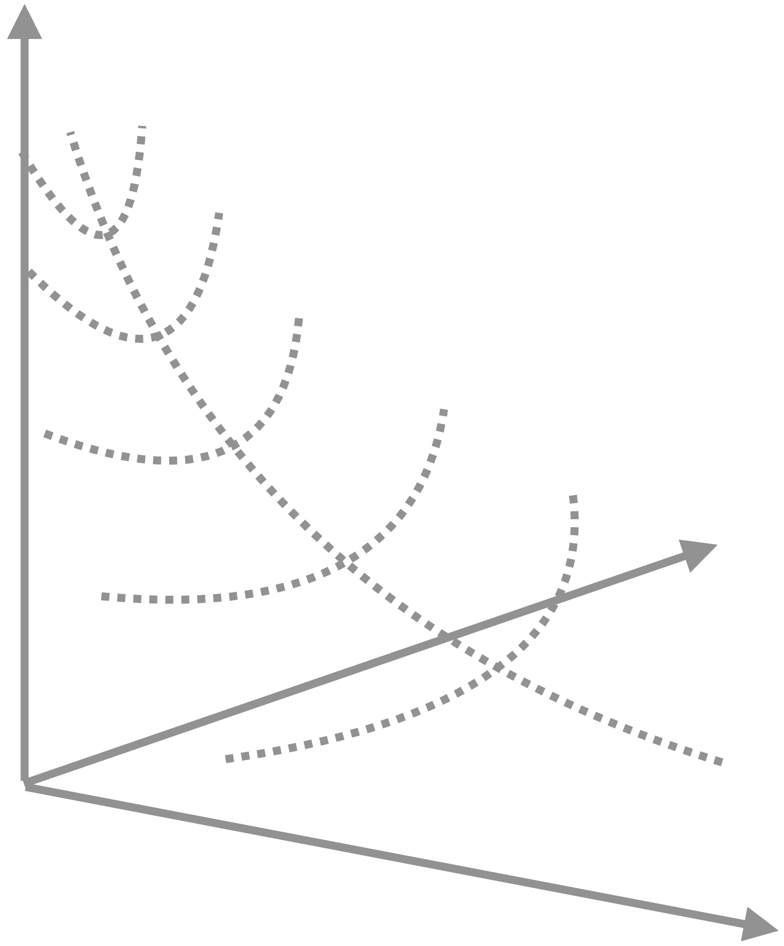

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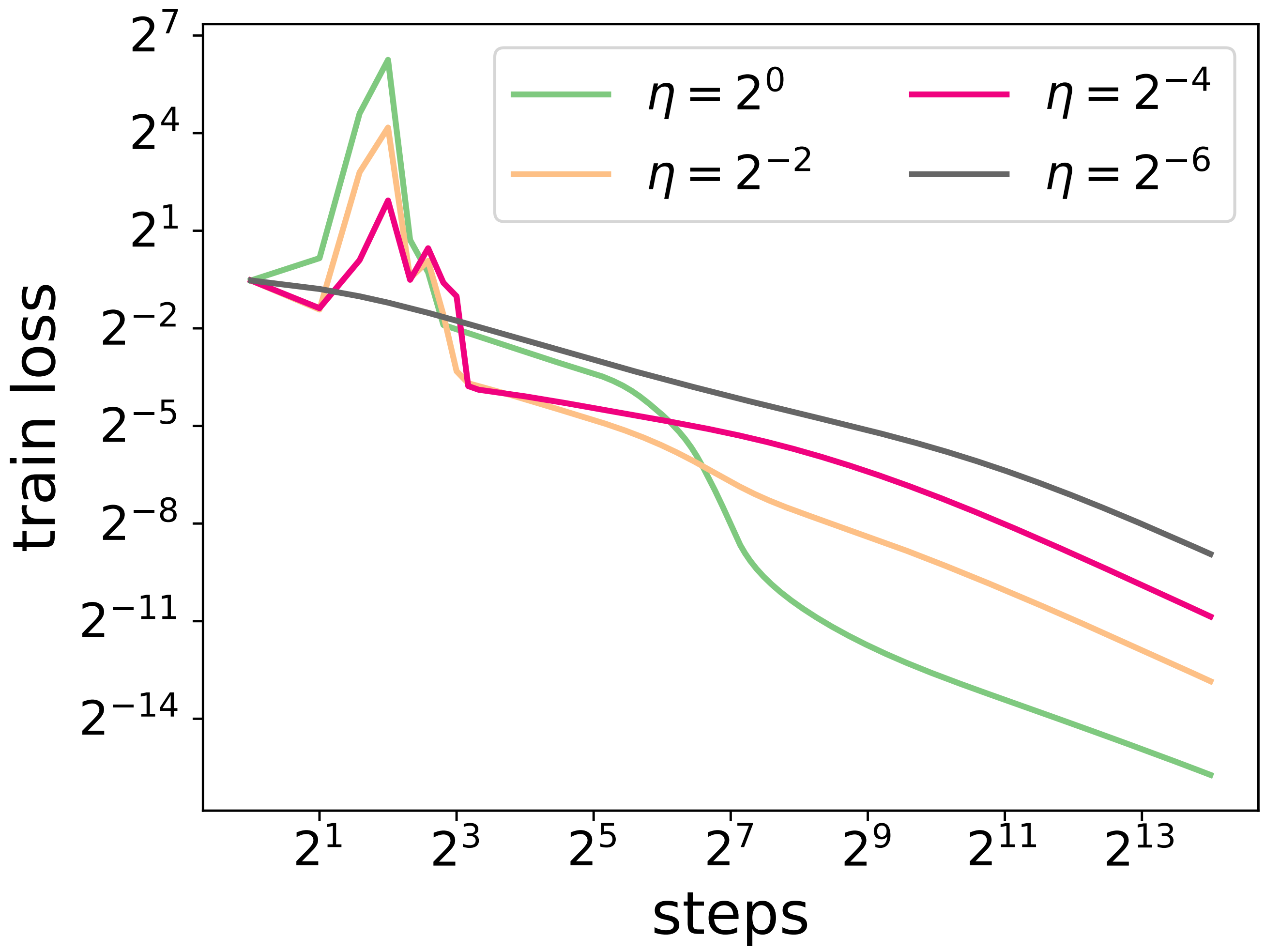

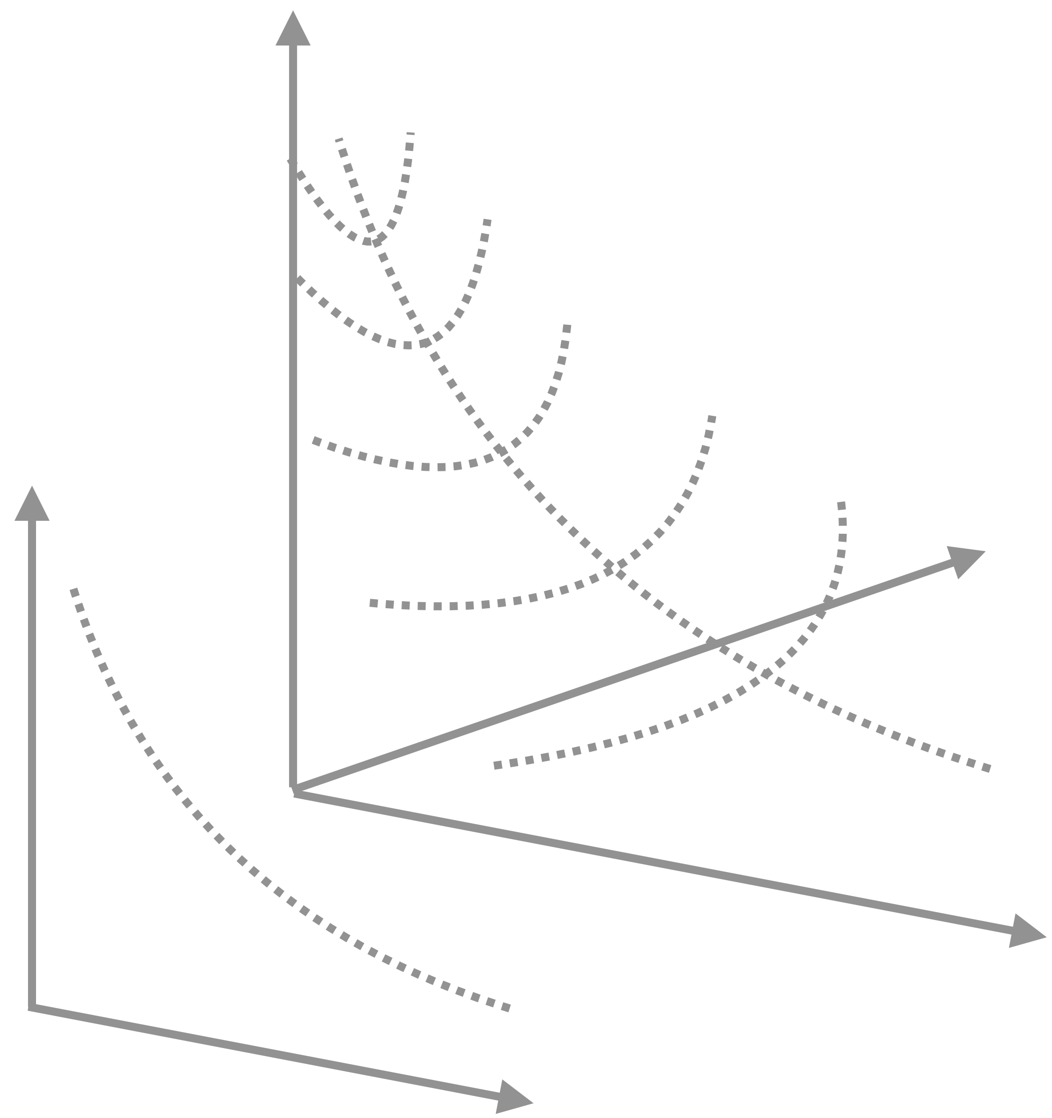

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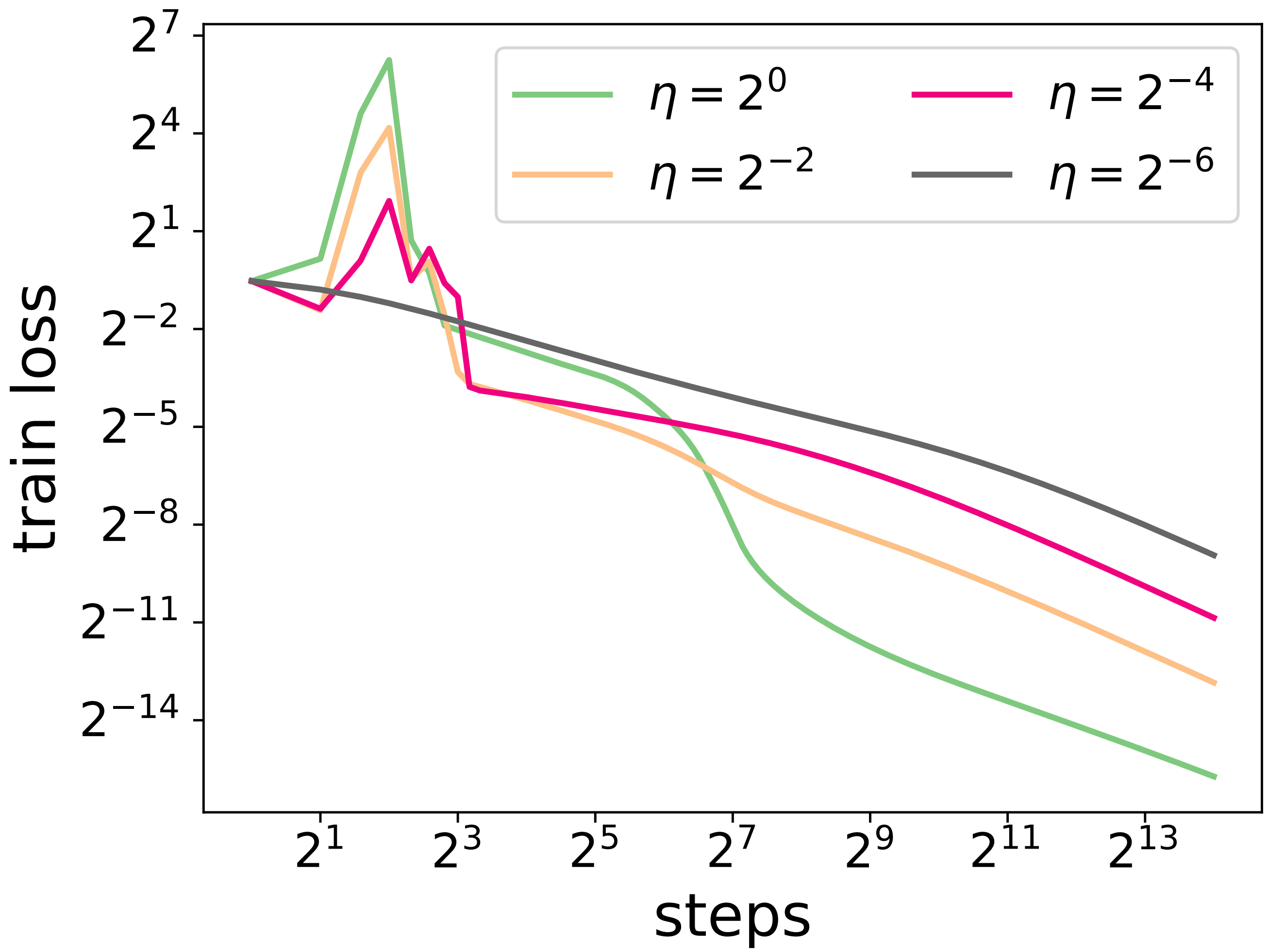

