Towards a Less Conservative Theory of Machine Learning

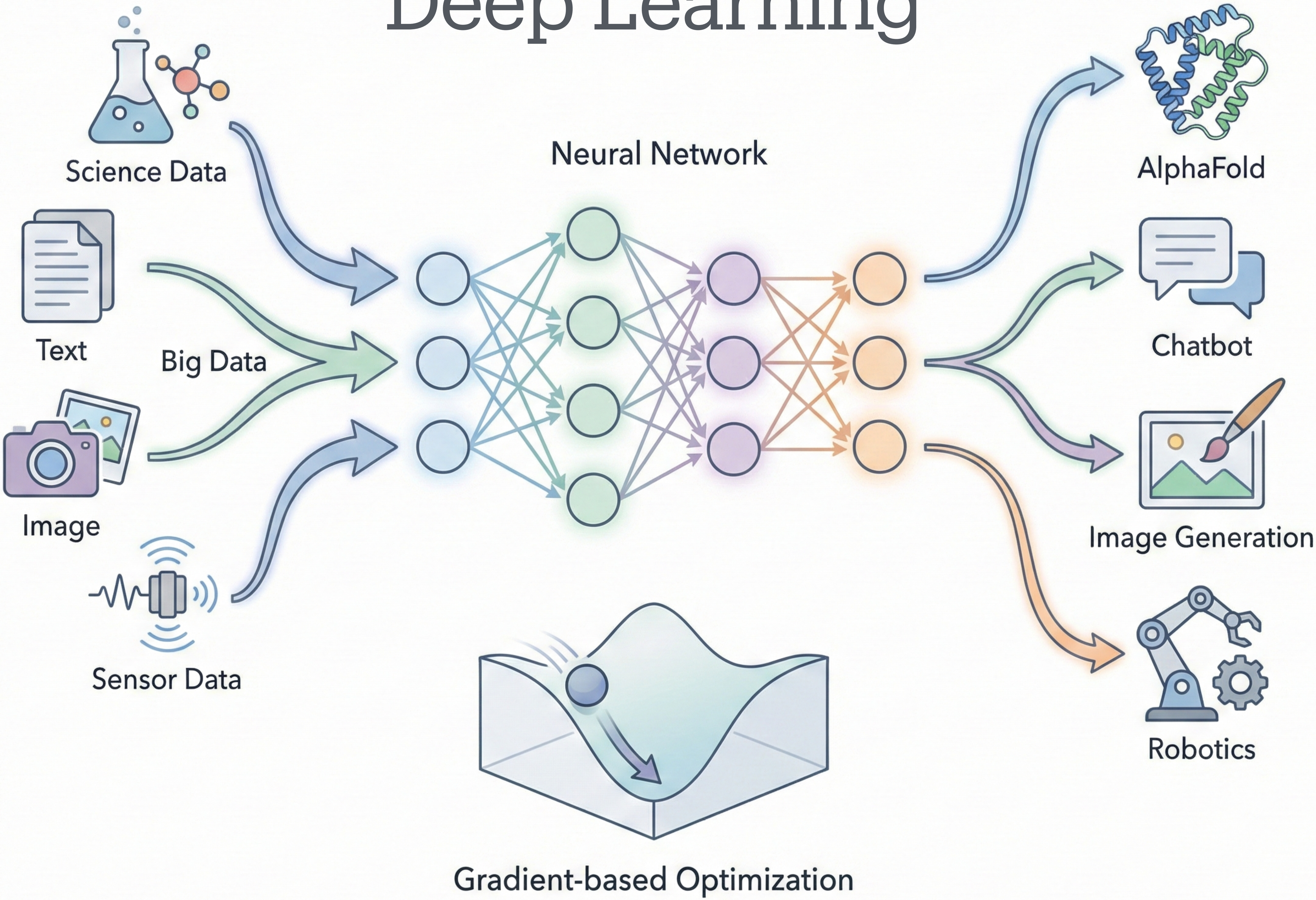
Unstable Optimization & Implicit Regularization

Jingfeng Wu

Simons Institute for the Theory of Computing

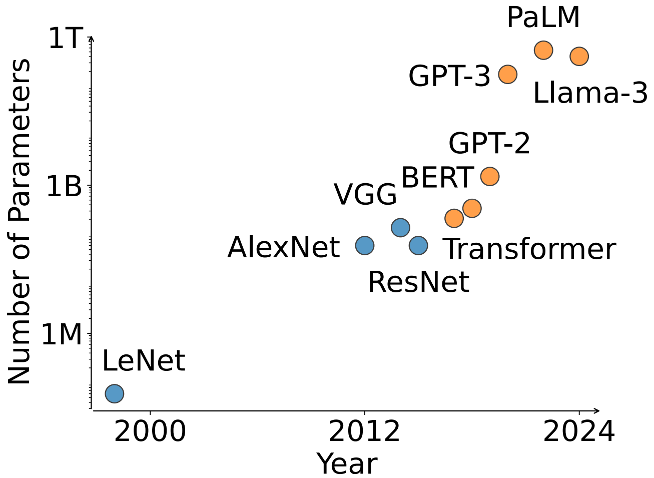
Berkeley
University of California

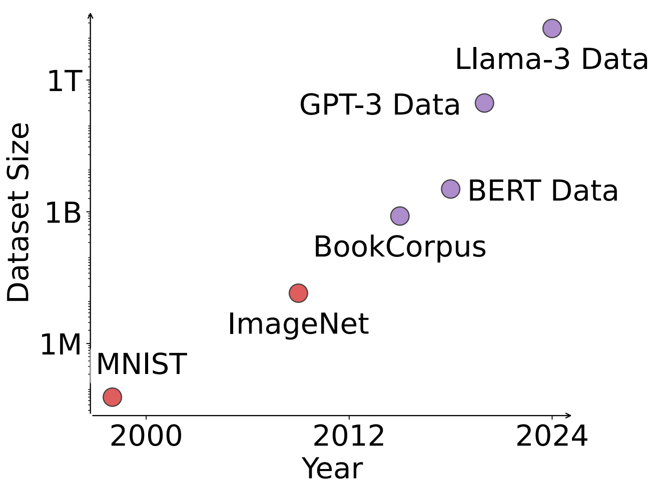
Deep Learning



What makes deep learning thrive?

scaling





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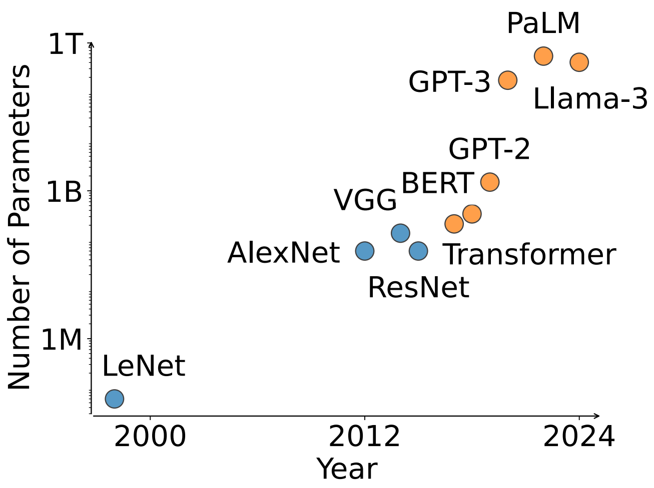
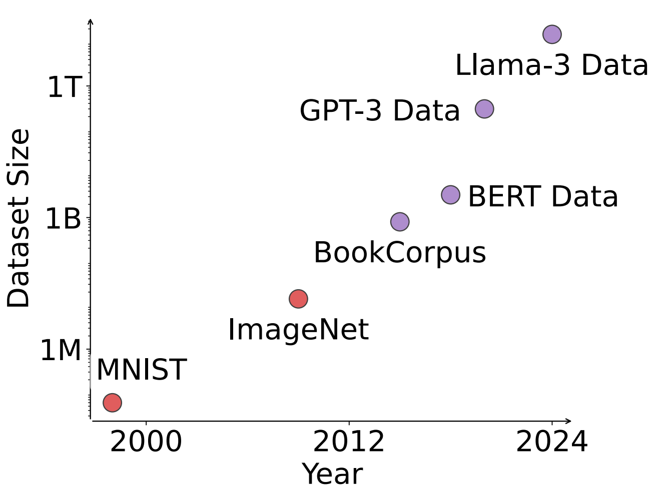
scaling	new mechanisms