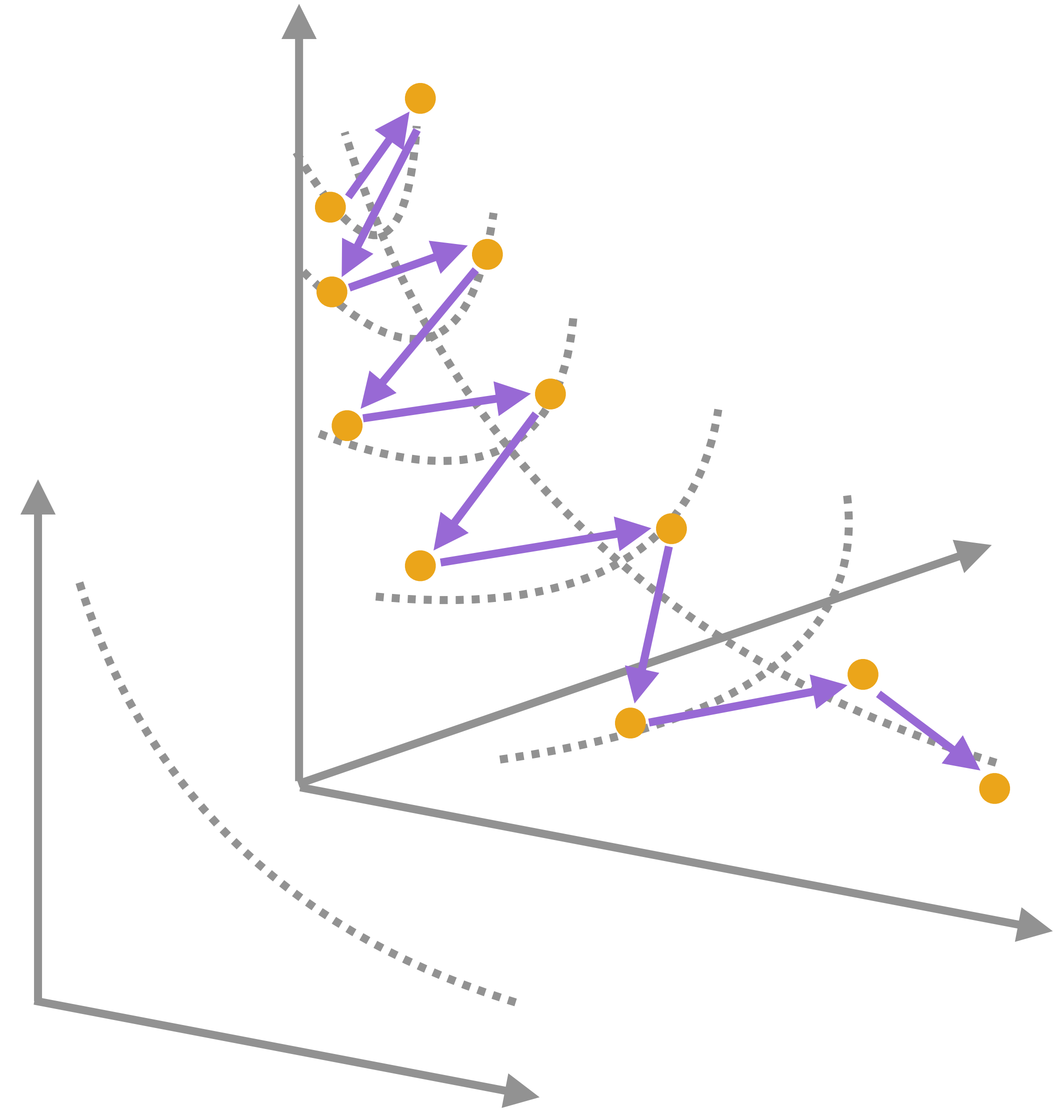

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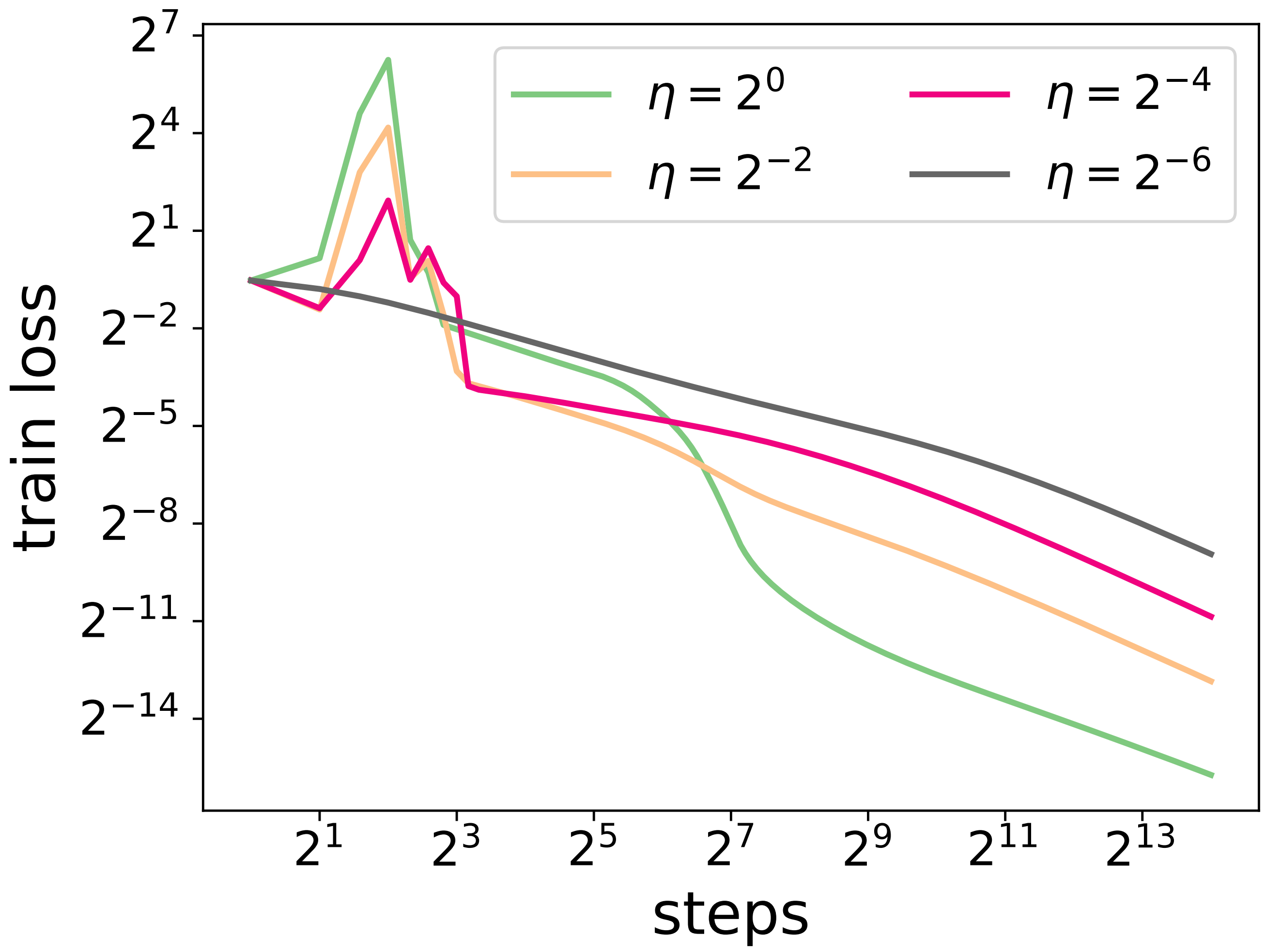

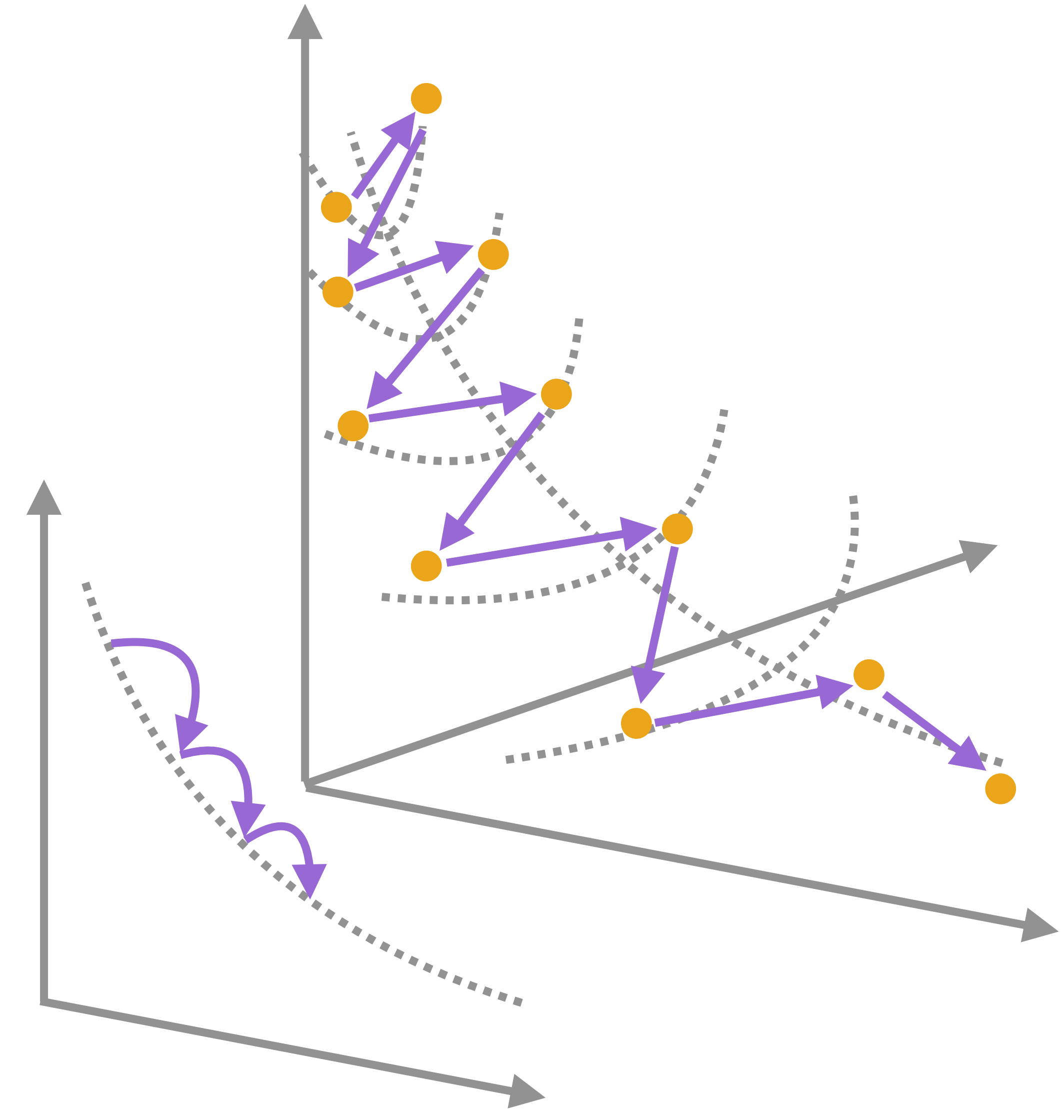

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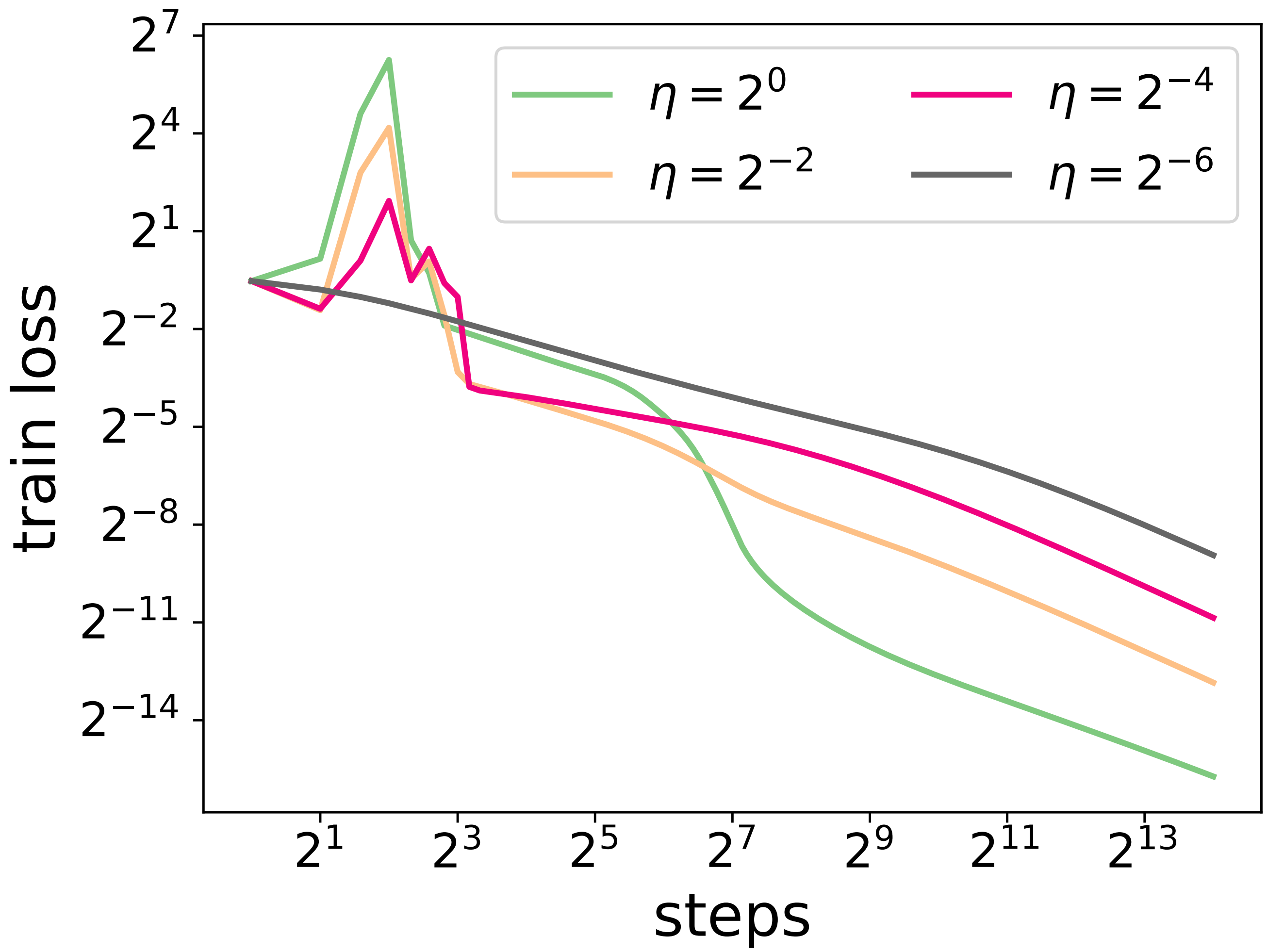
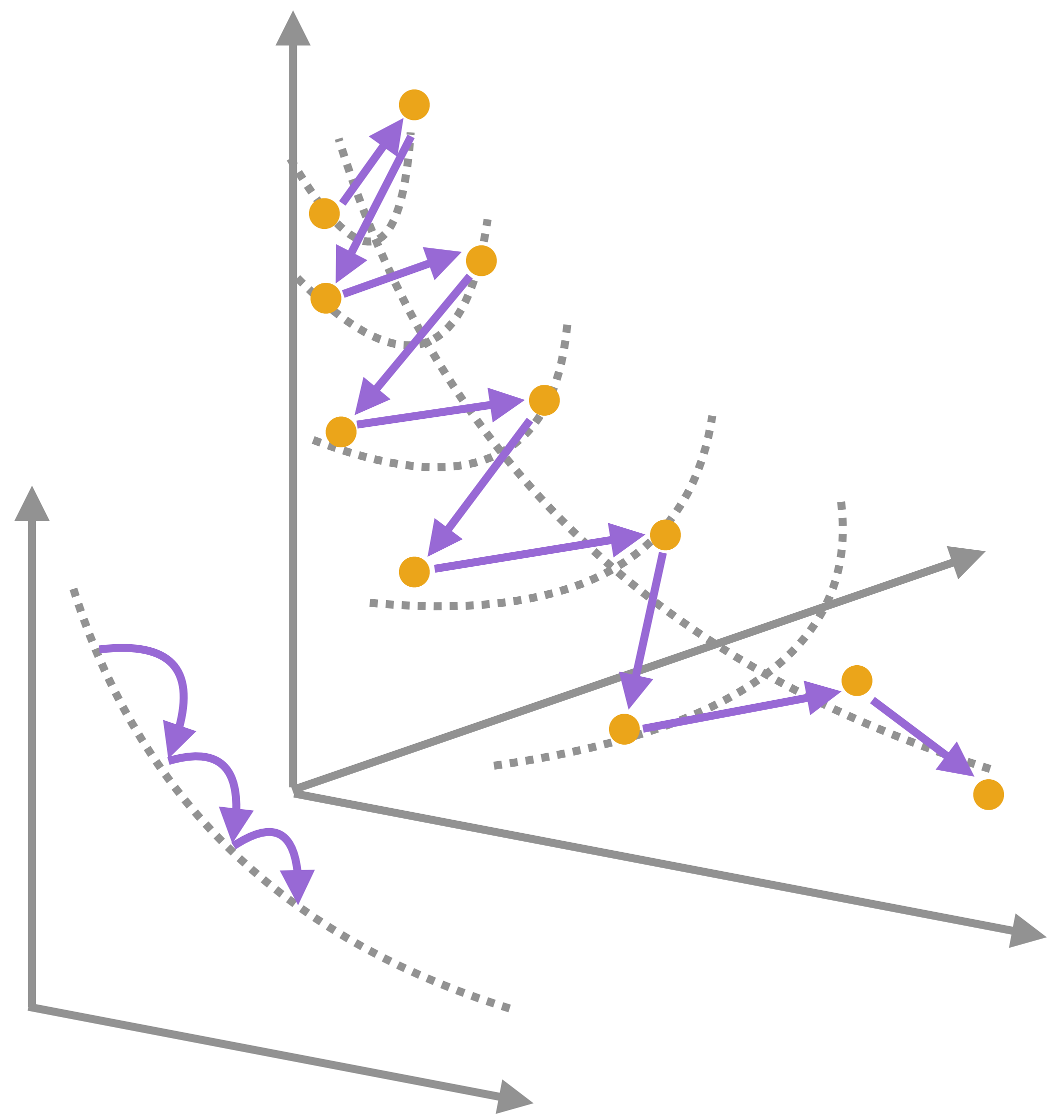
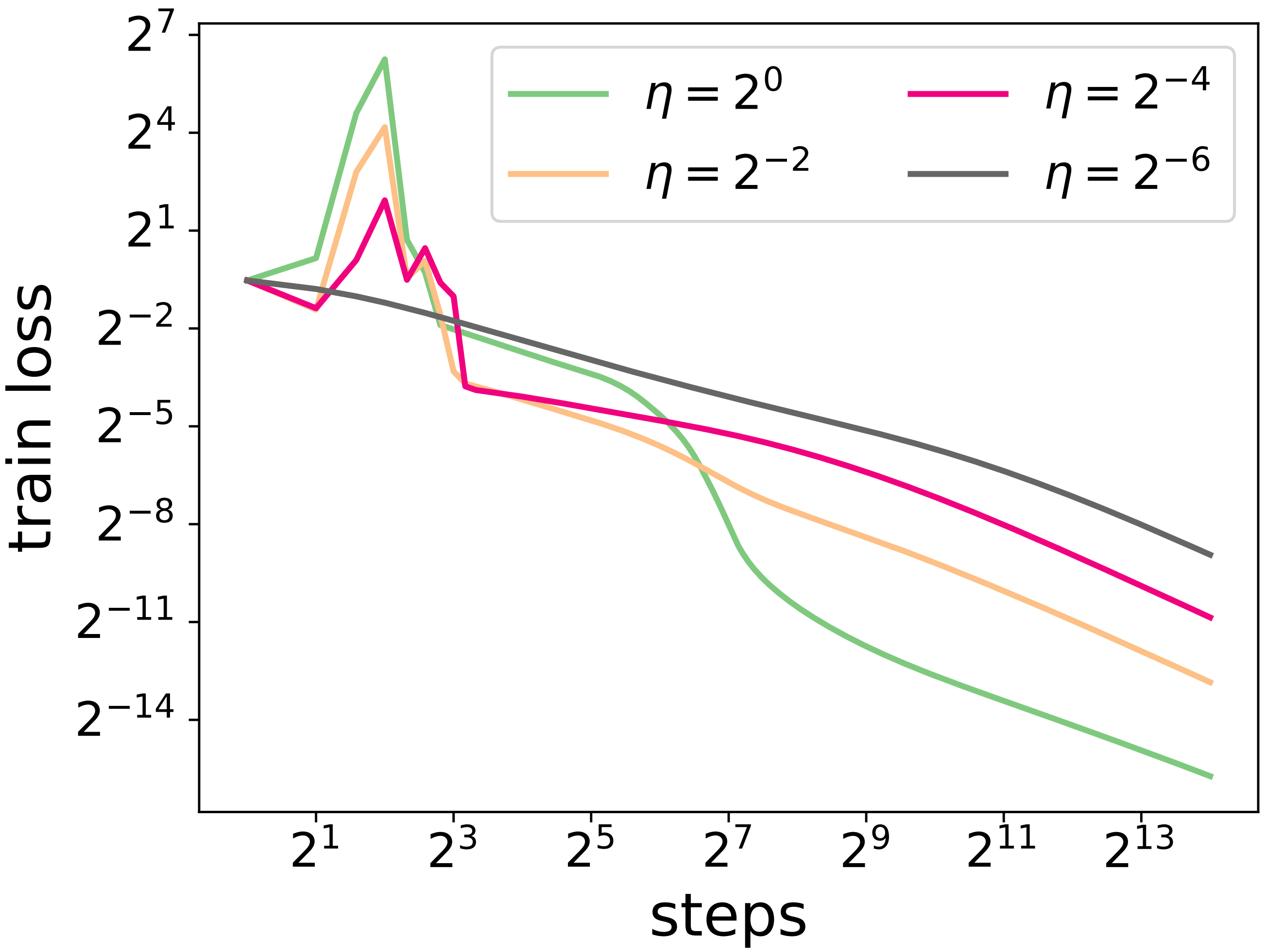




"open valley" as mental picture

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

More details



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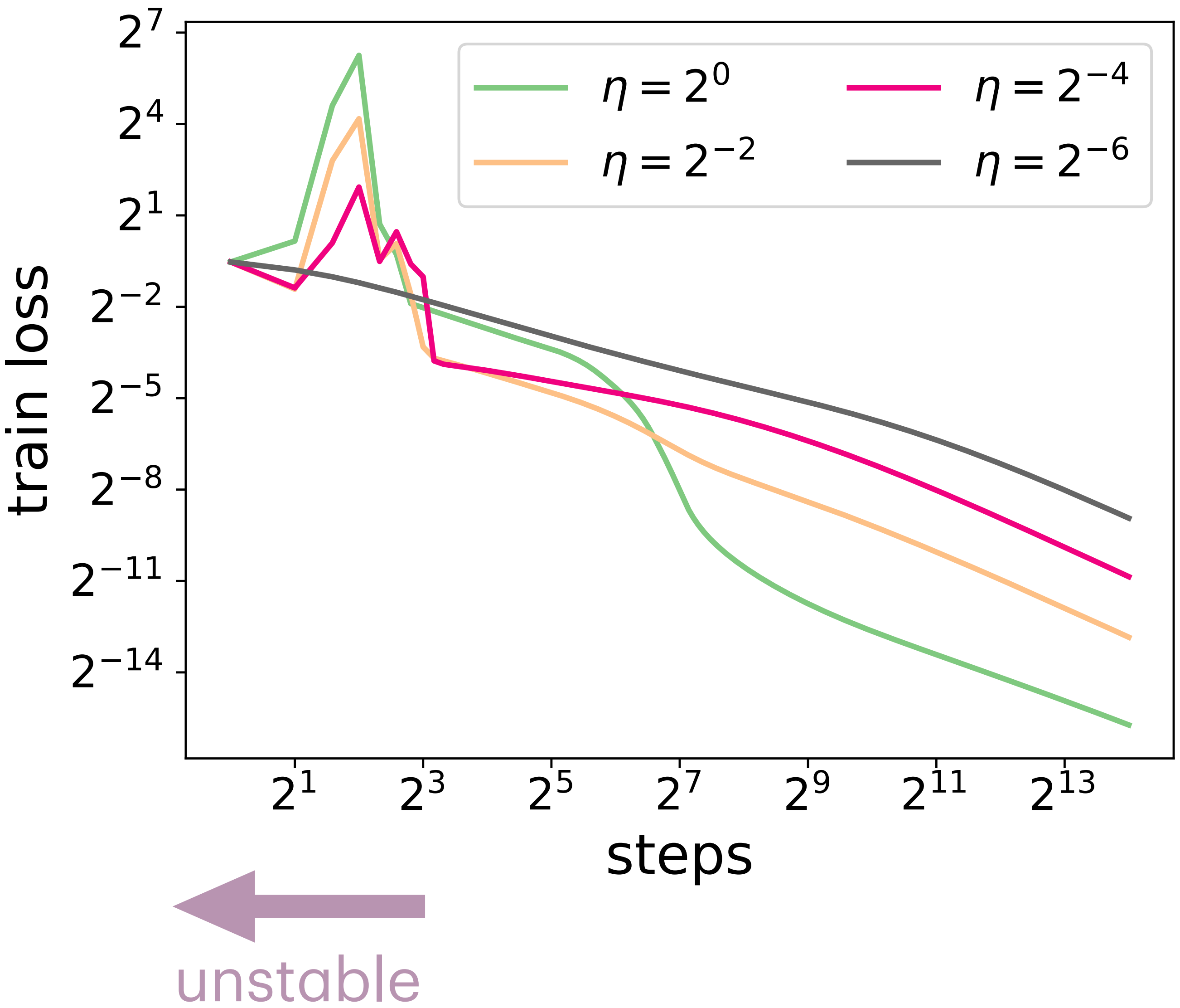

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- **Unstable phase:**

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

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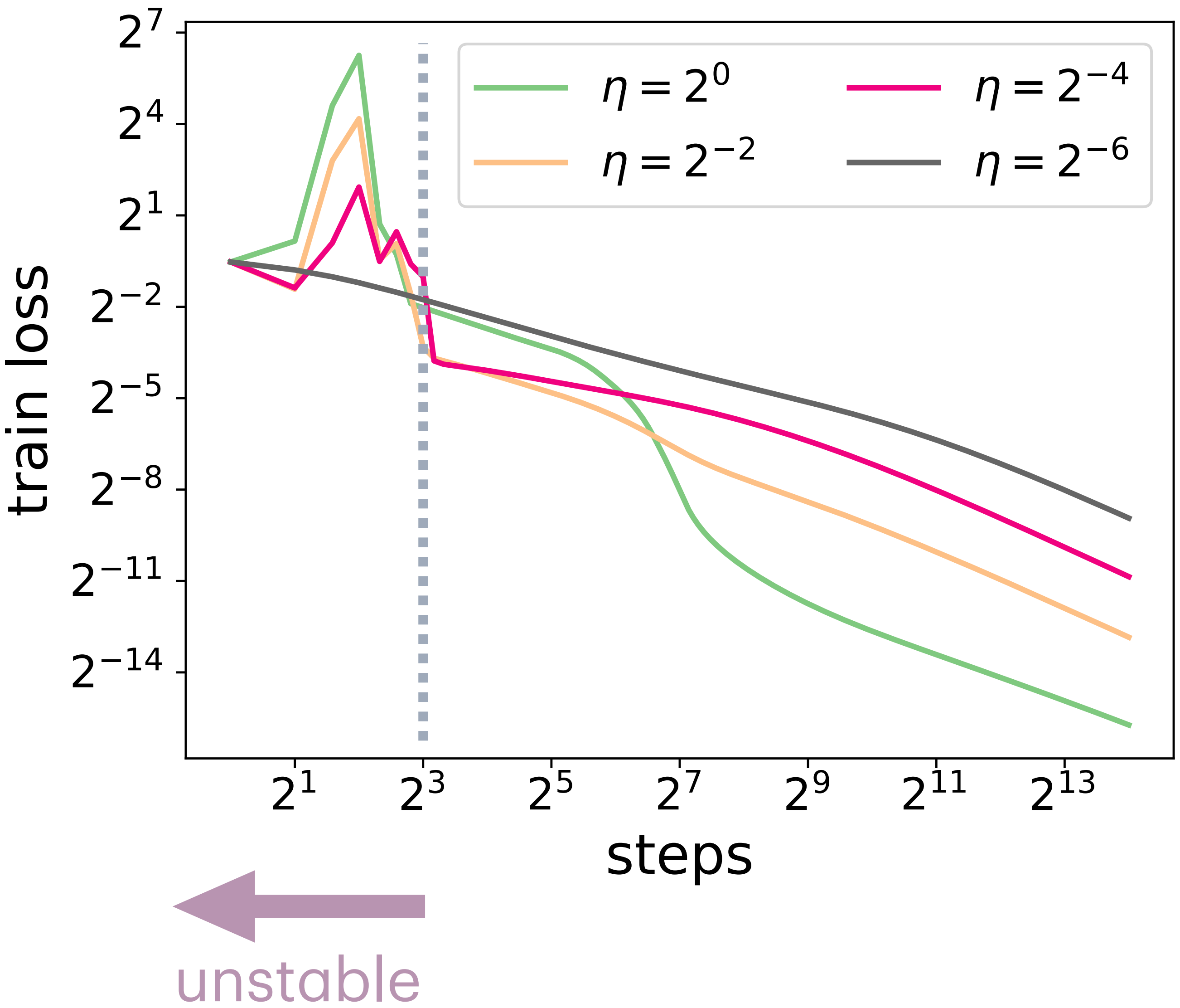

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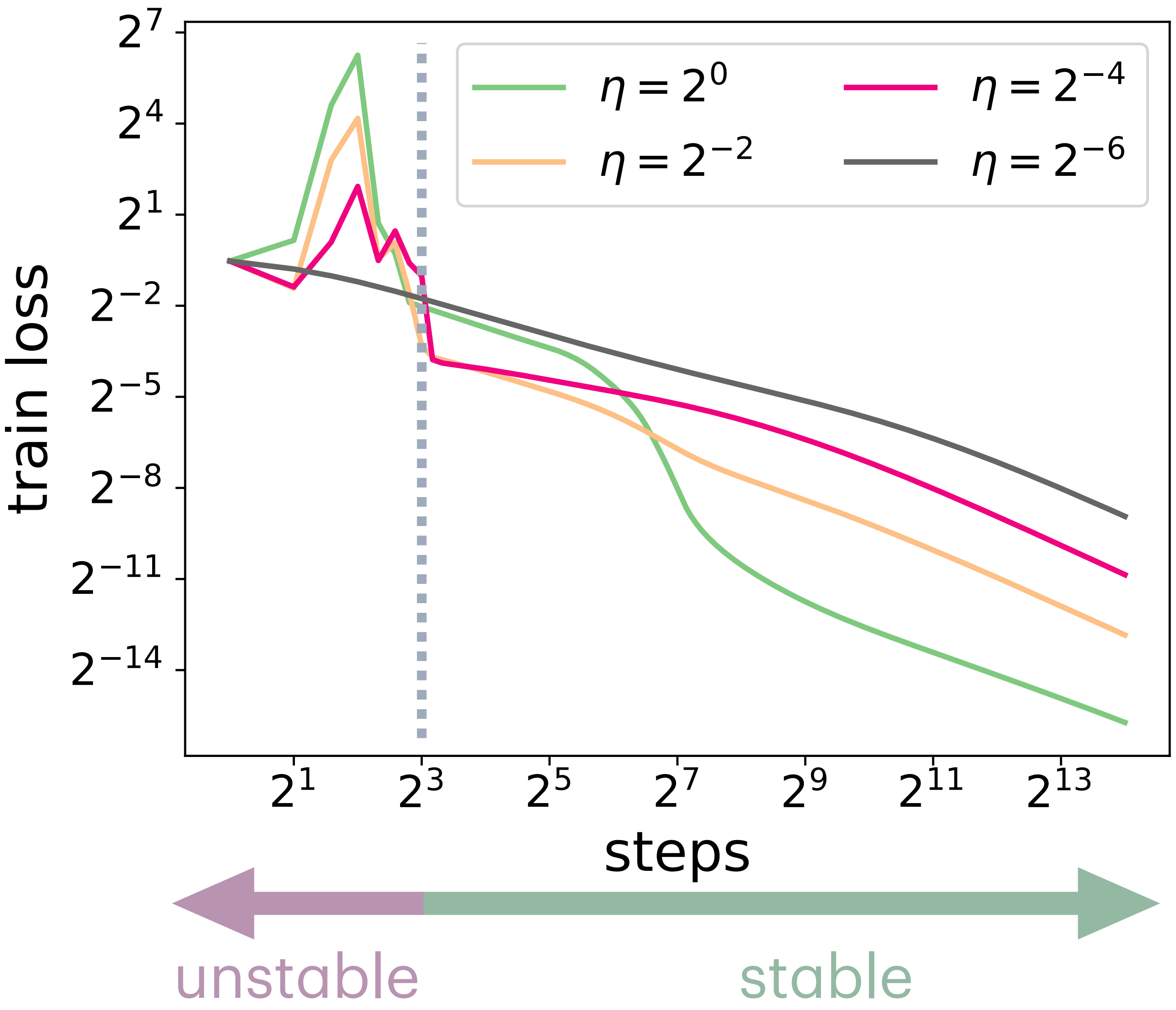