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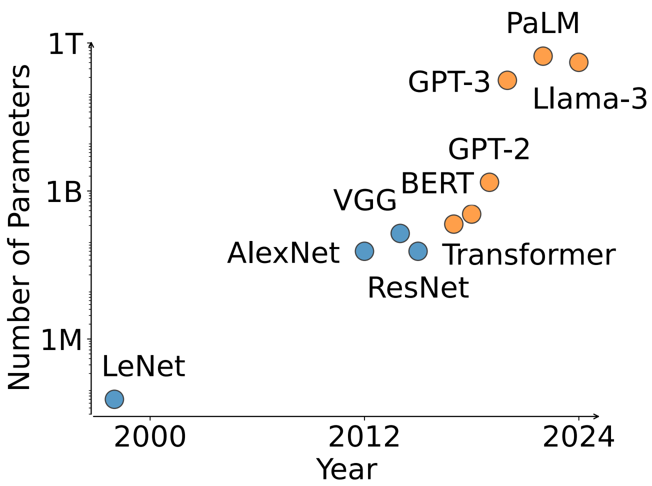
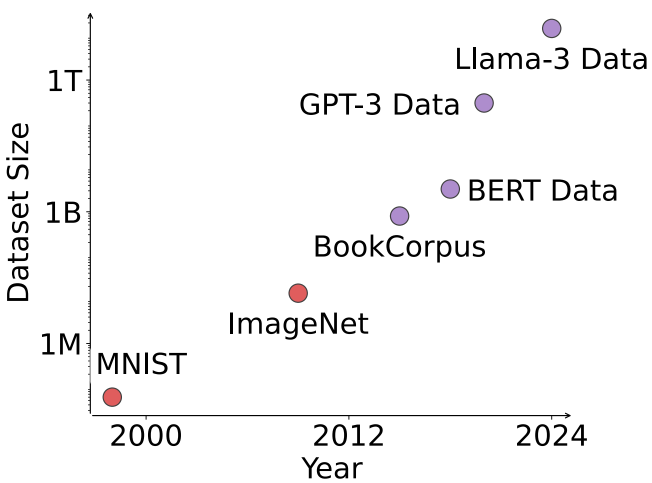
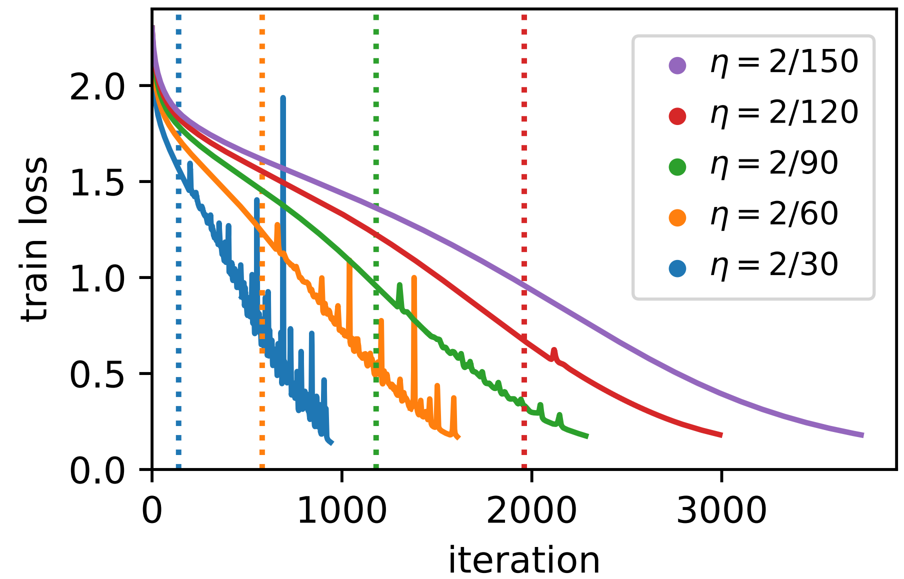




optimization



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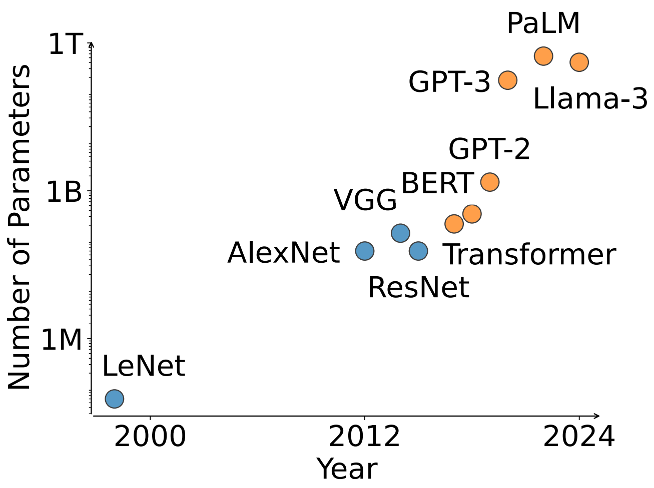

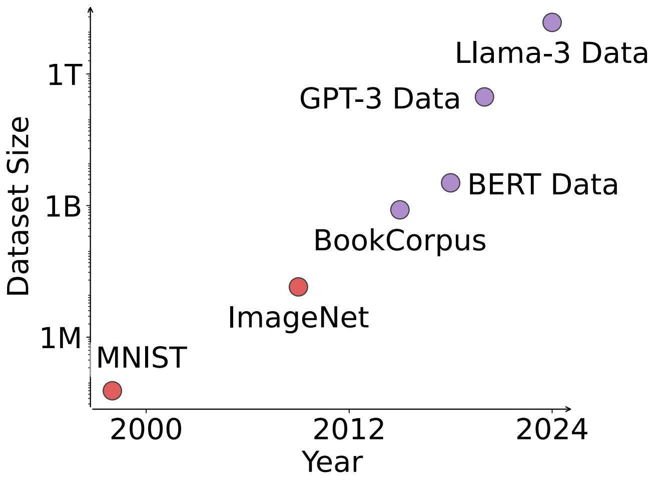

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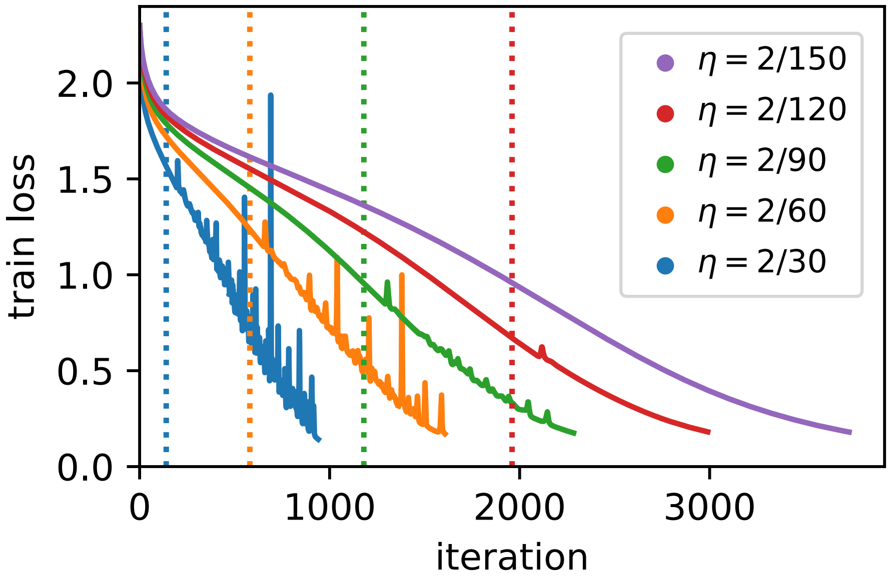

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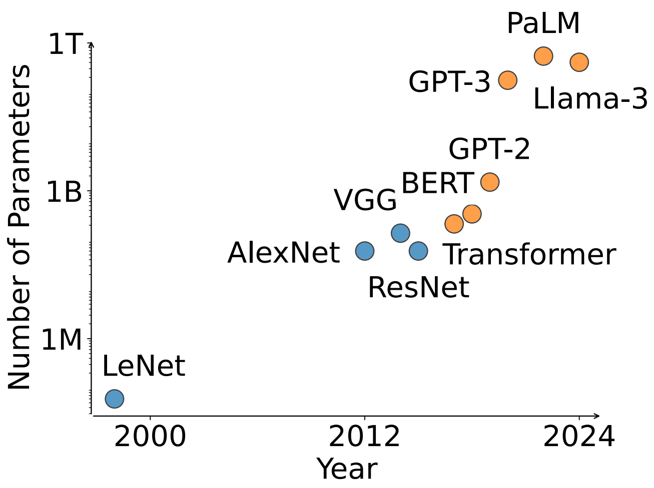

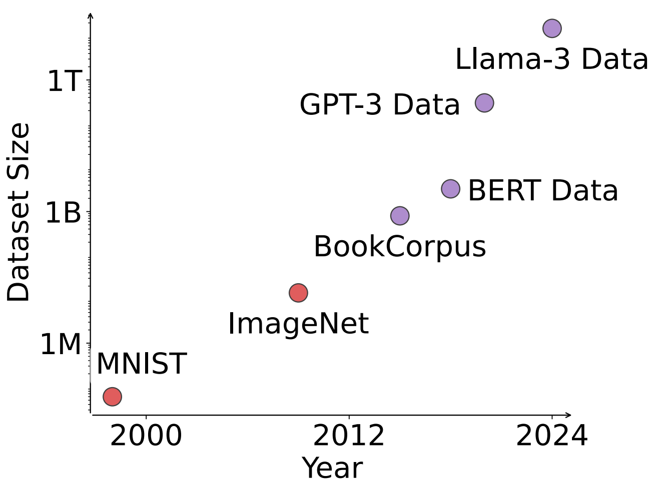

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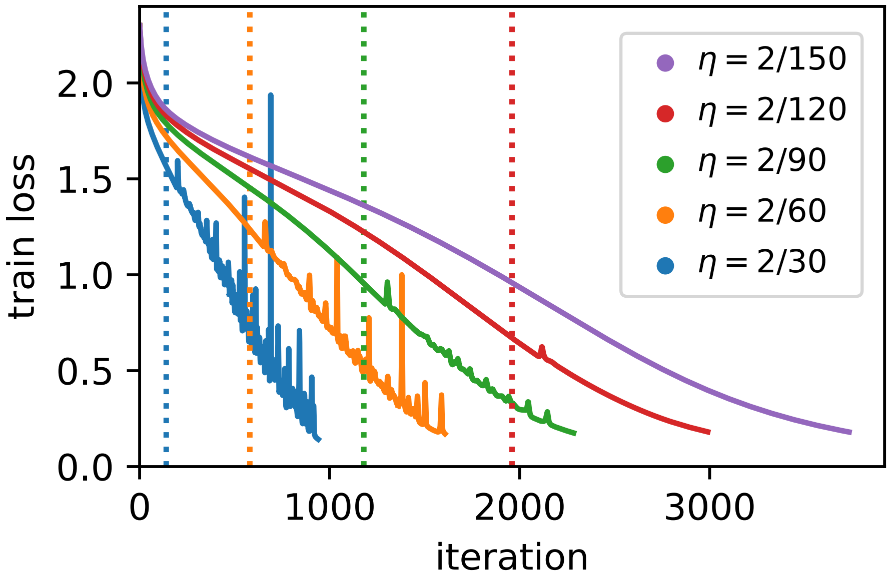

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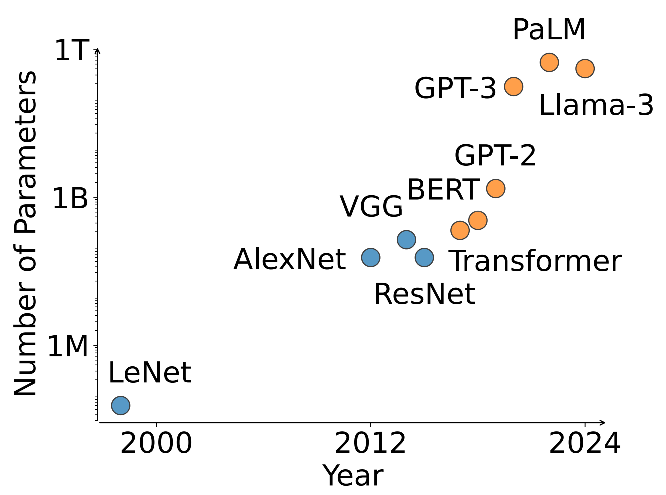

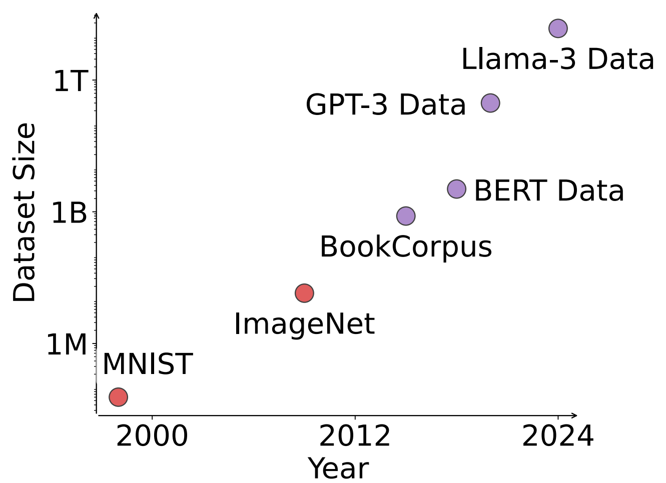

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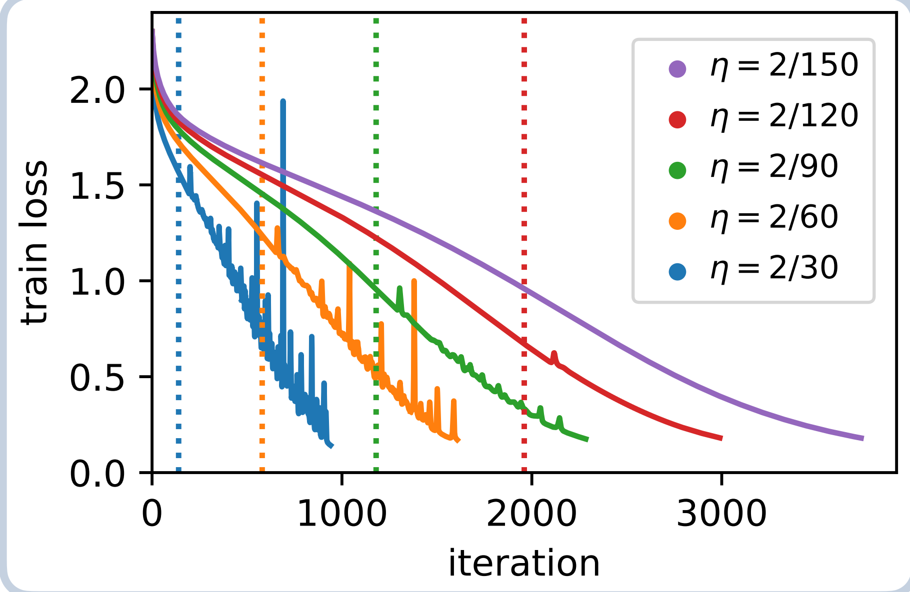

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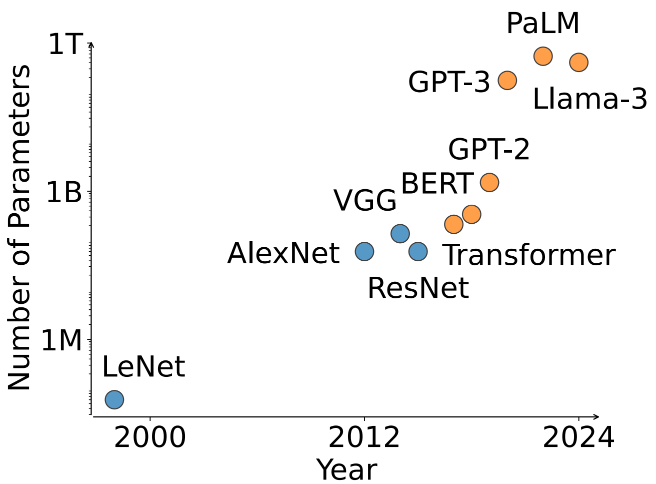

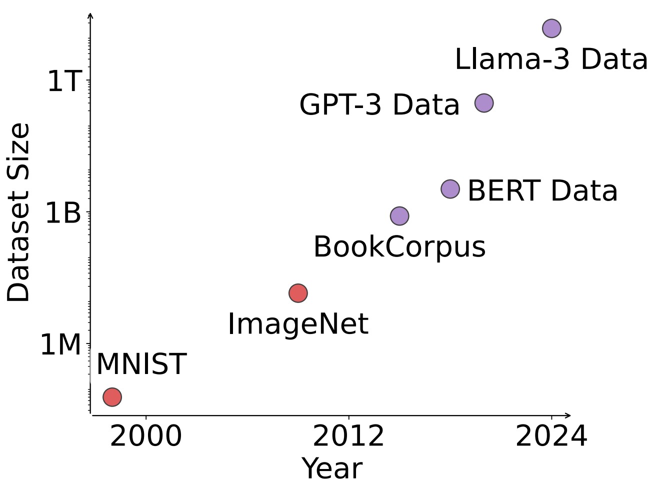

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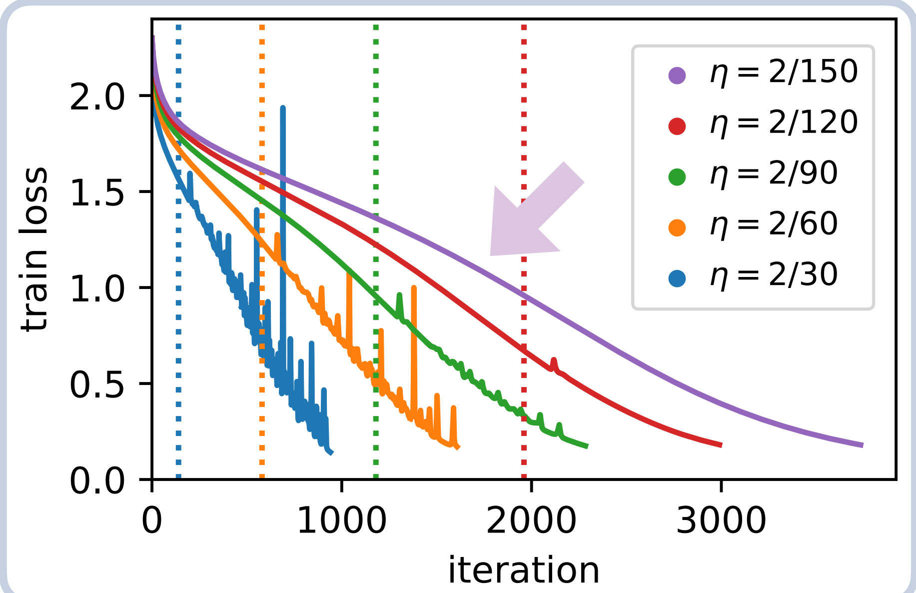

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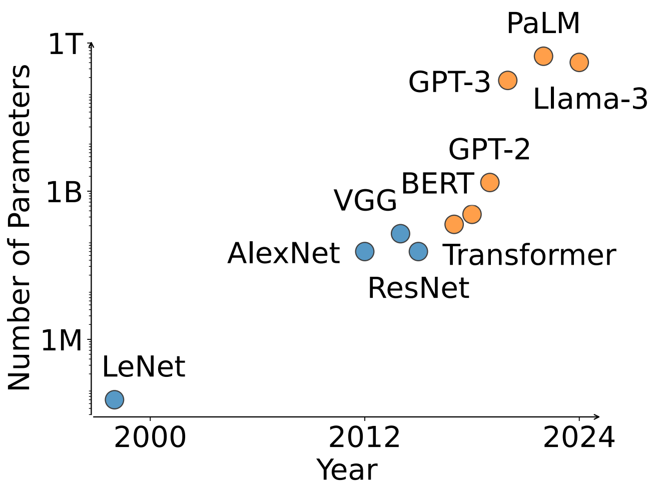