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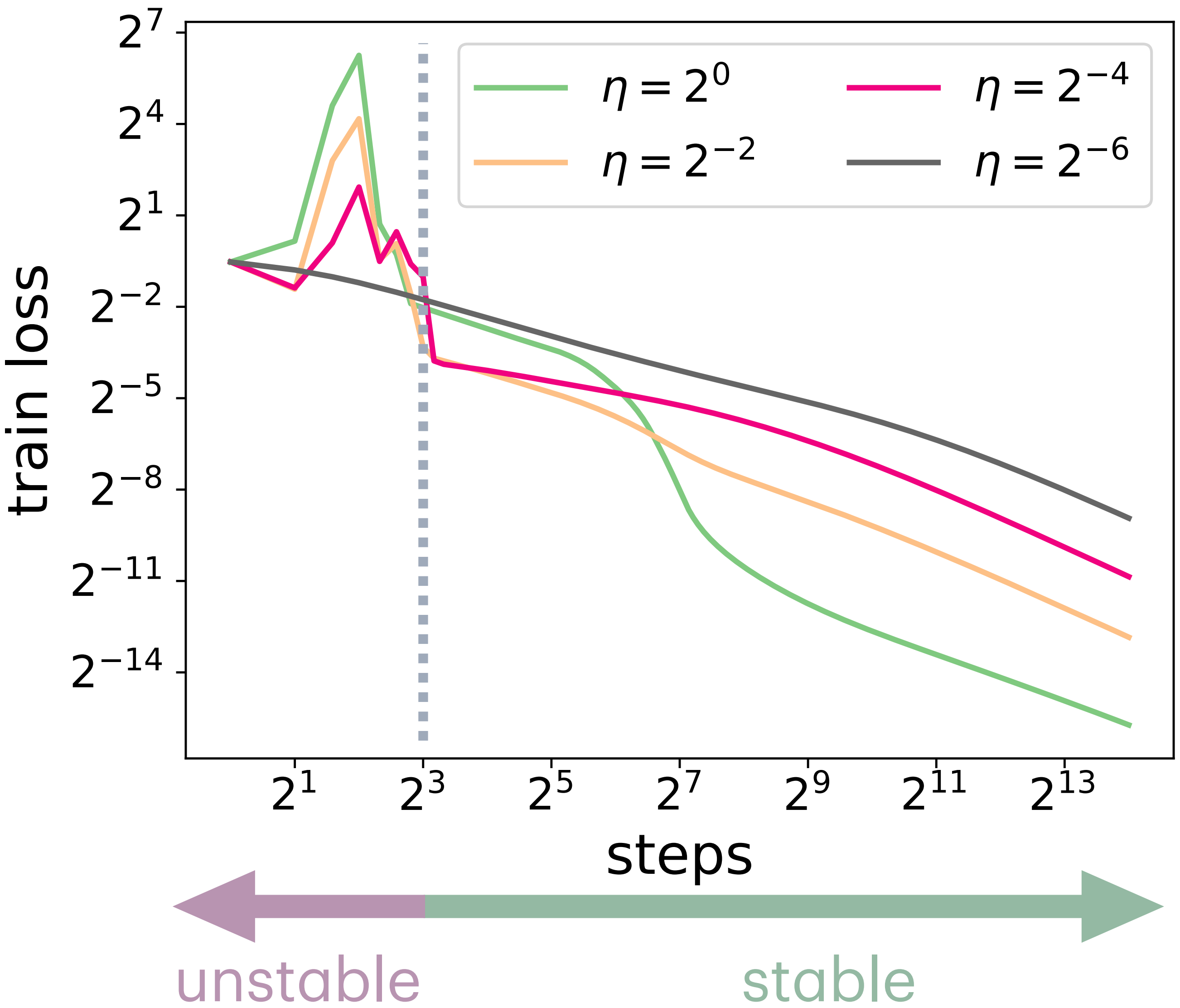

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Wu, Bartlett, Telgarsky, Yu. "Large stepsize gradient descent for logistic loss: non-monotonicity of the loss improves optimization efficiency." COLT 2024

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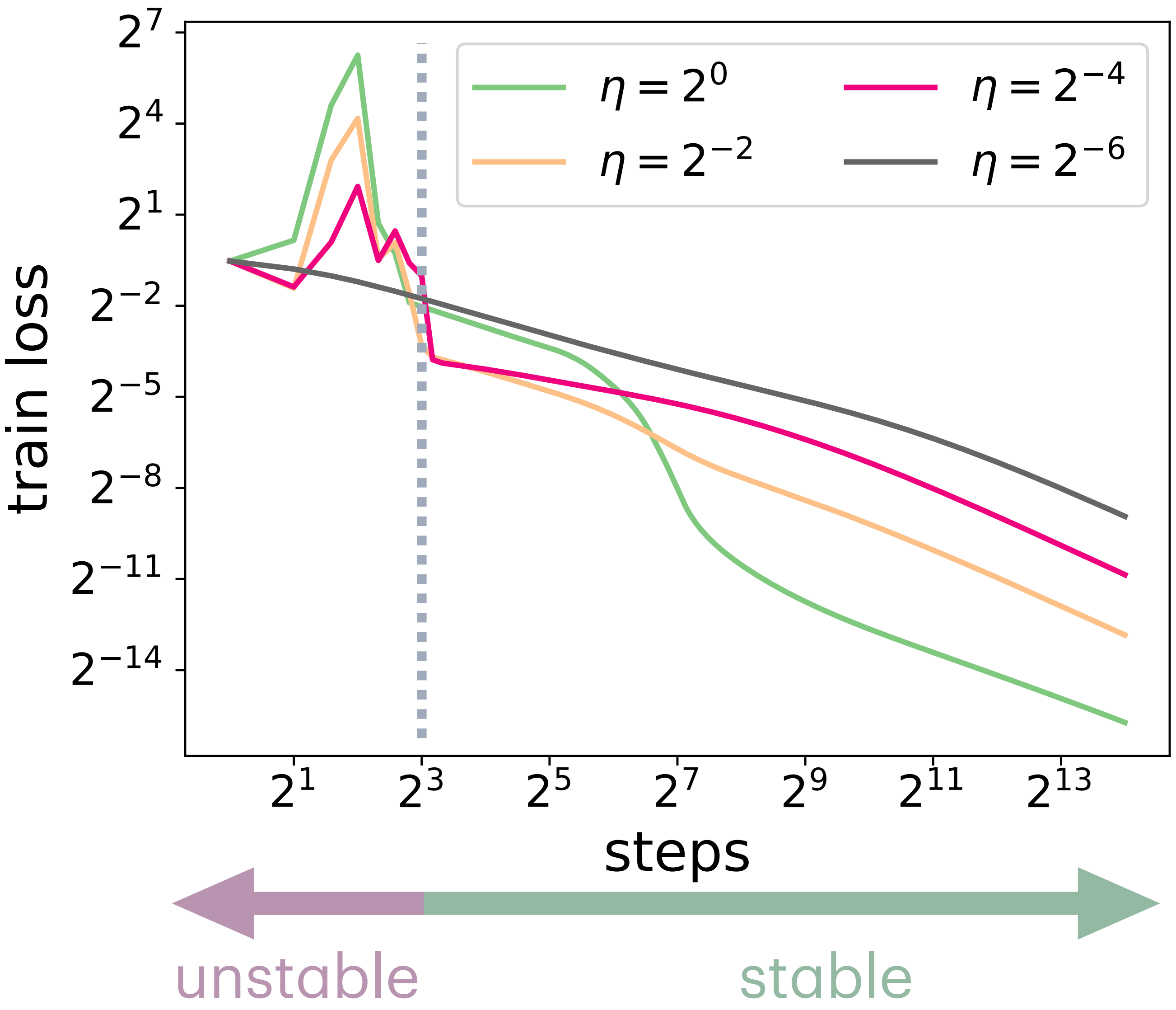

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"instability" is needed for acceleration

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

Regularized logistic regression

regularized empirical risk $\tilde{L}(\theta) = L(\theta) + \frac{\lambda}{2}||\theta||^2$

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Our theory. Assume $\lambda \le \Theta(1)$. For $\eta = \Theta\big(\sqrt{\kappa}\big)$, we have

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Wu, Marion, Bartlett. "Large stepsizes accelerate gradient descent for regularized logistic regression." NeurIPS 2025

Regularized logistic regression

regularized empirical risk $\tilde{L}(\theta) = L(\theta) + \boxed{\frac{\lambda}{2}\|\theta\|^2}$

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

$\Theta(1)$-smooth, λ-strongly convex $\Rightarrow$ condition number $\kappa = \Theta(1/\lambda) \gg 1$

Classical theory. For $\eta = \Theta(1)$, we have $\tilde{L}(\theta_t) \downarrow$ and

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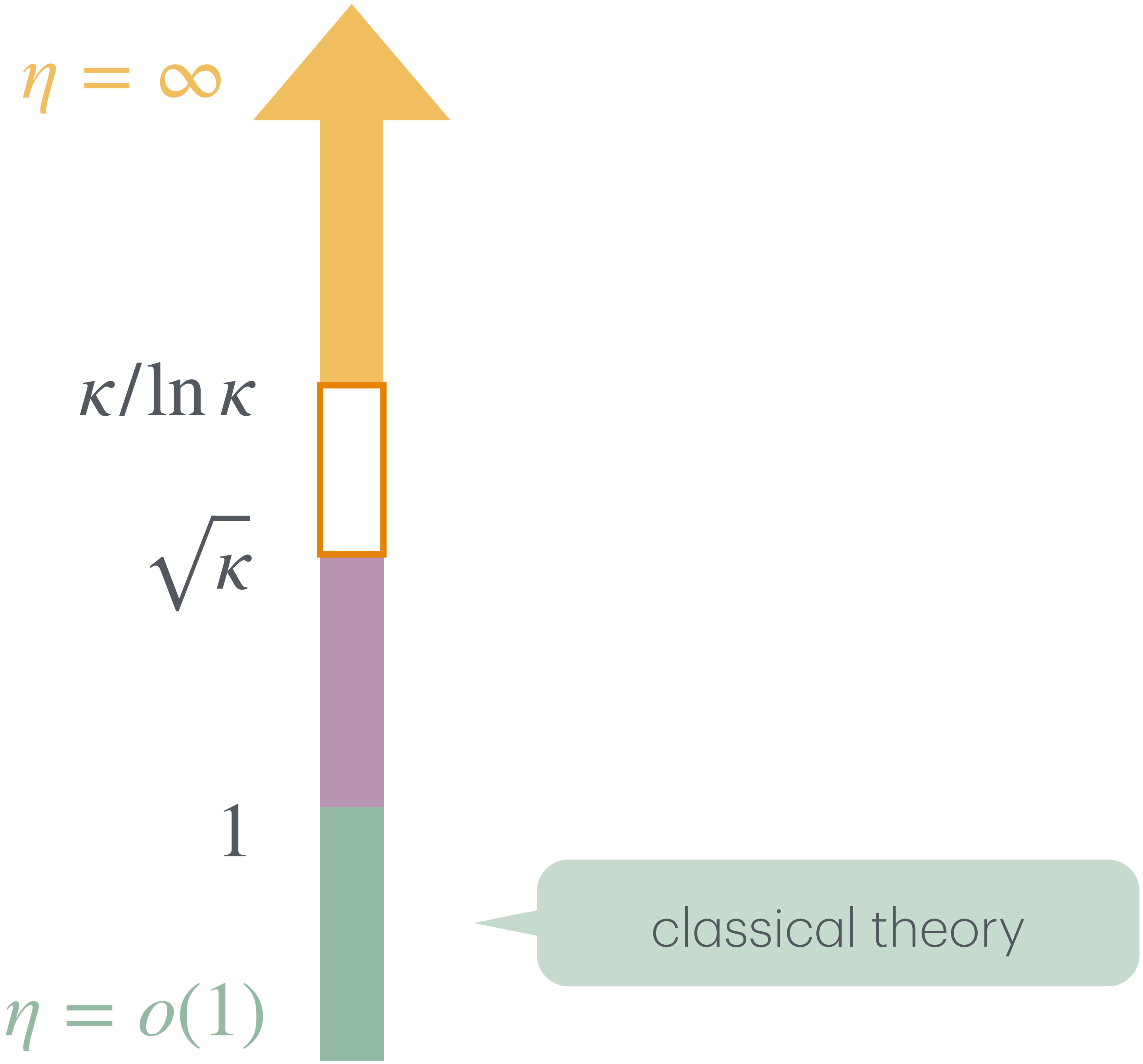
Stepsize diagram revisited



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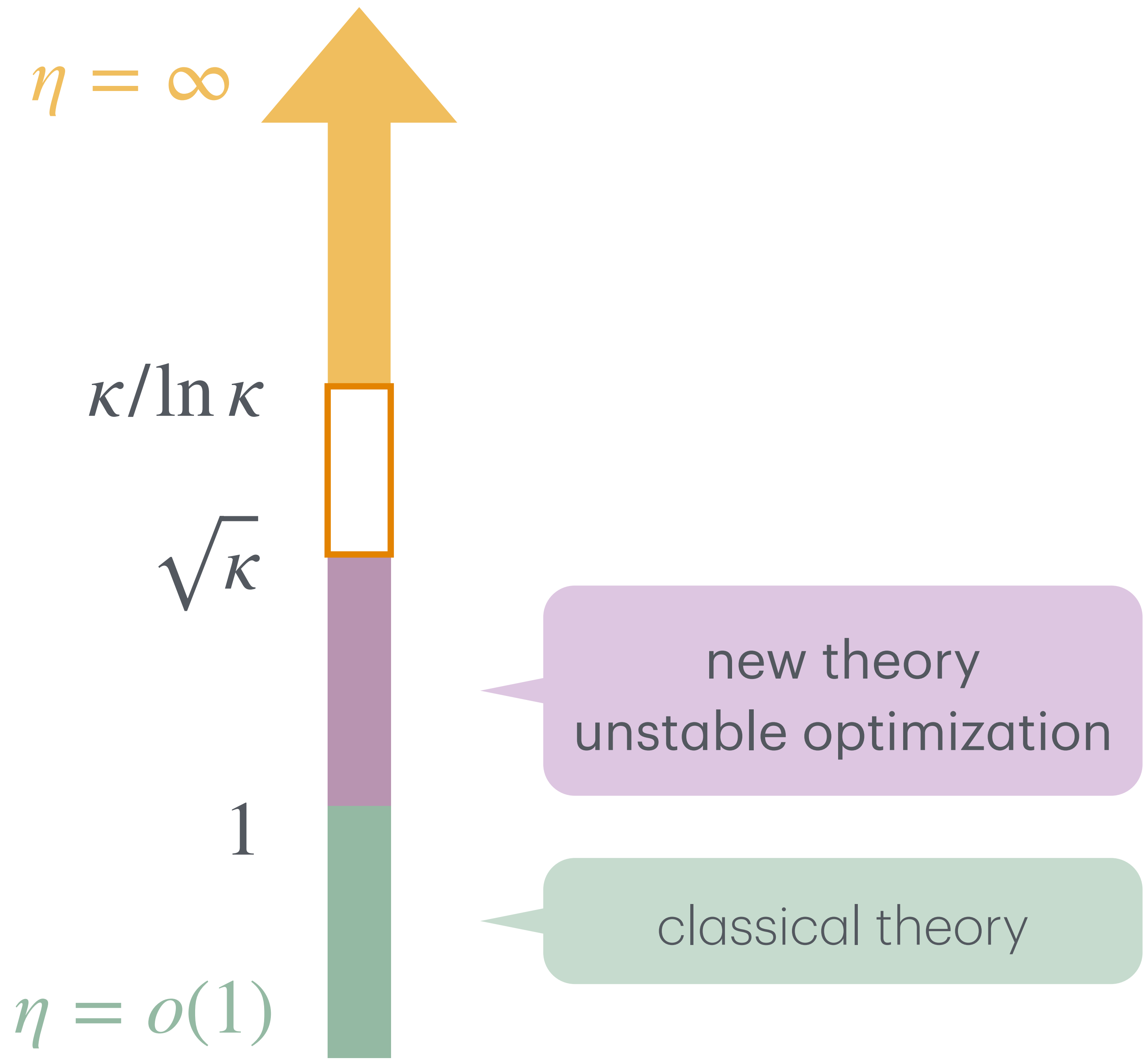