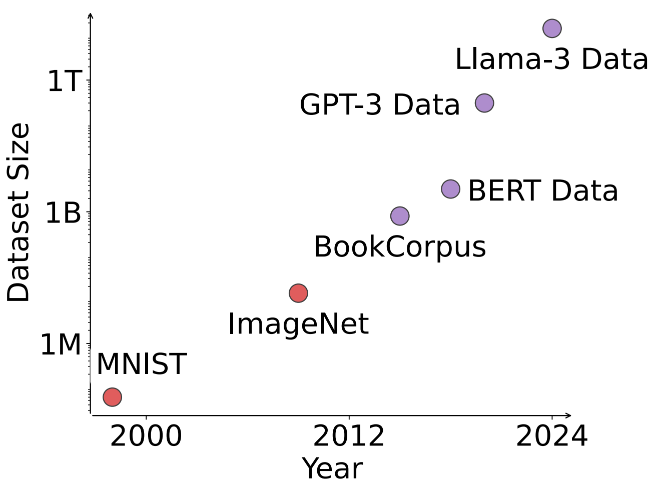

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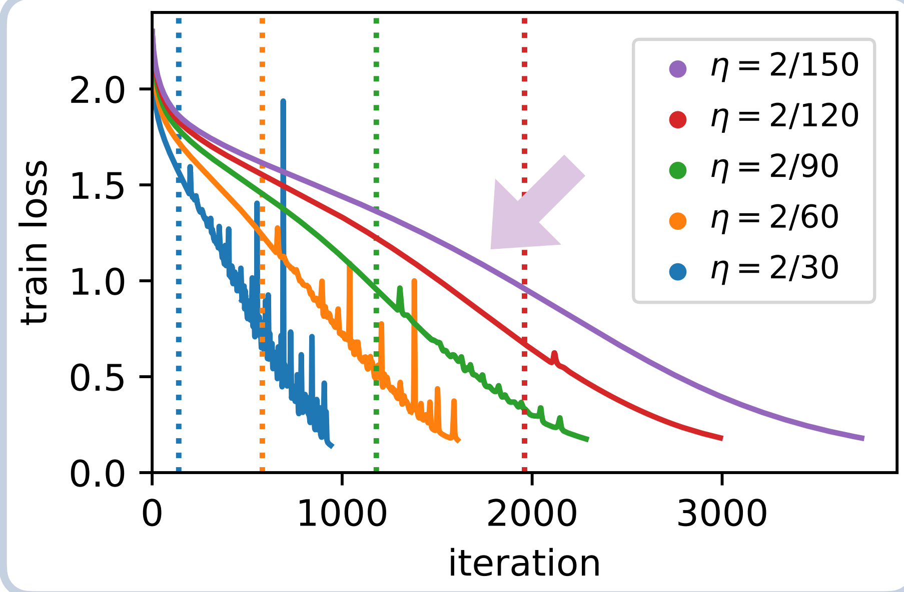

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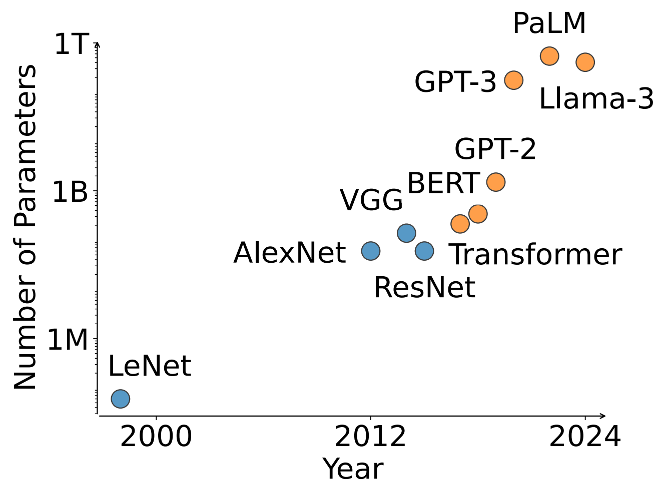

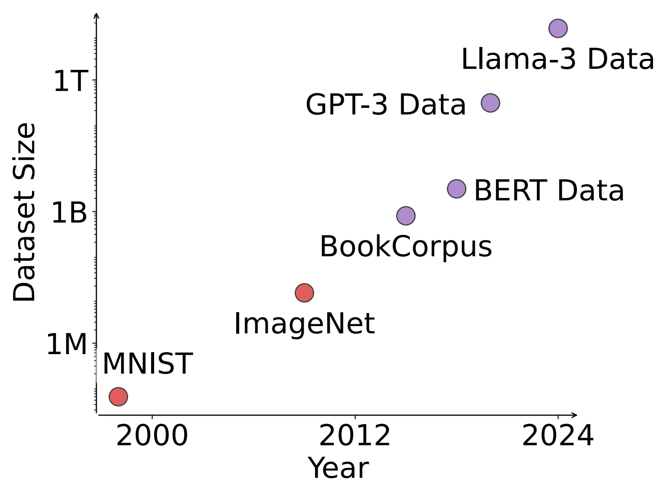

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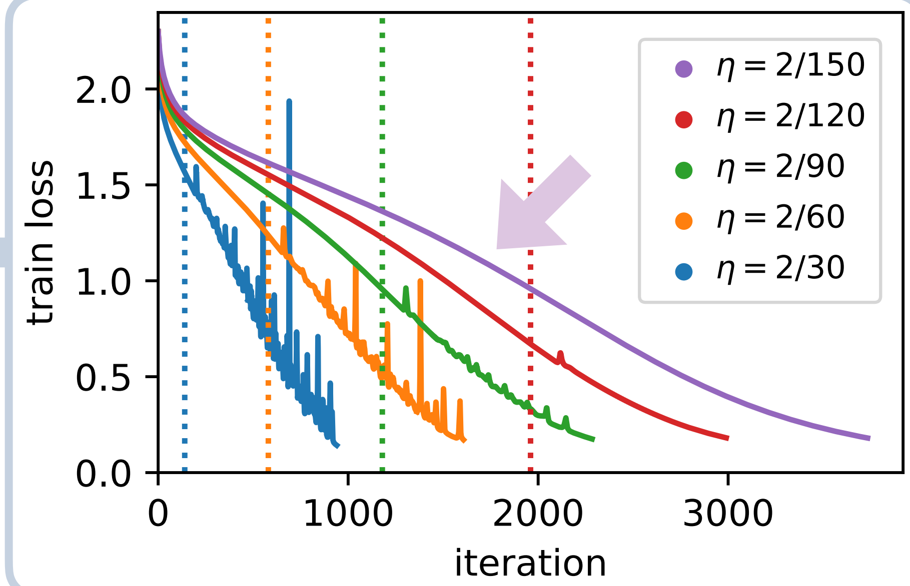
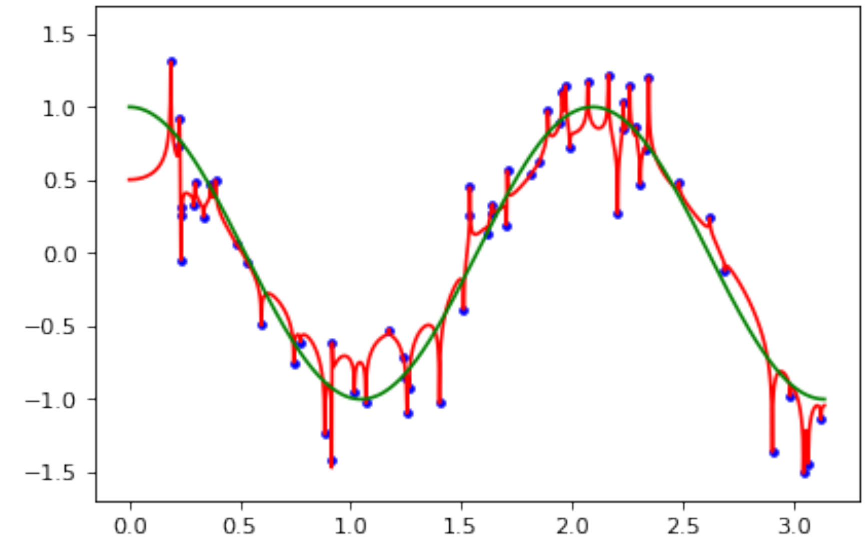


generalization



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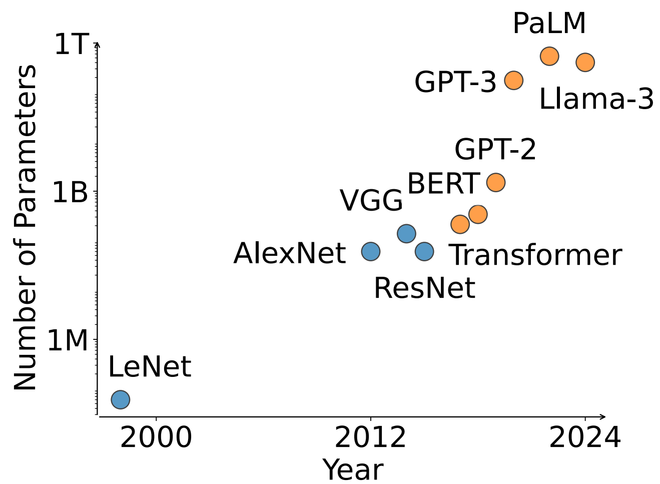

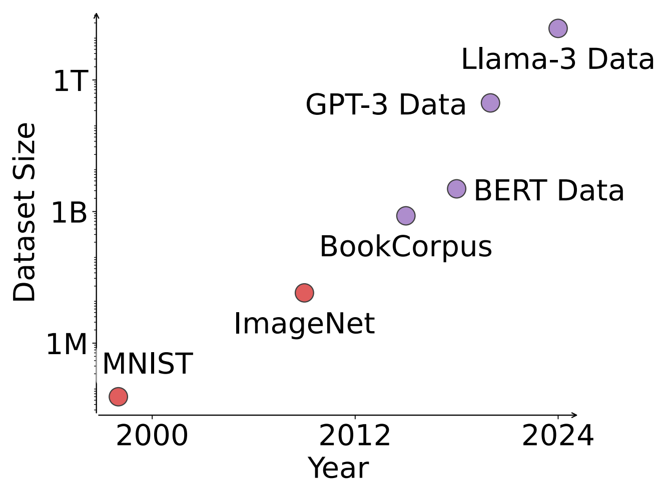

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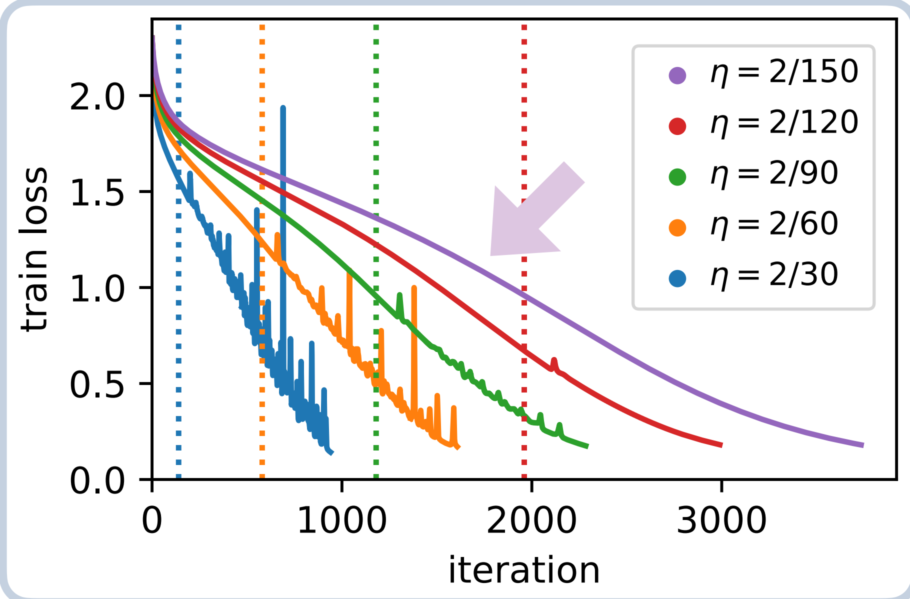
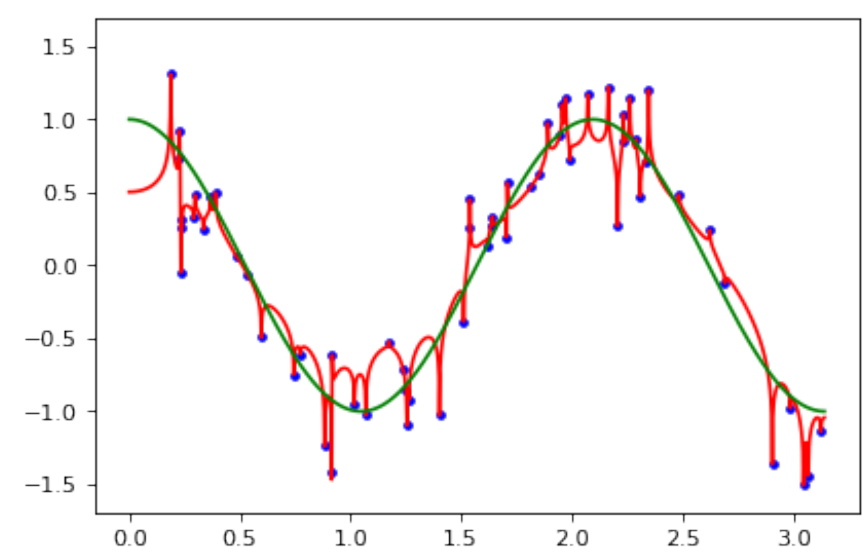


generalization

overparameterization



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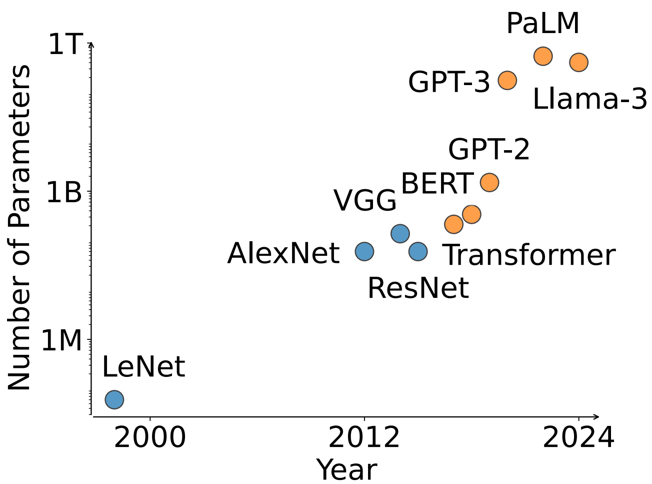

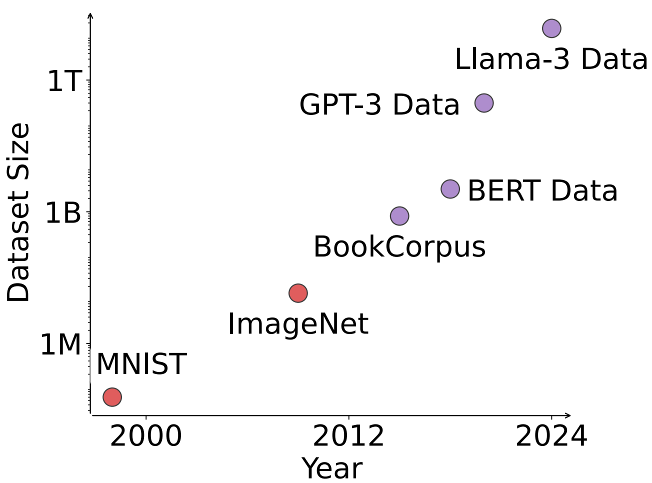

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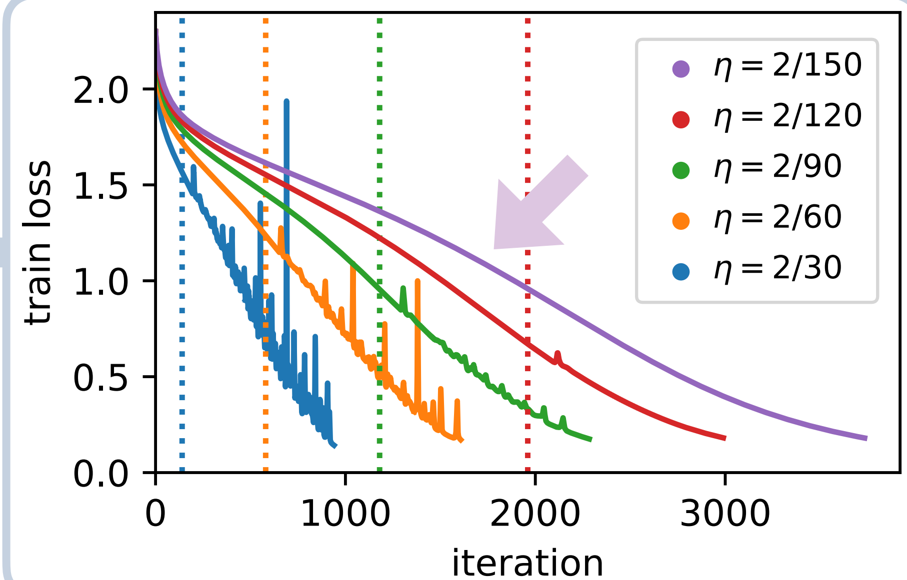

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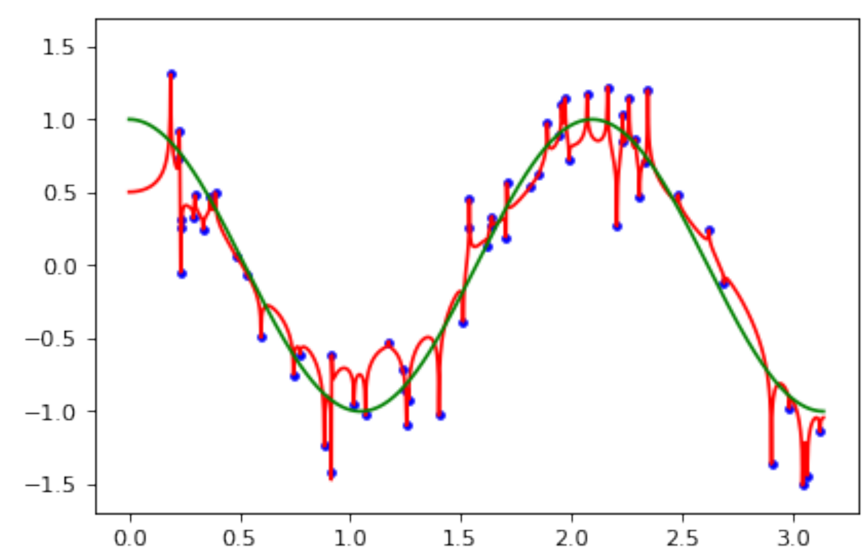

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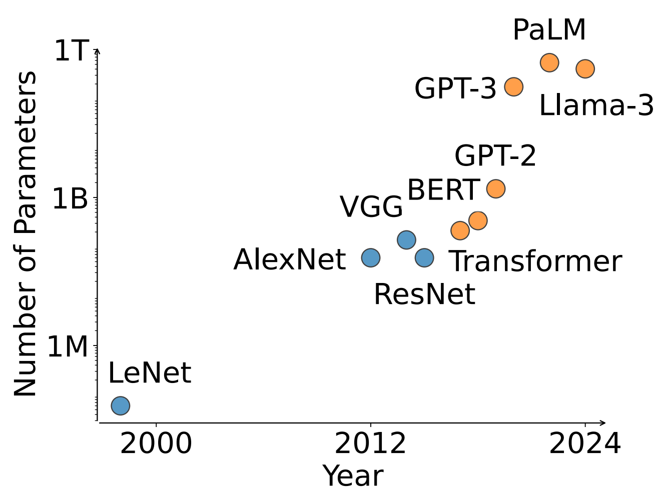