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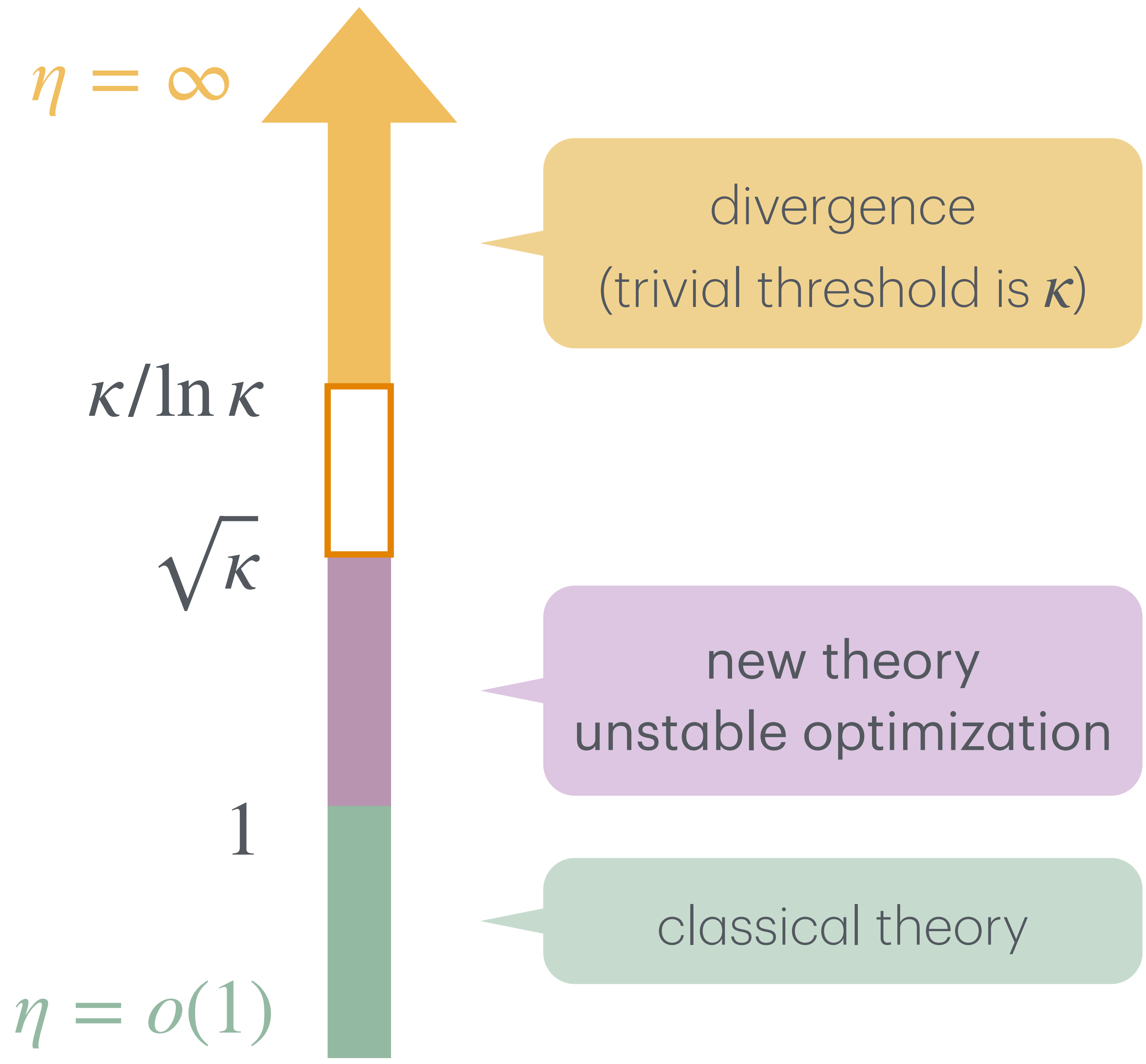

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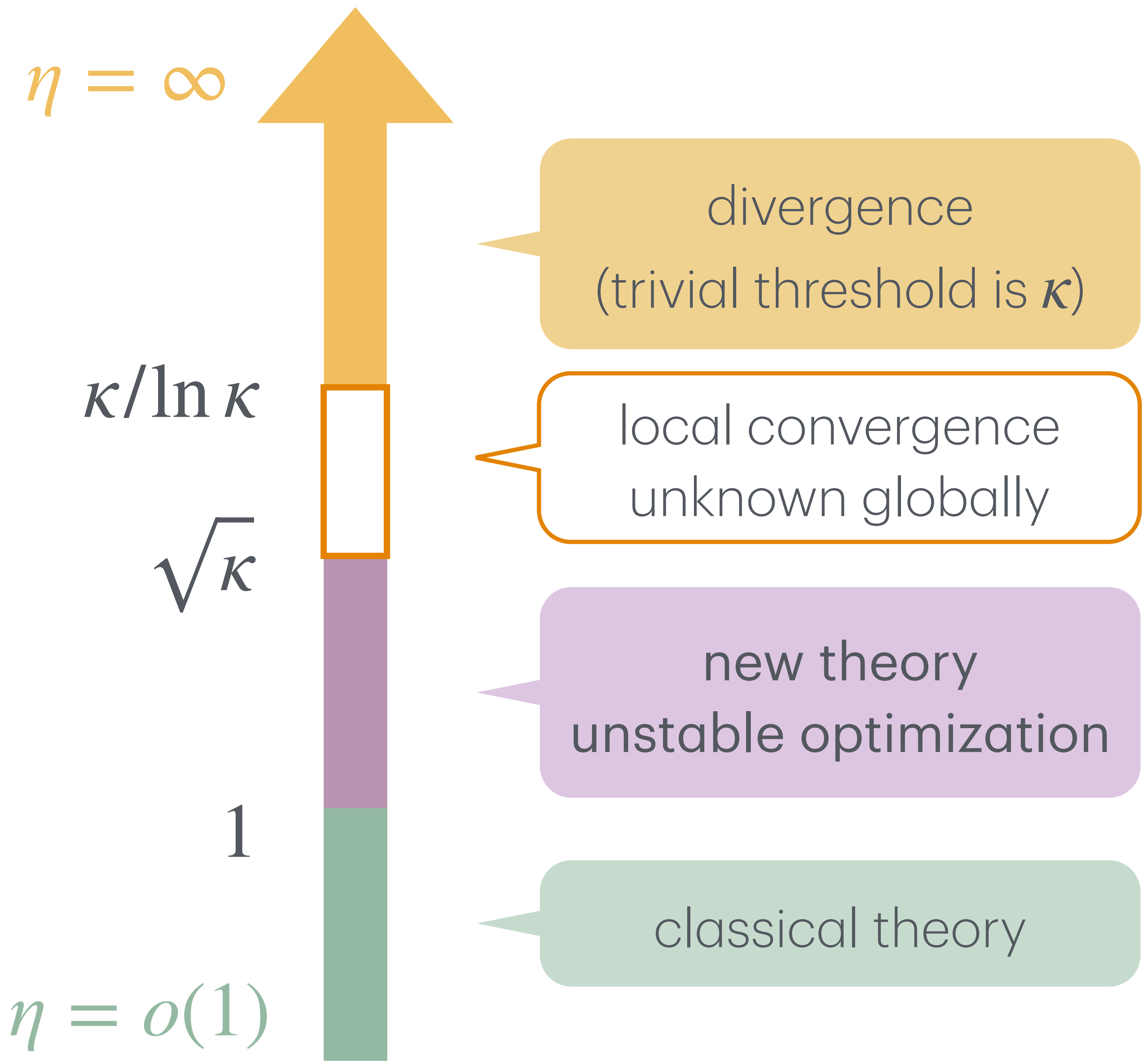

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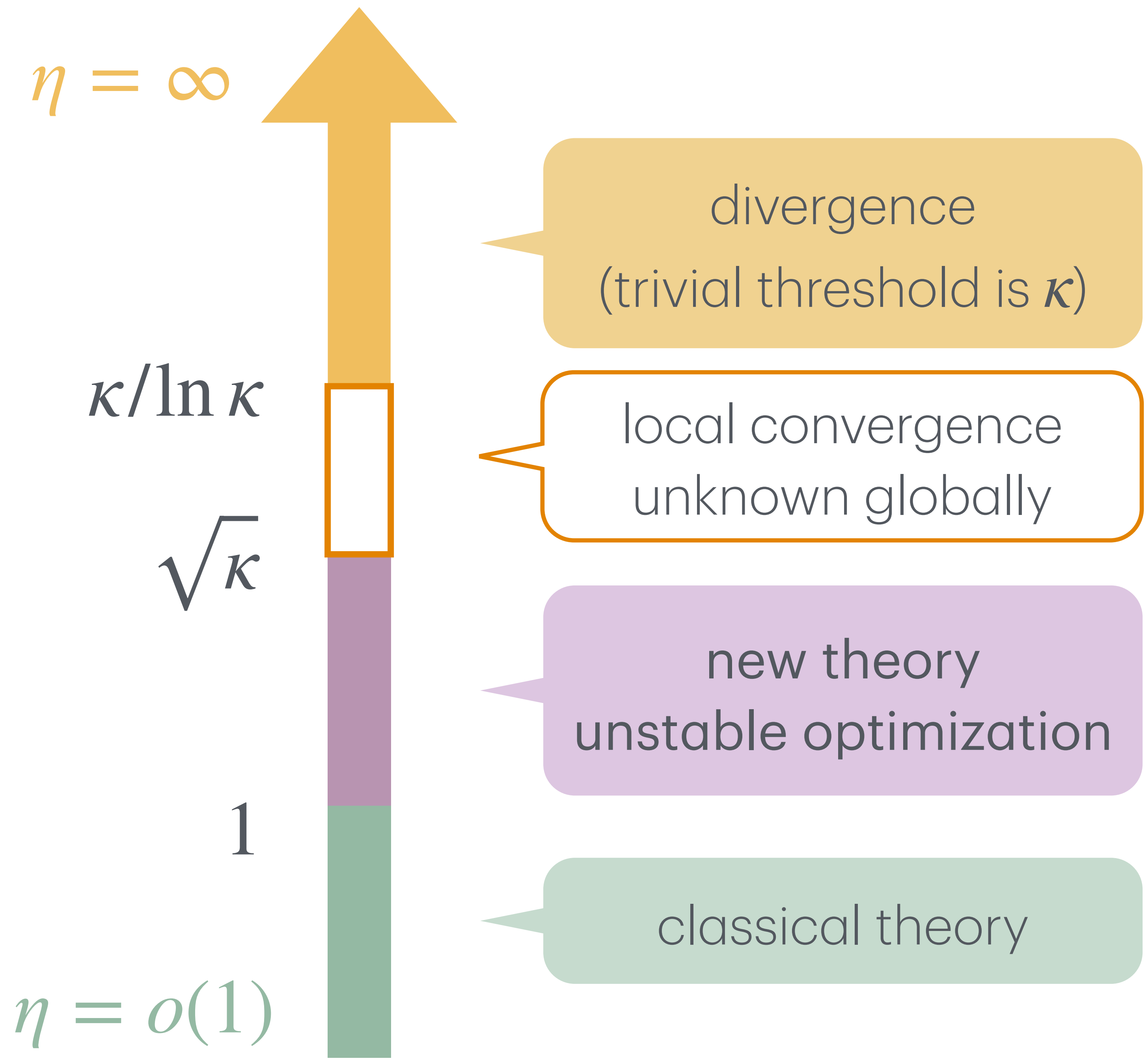

three extensions

- general loss functions (WBTY'24)
- *two-layer networks (WBTY'24, CWMLB'24)
- large adaptive stepsizes (ZWLB'25)

Wu, Marion, Bartlett. "Large stepsizes accelerate gradient descent for regularized logistic regression." NeurIPS 2025

Cai, **Wu**, Mei, Lindsey, Bartlett. "Large stepsize GD for non-homogeneous two-layer networks: margin improvement and fast optimization." NeurIPS 2024

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

Contribution 2: implicit regularization

gradient descent dominates ridge regression in linear regression

- “Risk comparisons in linear regression: implicit regularization dominates explicit regularization”
  W, Peter Bartlett, Jason Lee, Sham Kakade, Bin Yu
  arXiv 2025.09

Implicit regularization

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Sandbox:

linear regression

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For **all** linear regression problems (Gaussian-design):

early-stopped GD is

- always no worse
- sometimes much better

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$$x \sim \mathsf{N}(0, \Sigma), \quad y = x^\top \theta^* + \mathsf{N}(0, 1) \;\; \text{for} \;\; \|\theta^*\|_\Sigma \lesssim 1$$

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n iid samples $(x_1, y_1), \ldots, (x_n, y_n)$

$$X = \begin{bmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{bmatrix} \quad Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

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empirical risk $\quad L(\theta) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}(x_i^\top\theta - y_i)^2$

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- for $s = 1, \ldots, t$

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fix $0 < \eta \leq 1/\|\nabla^2 L\|$; otherwise, rescale time

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Theorem. For **every** (Σ, θ^*), $n \geq 1$, $\lambda \geq 0$, there exists $t \geq 0$ such that, w.p. ≥ 0.99

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GD dominates ridge instead of "GD = ridge"

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(TB'23) There is an analytic function f such that, w.p. ≥ 0.99

$$\text{risk}\left(\hat{\theta}_t^{\text{gd}}\right) \lesssim f(\Sigma, \theta^*, n, \lambda) \approx \text{risk}\left(\hat{\theta}_\lambda^{\text{ridge}}\right)$$

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more effective when θ^* decays fast

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Theorem. In linear regression, GD dominates ridge;

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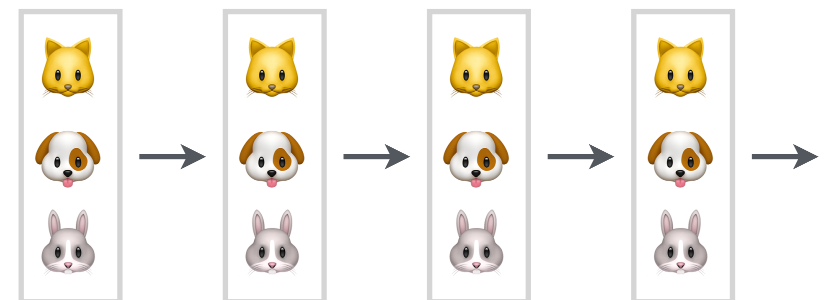

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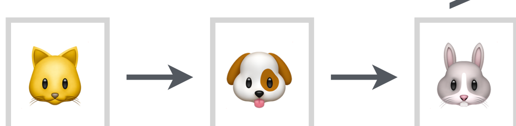

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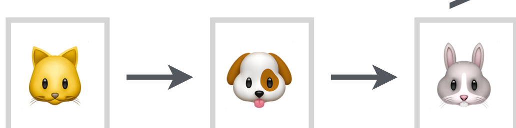

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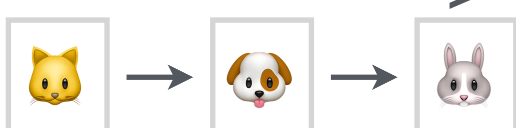

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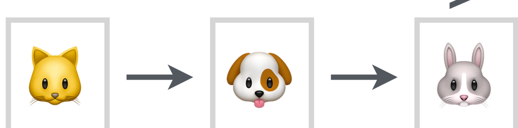