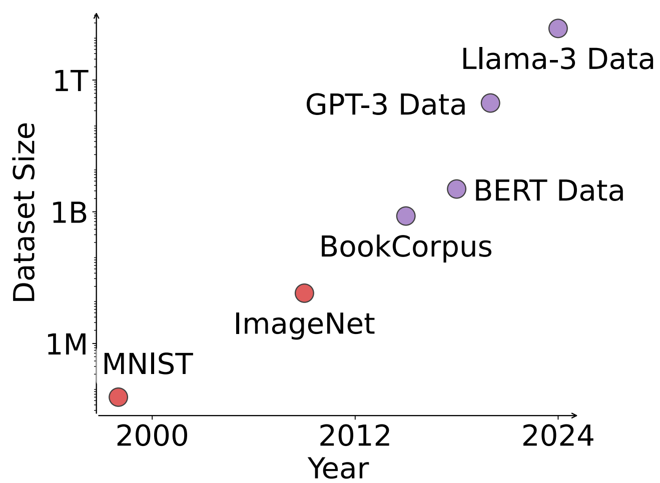

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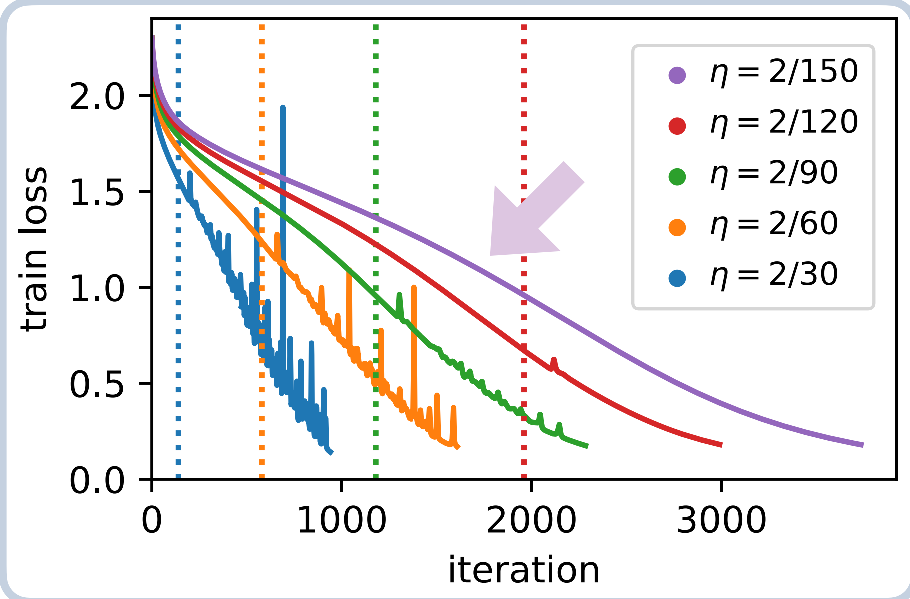

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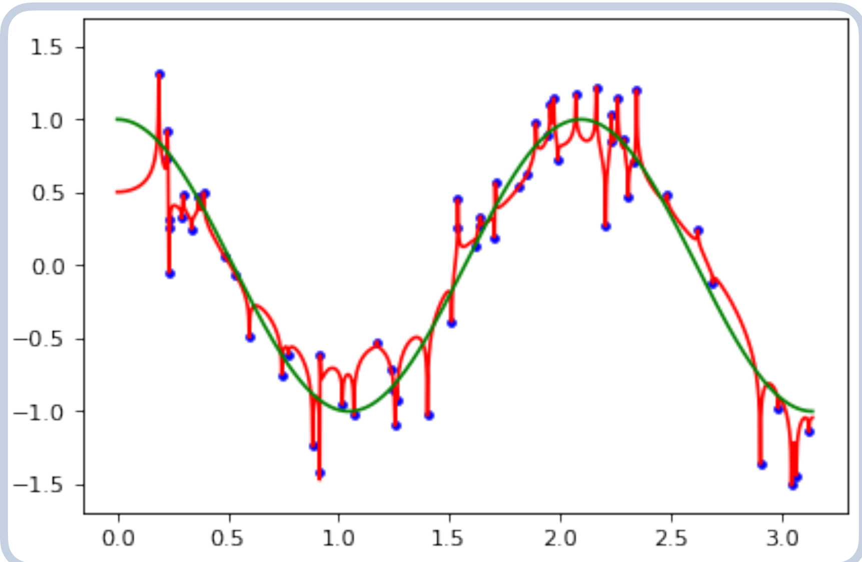

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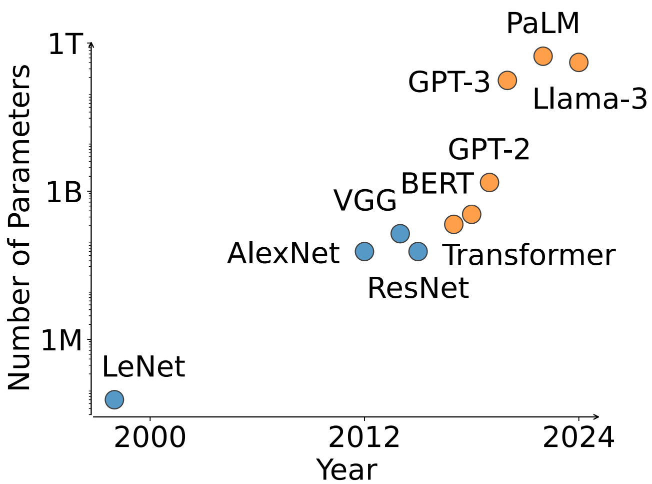

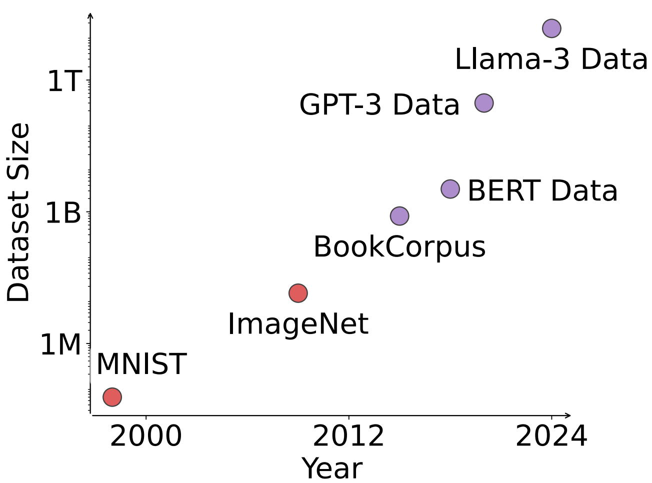

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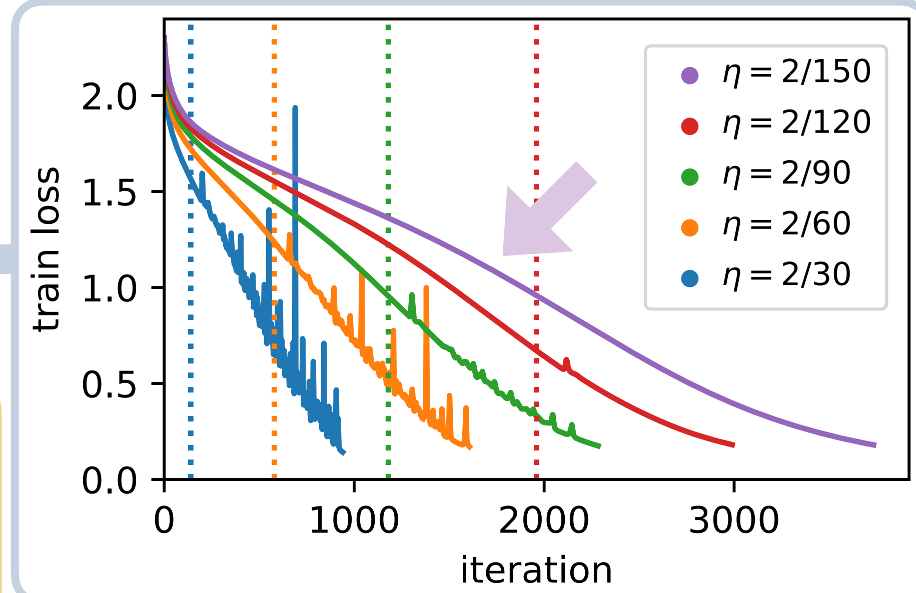

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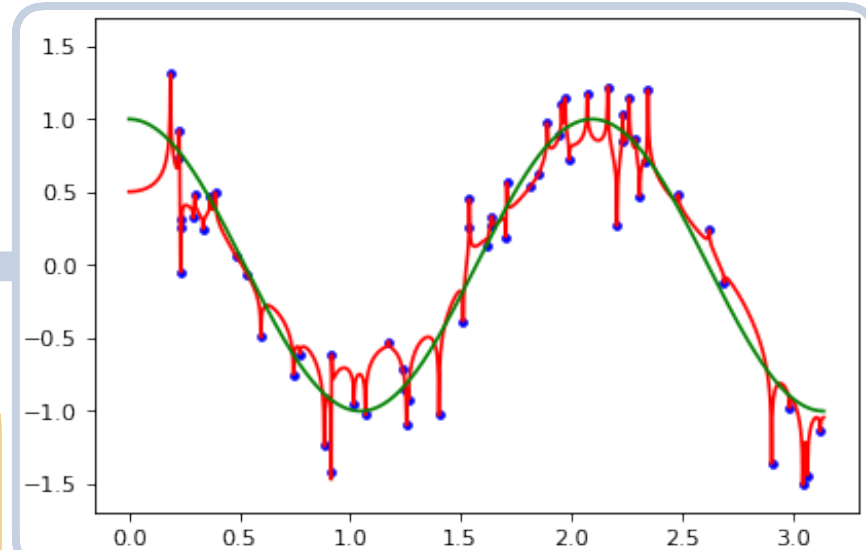
optimization path

implicit regularization



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My research

deep learning = scaling + new mechanisms

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not covered by classical theory

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not covered by classical theory

deep learning = scaling + new mechanisms

My research

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deep learning = scaling + new mechanisms

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ML fields (beyond DL)

not specific to deep learning

✨✨✨

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Approach. Demystify new mechanisms in **sandboxes**

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simple

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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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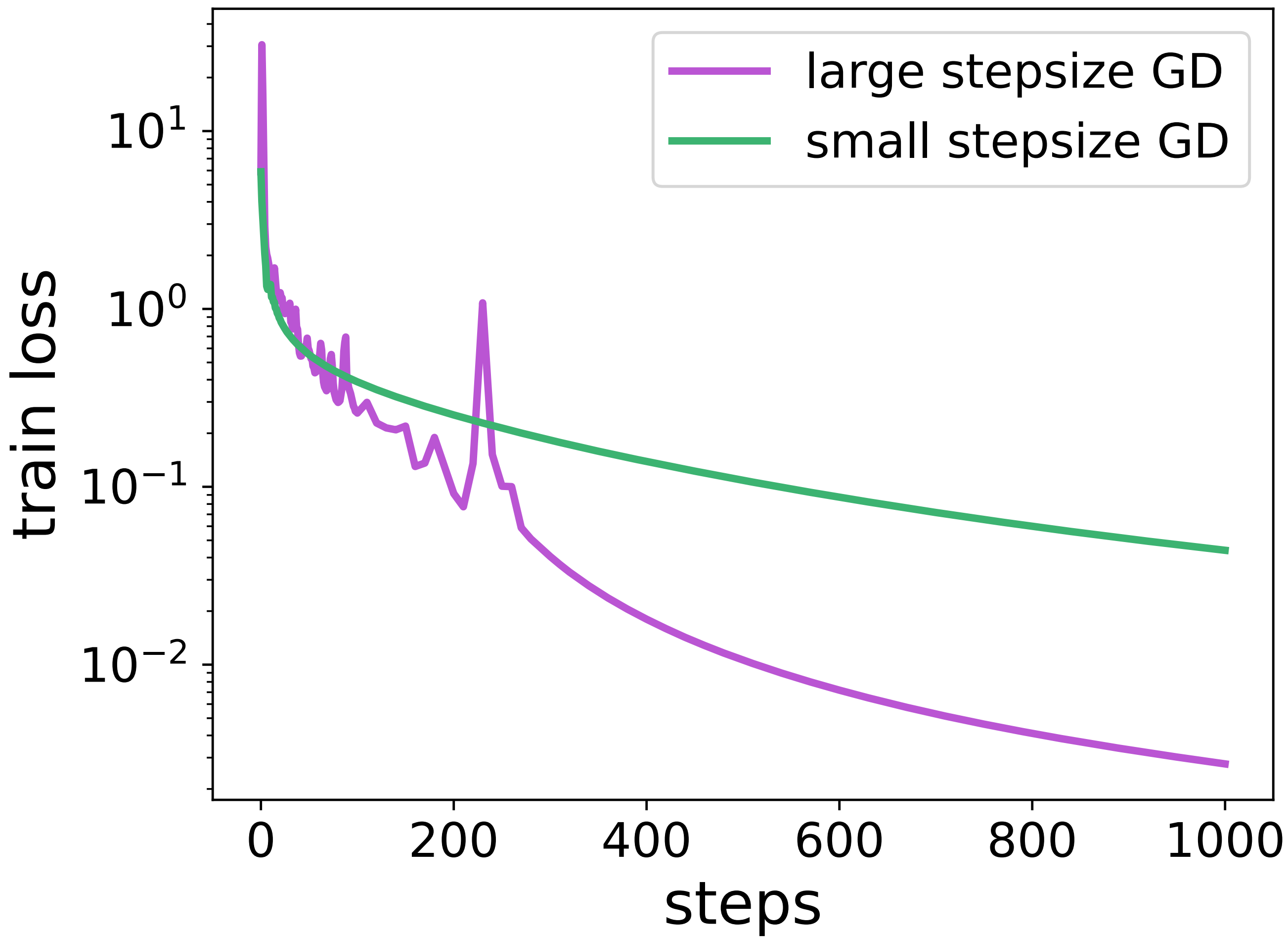

MLP, GD, classification task

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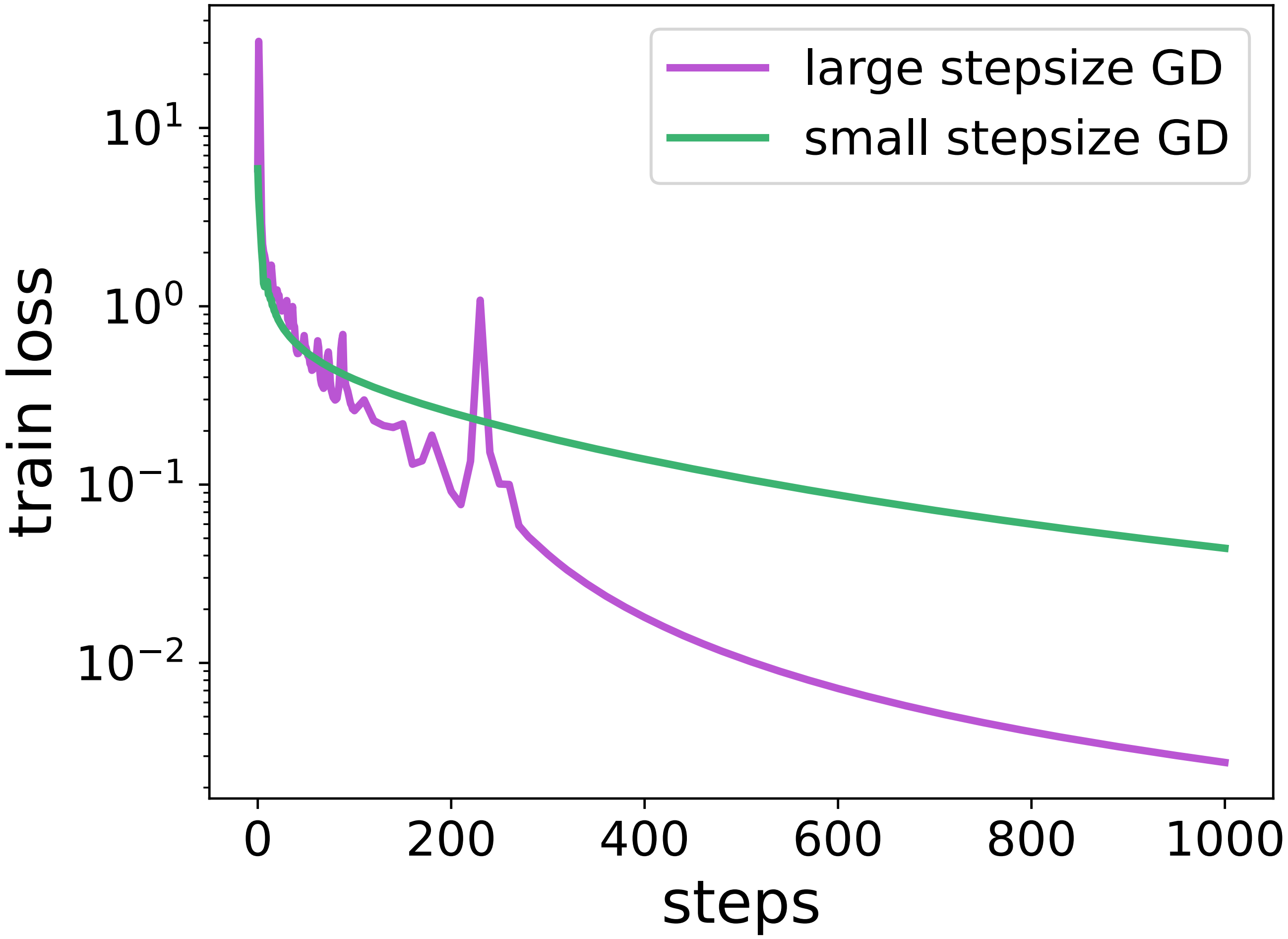

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practice:
best stepsize is large
oscillatory loss

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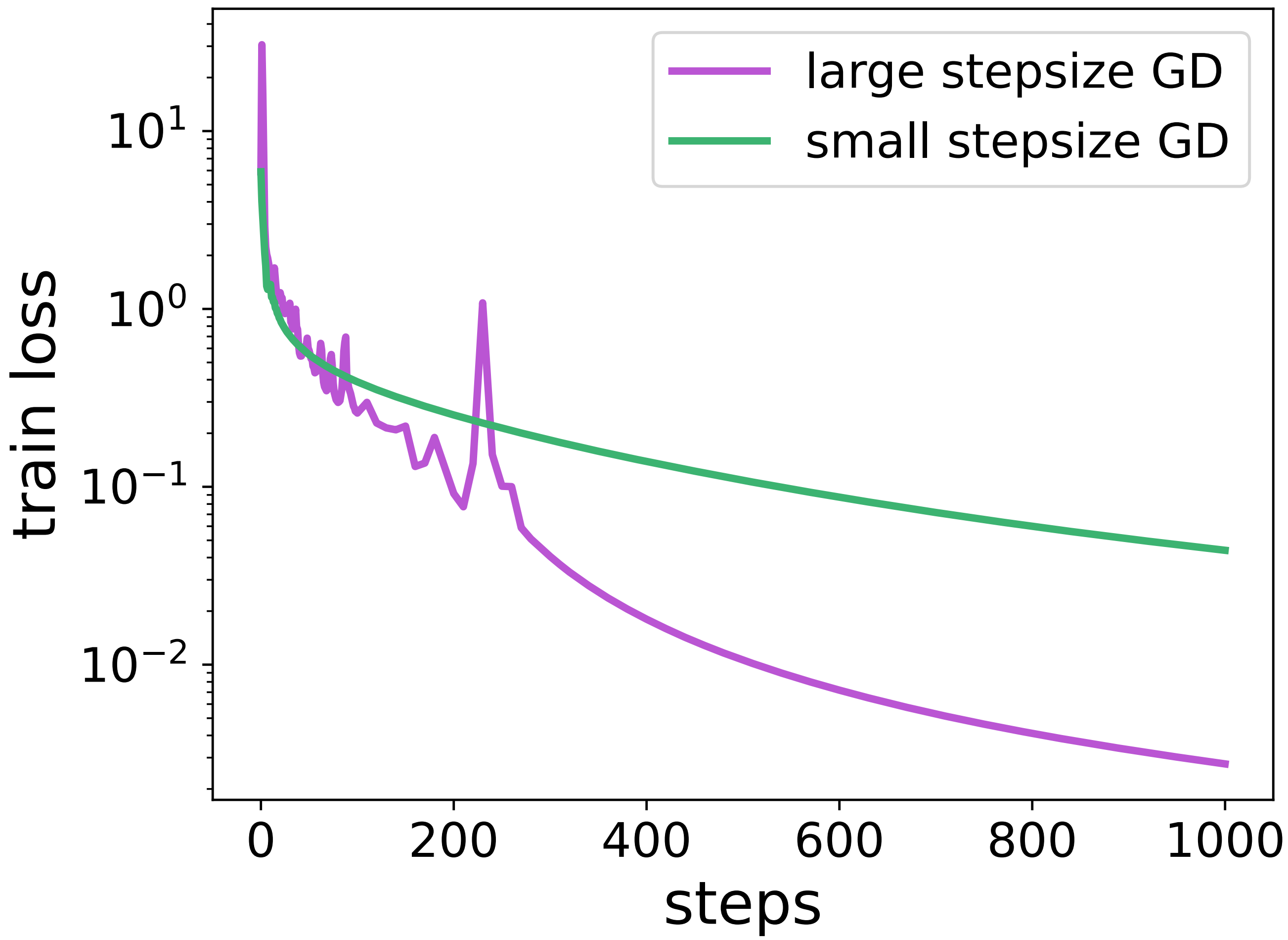