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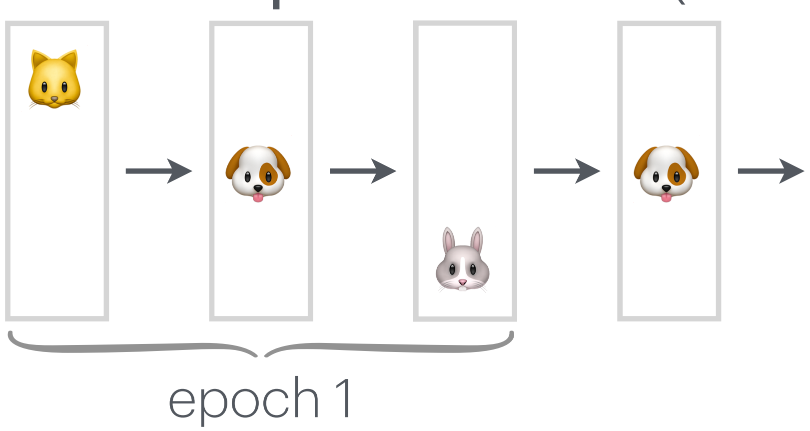

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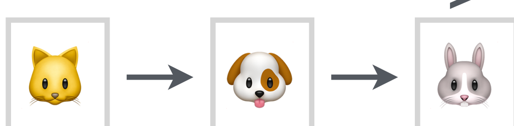

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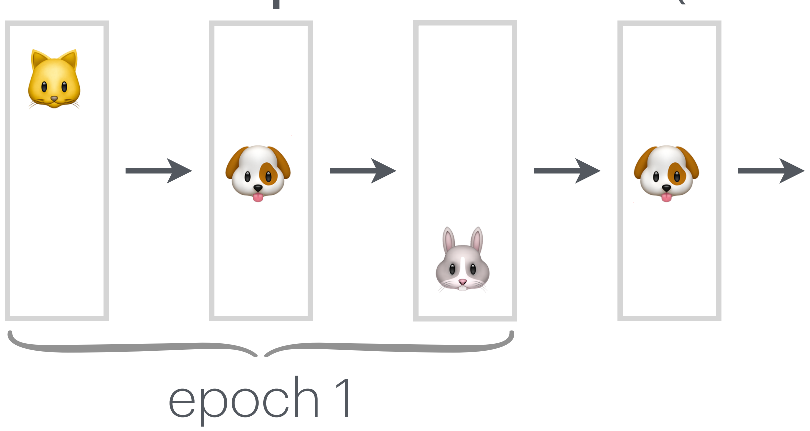

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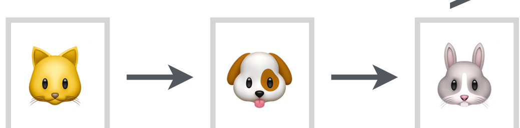

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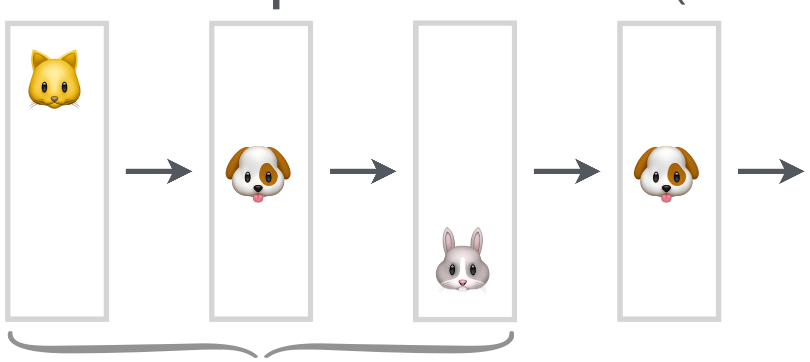

the SGD variant used in deep learning

Wu, Bartlett, Lee, Kakade, Yu. "Risk comparisons in linear regression: implicit regularization dominates explicit regularization." arXiv 2025.09

Contribution 3: from theory to practice

principled parallelization method for training language models

- "*Seesaw*: accelerating training by balancing learning rate and batch size scheduling"
  Alexandru Meterez*, Depen Morwani*, W, Costin-Andrei Oncescu, Cengiz Pehlevan, Sham Kakade
  ICLR 2026

Language Model (LM) training

Practice. LM training is “online”: #data ∝ #flops

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Question. Fixing #flops, same test error with fewer steps?

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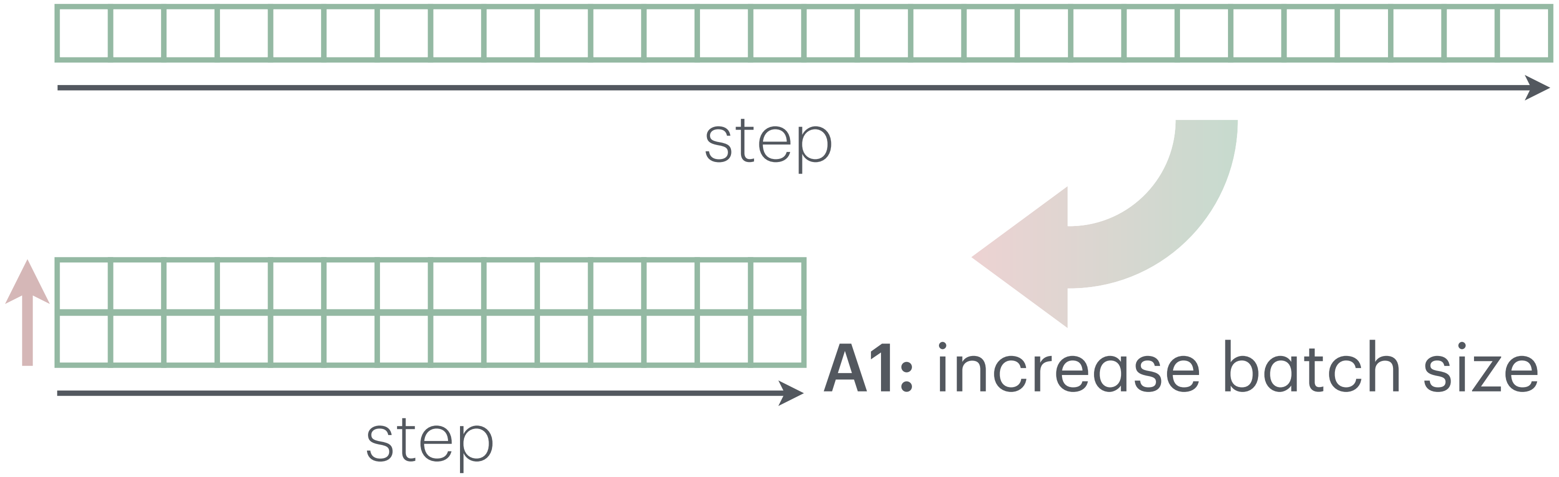

A1: increase batch size

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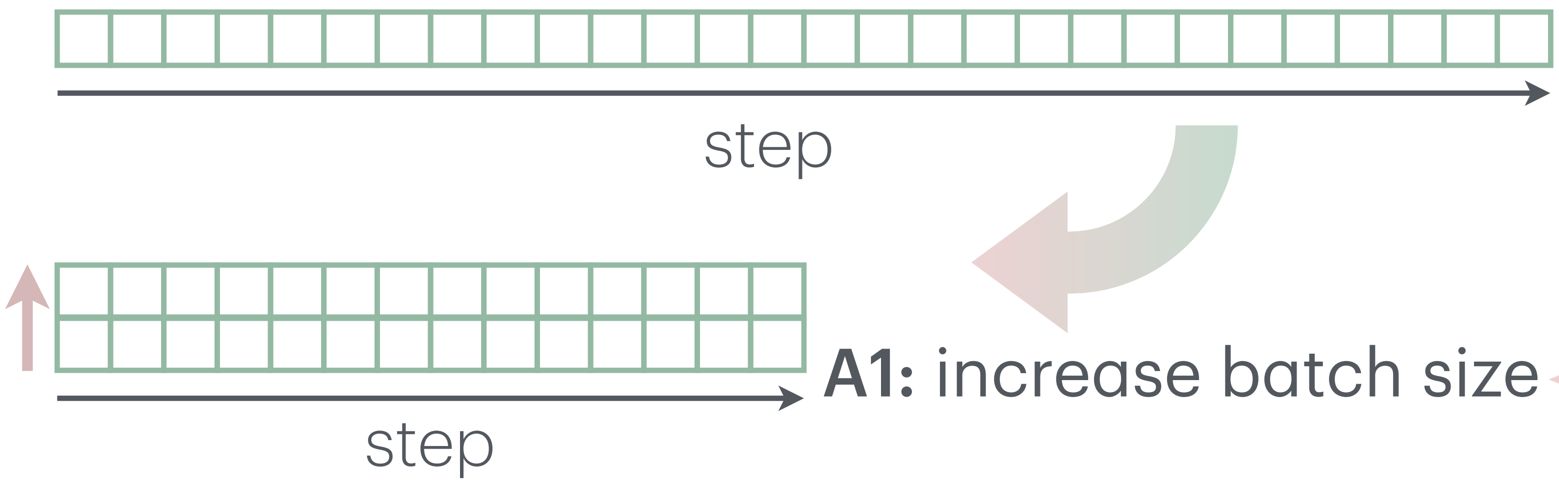

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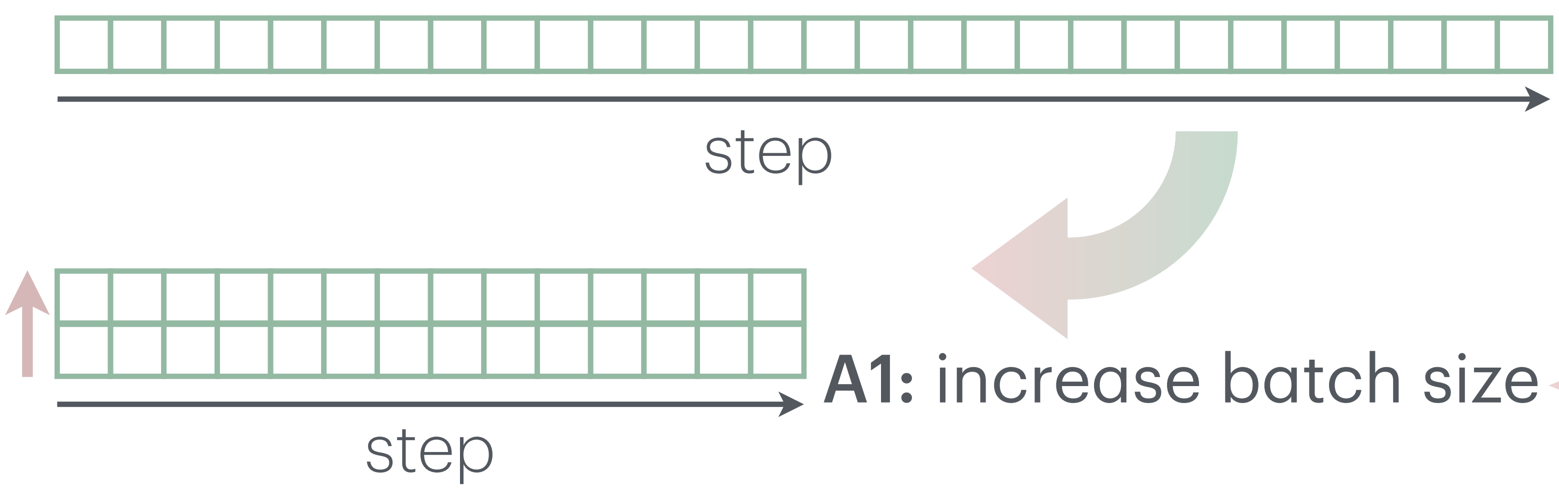

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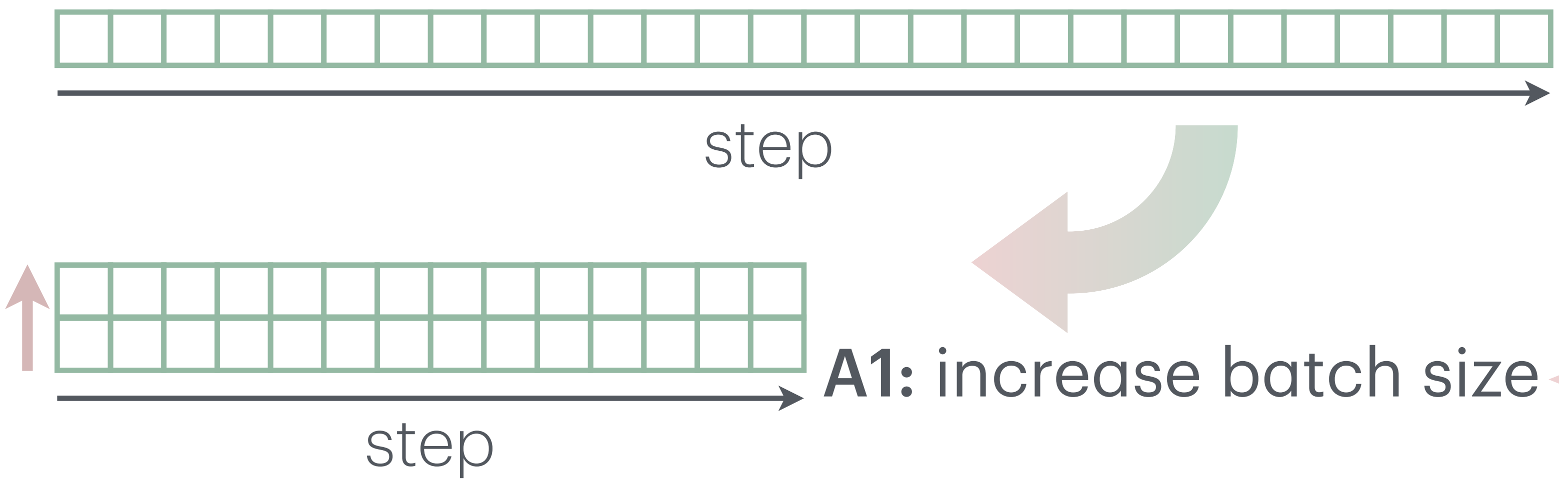

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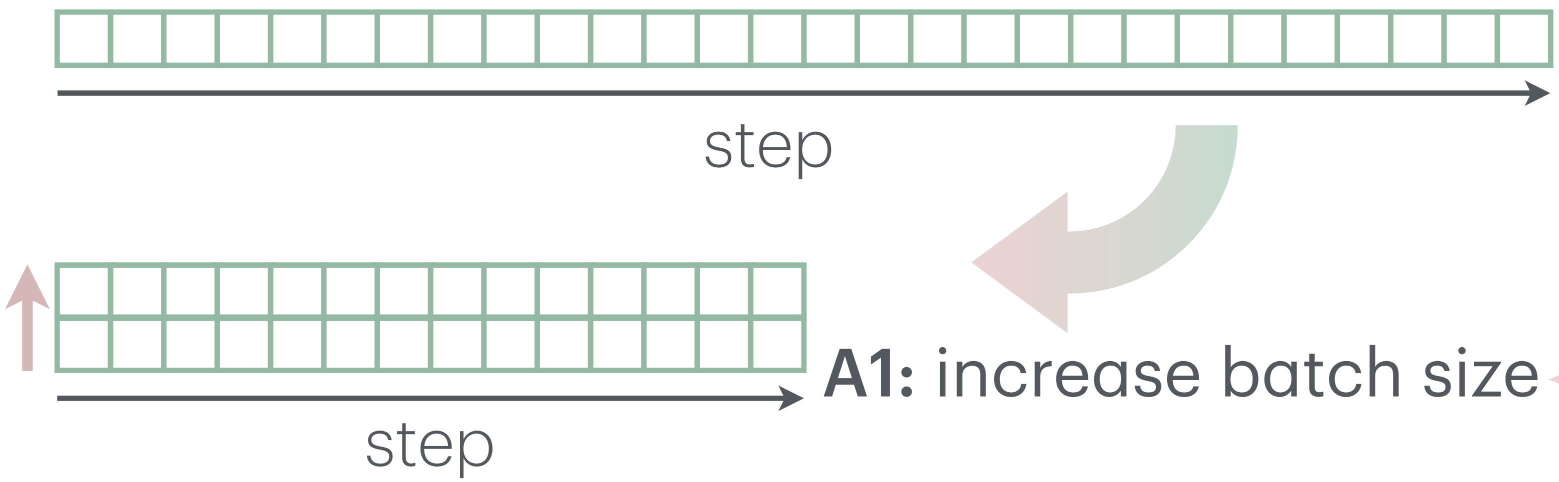

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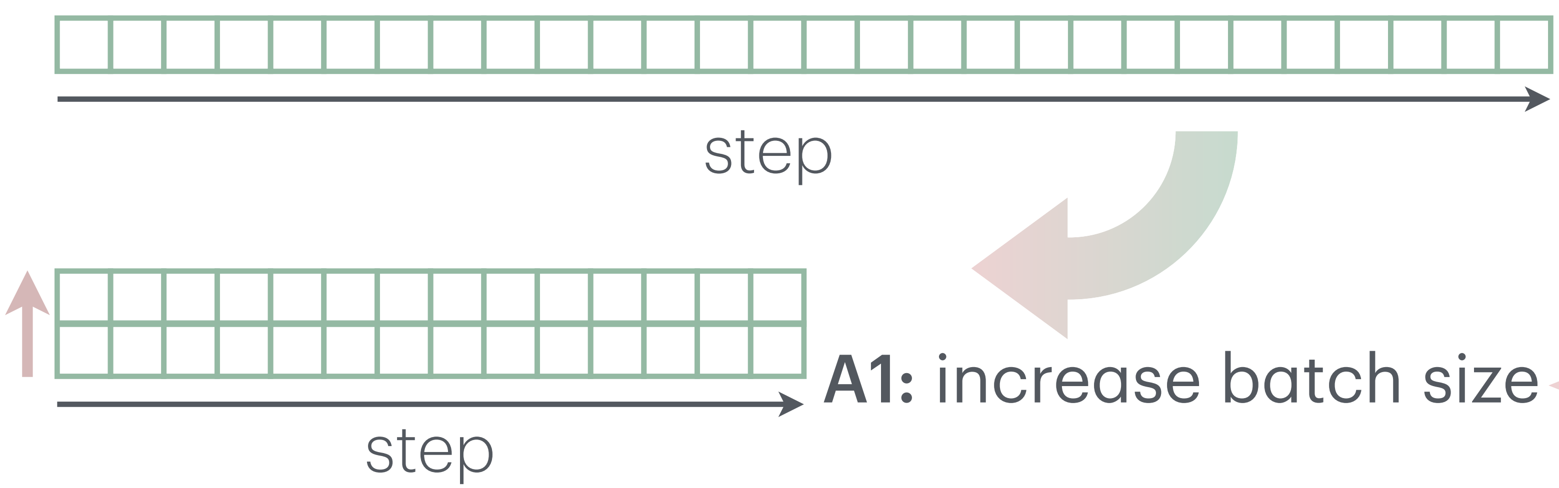

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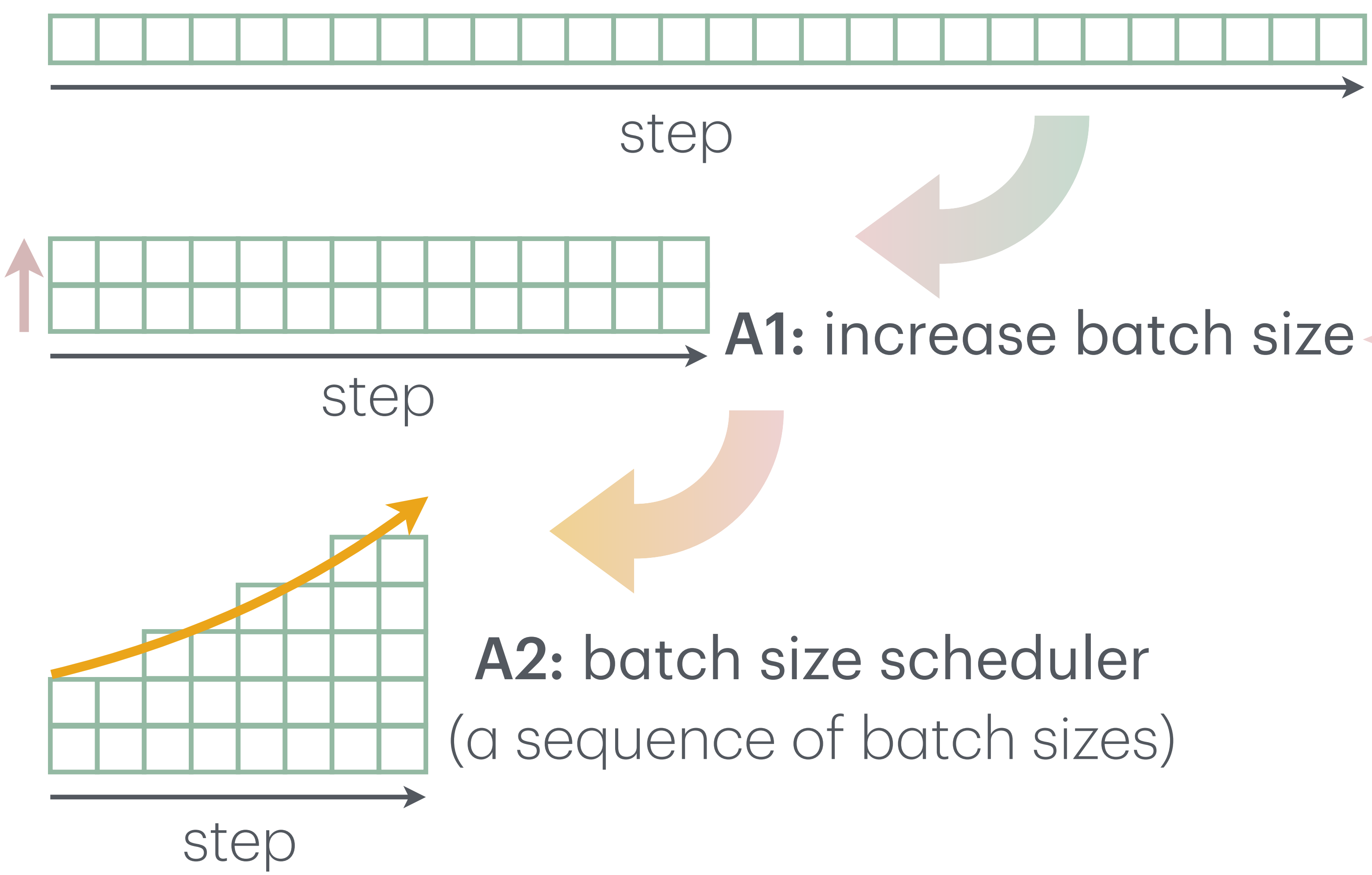

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Seesaw — a principled batch size scheduler

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Theorem (informal). For normalized SGD, "default" and "*Seesaw*" achieve same test error rate for all linear regression problems

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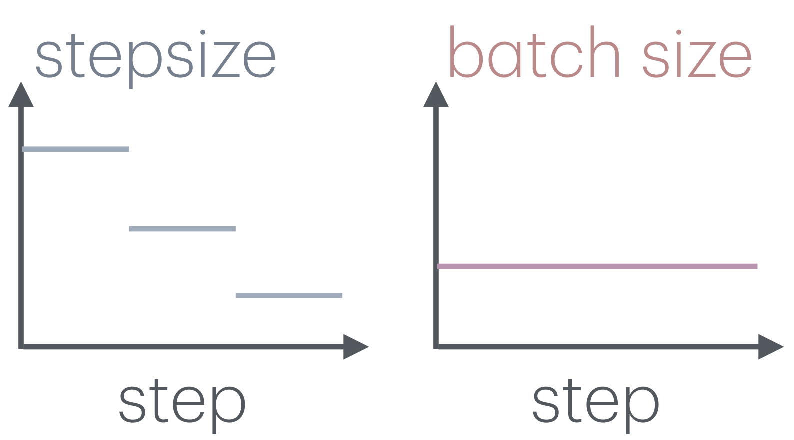
default: stepsize scheduler

$\eta \to \eta/1.1$, B fixed



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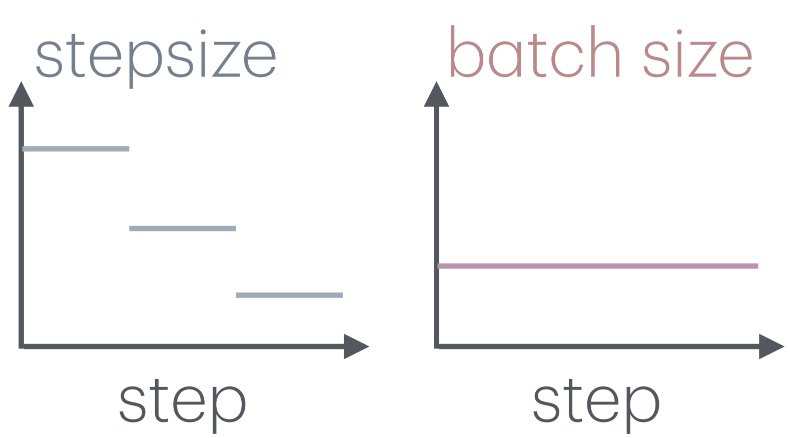
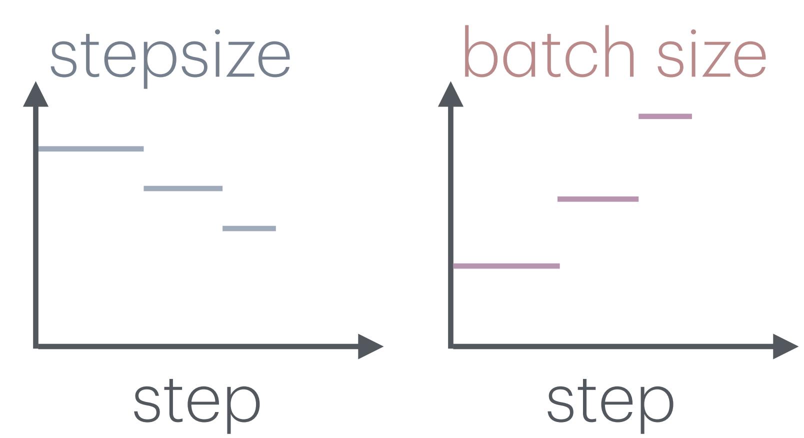


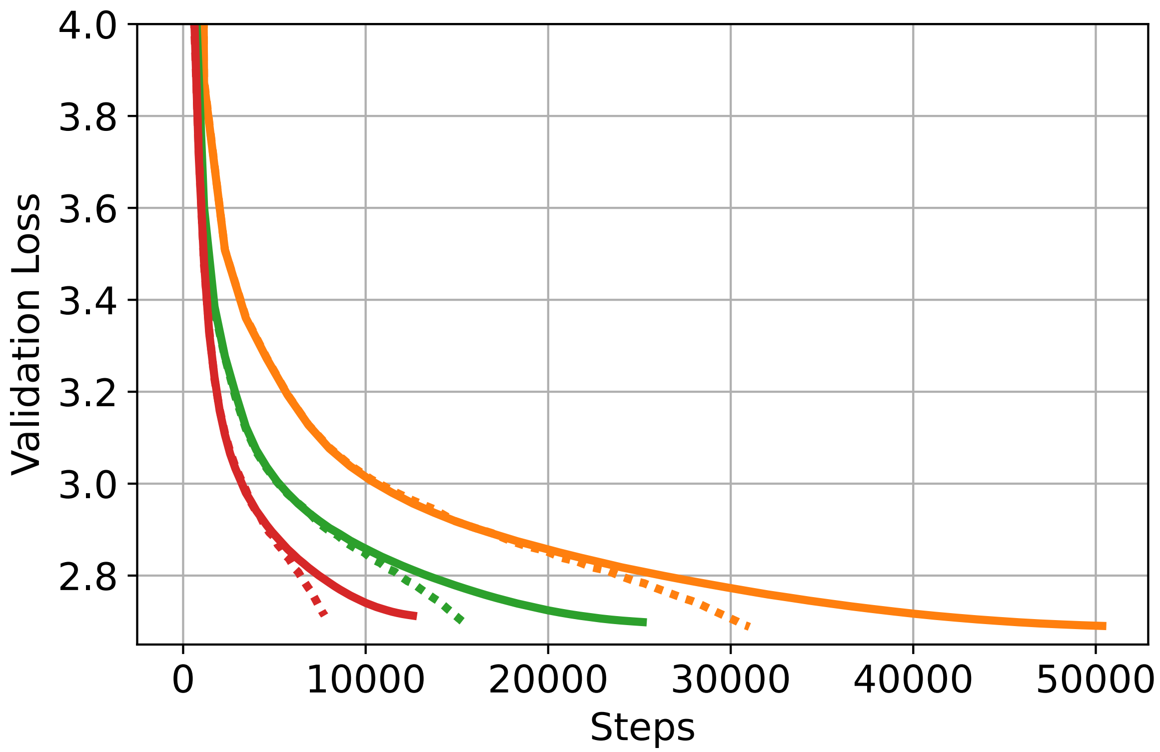
***Seesaw*:** joint scheduler

$\eta \to \eta/\sqrt{1.1}$, $B \to 1.1B$



Meterez, Morwani, **Wu**, Oncescu, Pehlevan, Kakade. “*Seesaw*: accelerating training by balancing learning rate and batch size scheduling.” ICLR 2026

Same error (±0.17%), 36% fewer steps



transformer (600M), Adam, C4

initial batch size: 2^8, 2^9, 2^{10} (= CBS)
solid curve: **default** (fixed batch size, cosine stepsize scheduler)
dotted curve: *Seesaw* (ours)

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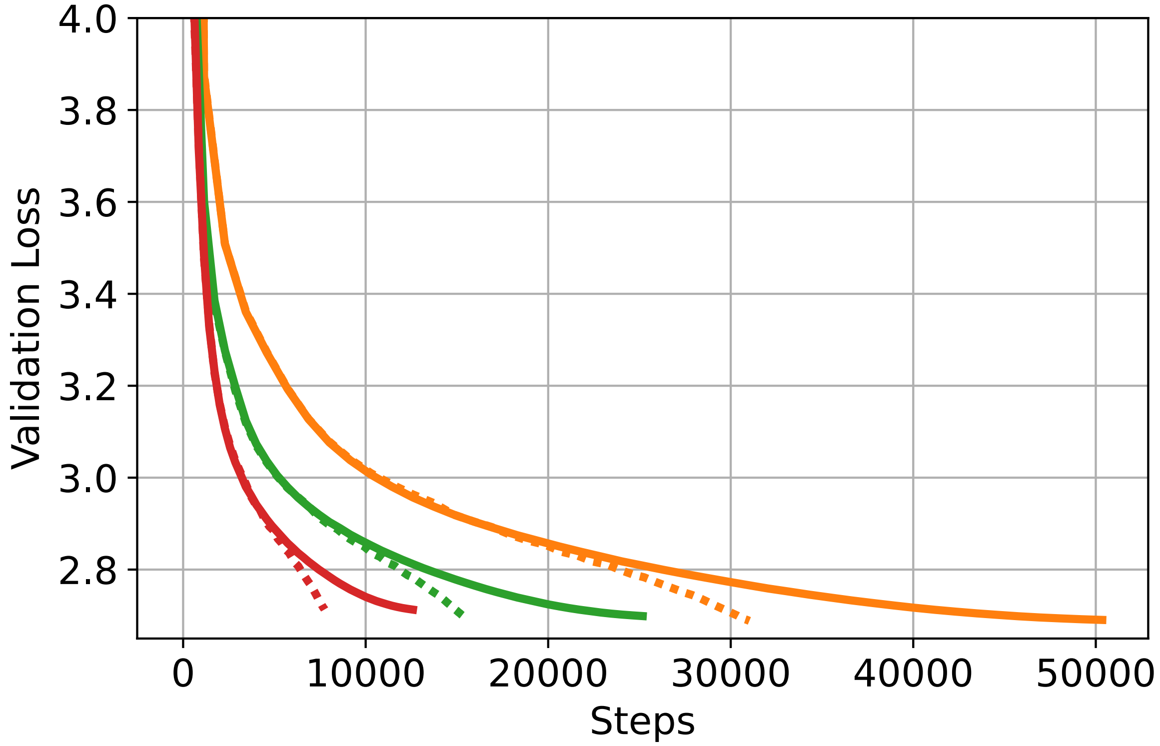

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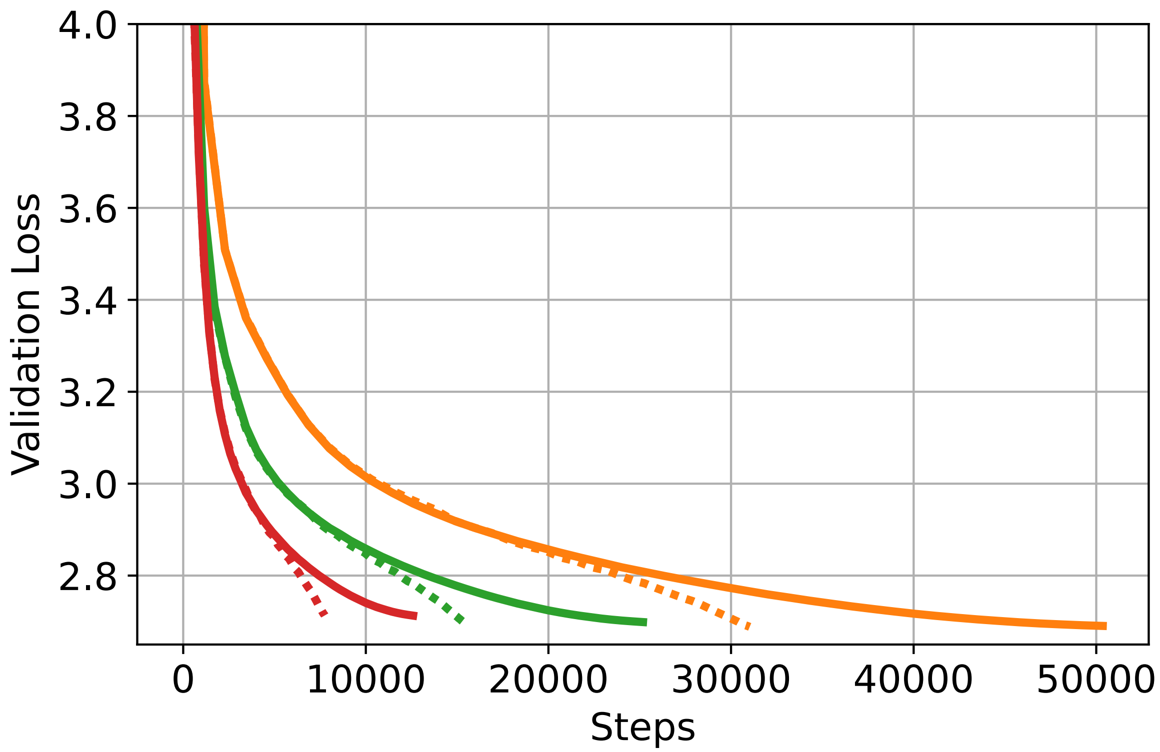

transformer (600M), Adam, C4

Seesaw

- theory based, practice verified
- blackbox — no extra measures
- #GPU ⬆️ — no free lunch

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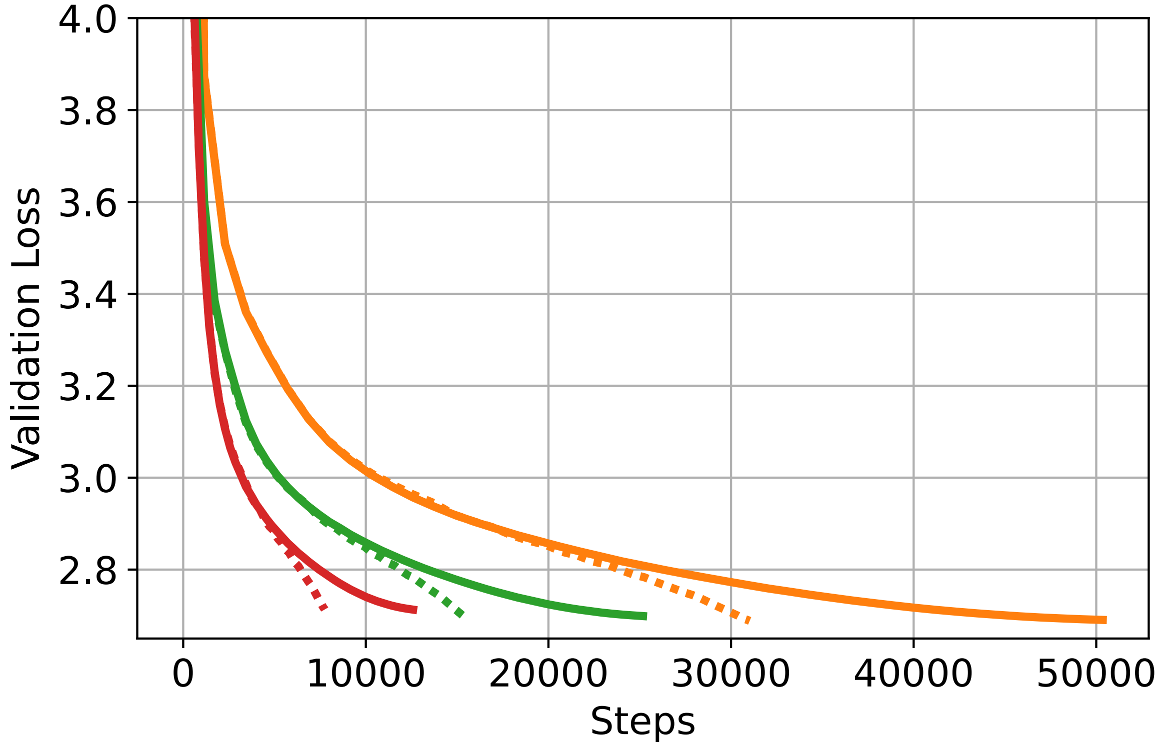

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Seesaw

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simple, meaningful sandbox can be predictive!

initial batch size: 2^8, 2^9, 2^{10} (= CBS)
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Summary

Contribution 1: unstable optimization

large stepsize accelerates gradient descent in logistic regression

Contribution 2: implicit regularization

gradient descent dominates ridge regression in linear regression

Contribution 3: from theory to practice

principled parallelization method for training language models

Summary

💡 💡 💡

not covered by classical theory

deep learning = scaling + new mechanisms

ML systems (beyond DL)

not specific to deep learning

✨✨✨

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Summary

classical theory: conservative

“worst-case”, “stable”, ...

optimization | statistics

Summary

my research: less conservative

"instance-wise", "unstable", ...

optimization x statistics

classical theory: conservative

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Summary

my aim: theory that is explanatory, predictive, inspirational

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“instance-wise”, “unstable”, ...

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Going forward

my aim: theory that is explanatory, predictive, inspirational

Going forward

my aim: theory that is explanatory, predictive, inspirational

1. embrace *instability* in optimization theory

Going forward

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1. embrace *instability* in optimization theory
2. explore *synergies* between statistics & optimization

Going forward

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instability

new technique?
model, data?
other instabilities?

*check out our tutorial for more discussions

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stats → opt

new criterion
hyperparameter?
data reuse?

opt → stats

opt algorithm as estimator?

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stats → opt

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opt algorithm as estimator?

practice

testbed
new question?
new sandbox?
other domain?

Going forward

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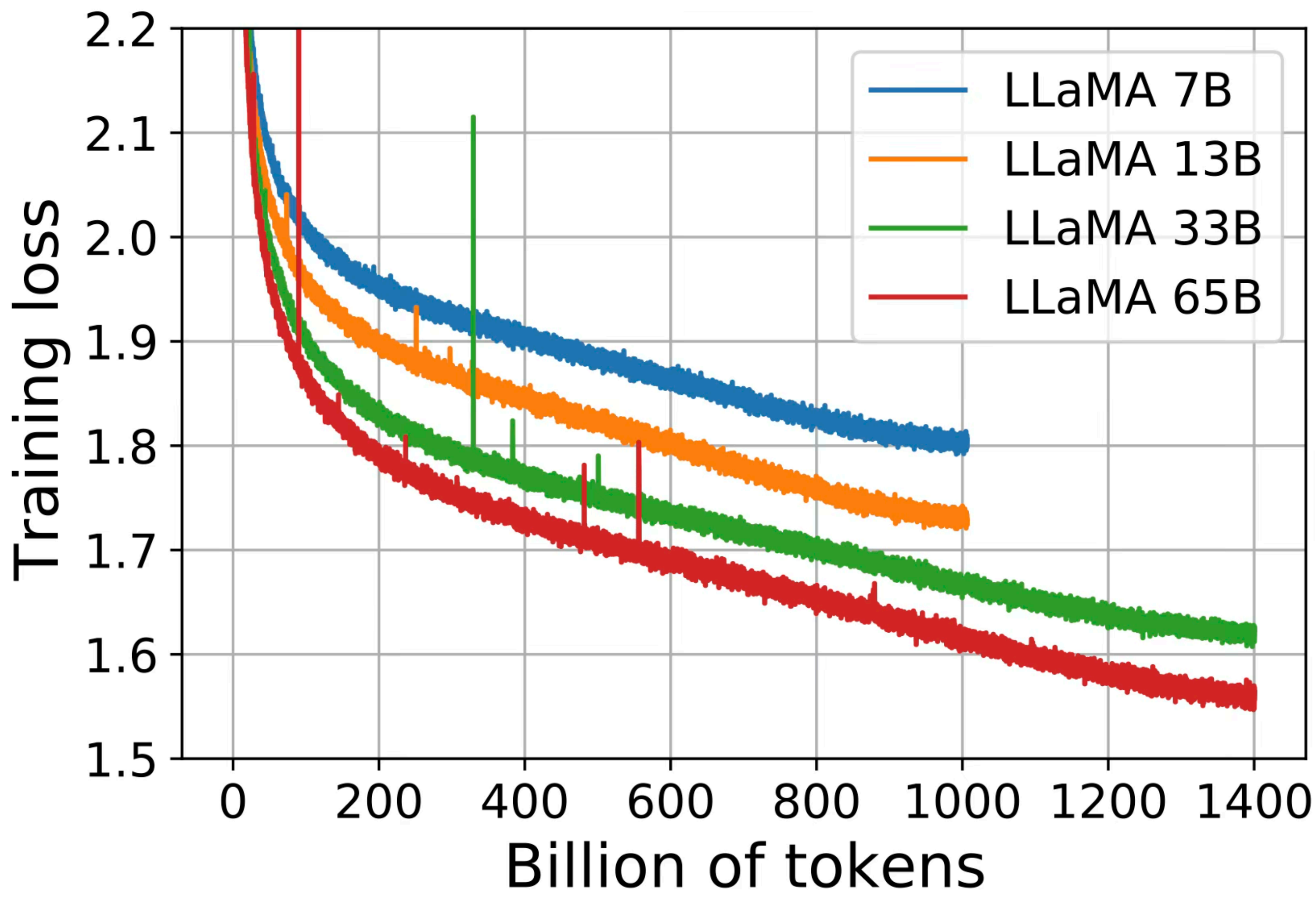
Backup slides

LM training instability



"online" AdamW, batch size = 4M, internet data, transformer

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

Large, adaptive stepsize

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

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Theorem. Assume separability with margin γ. For $t \geq 1/\gamma^2$,

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

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matching "Perceptron"
(Novikoff'1962, or earlier)

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

Online SGD beats GD

Theorem. Let $n \geq 1$. For a sequence of d-dim problems

$$d \geq n^2 \qquad \theta^* = \begin{bmatrix} n^{0.45} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} n^{-0.9} & & & \\ & 1/d & & \\ & & \ddots & \\ & & & 1/d \end{bmatrix}$$

we have $\|\theta^*\|_\Sigma \leq 1$; moreover, w.p. ≥ 0.99,

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online SGD decays bias exponentially; GD bias ≥ OLS bias

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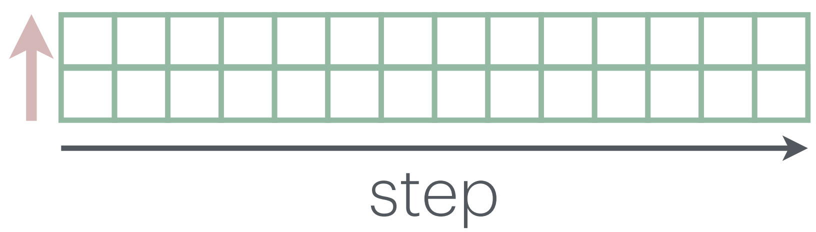
Comparing with (MLPA’22)

MLPA’22 setup

(constant batch size)

for *multiple* training runs with different constant batch size B, how to set (initial) stepsize η in each run?



Malladi, Lyu, Panigrahi, Arora. "On the SDEs and scaling rules for adaptive gradient algorithms." NeurIPS 2022

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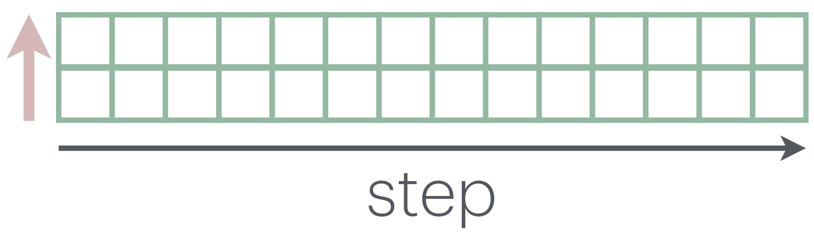

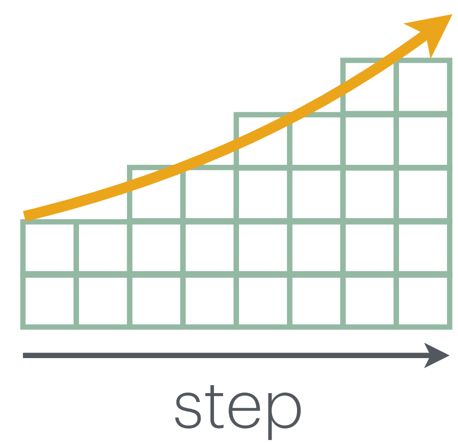

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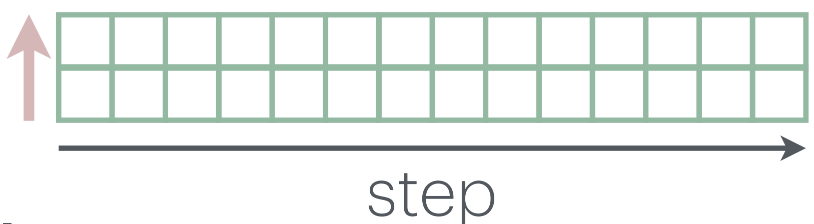

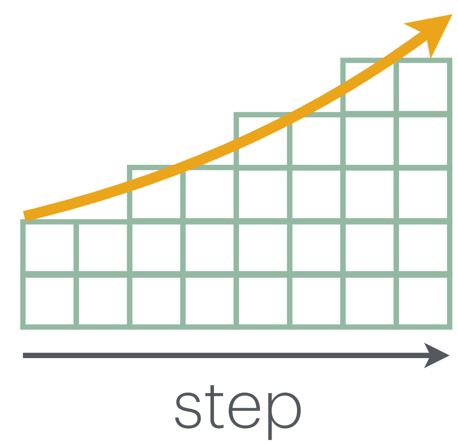

Details:

- constant batch size **vs** batch size scheduler
- SDE **vs** linear regression
- infinitesimal stepsize **vs** any stepsize scheduler
- batch **vs** online

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