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classical theory fails to predict best stepsize

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Classical theory

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

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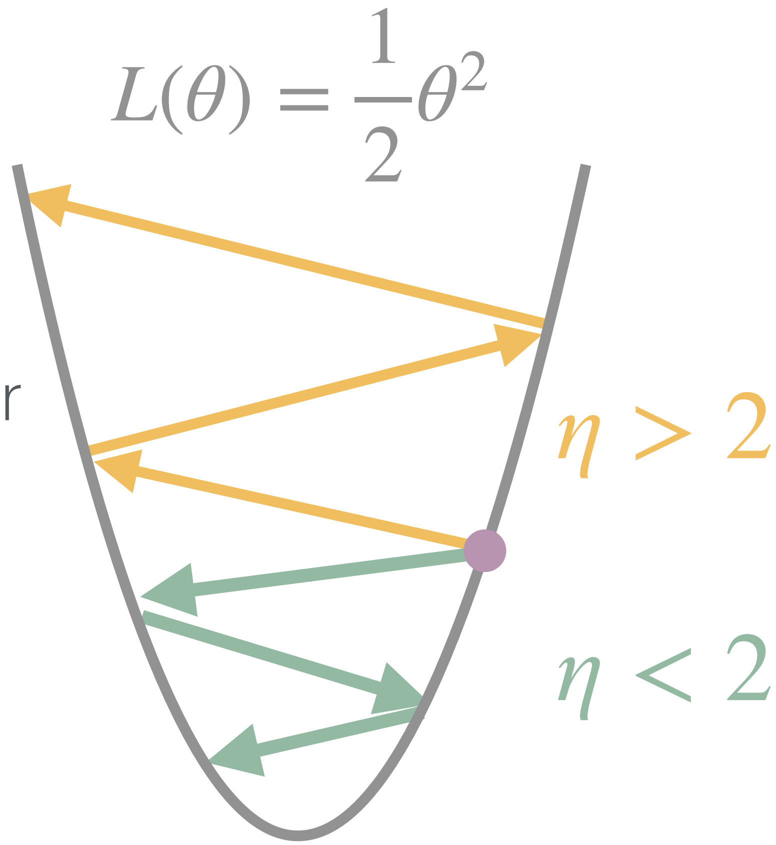
Let L be 1-smooth ($\|\nabla^2 L\| \leq 1$) with finite minimizer

Descent lemma.

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

Classical theory



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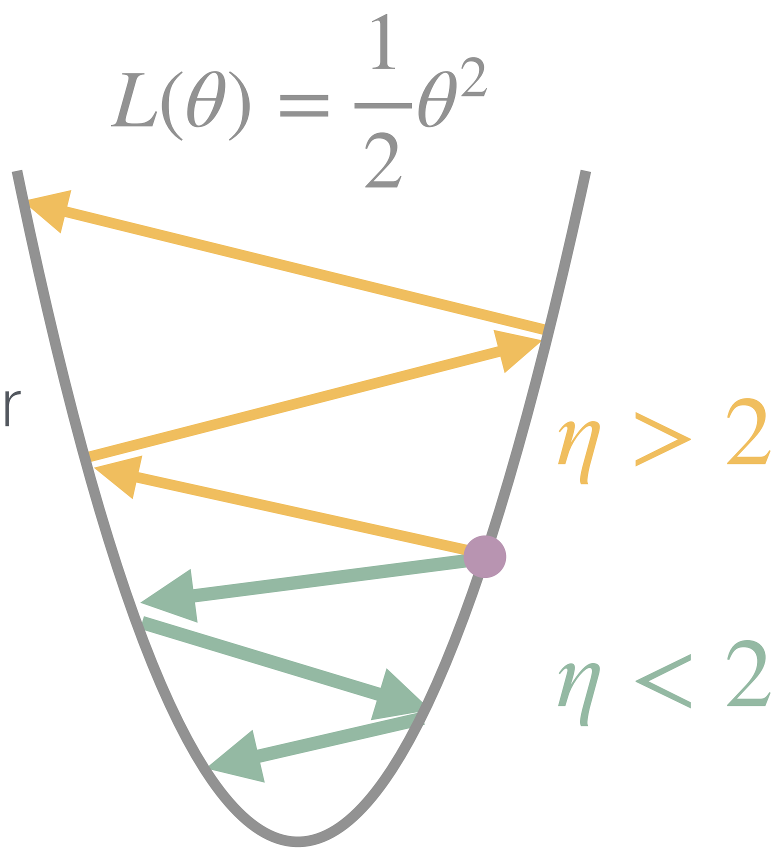

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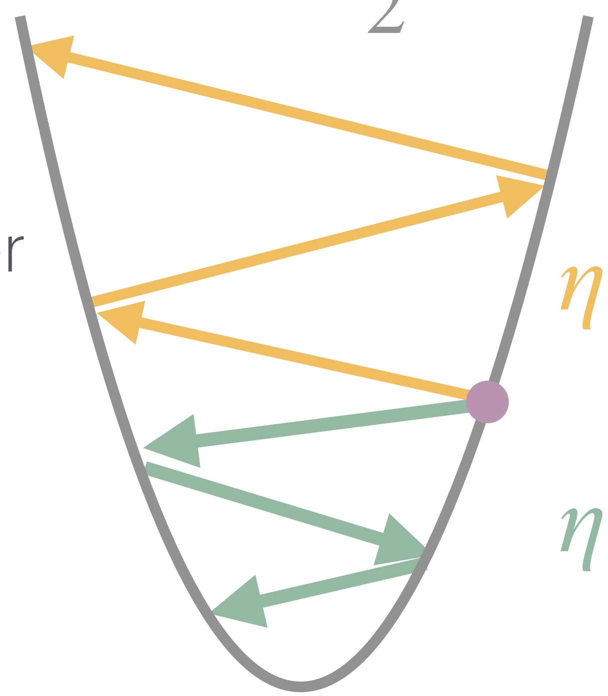

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Rates. GD with $\eta = 1$ achieves

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

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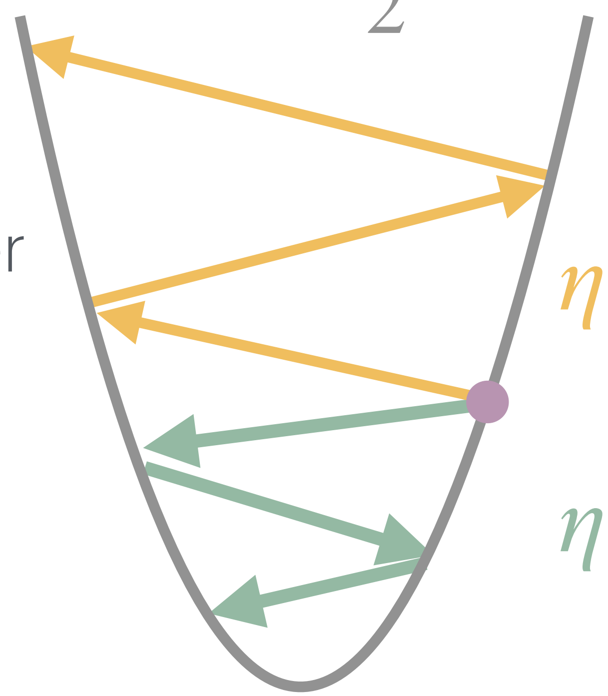

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condition number $\kappa = 1/\lambda \gg 1$

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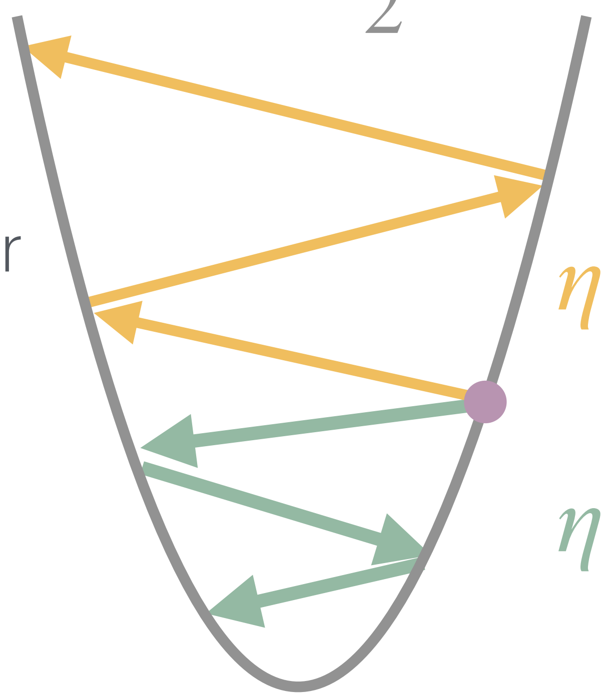

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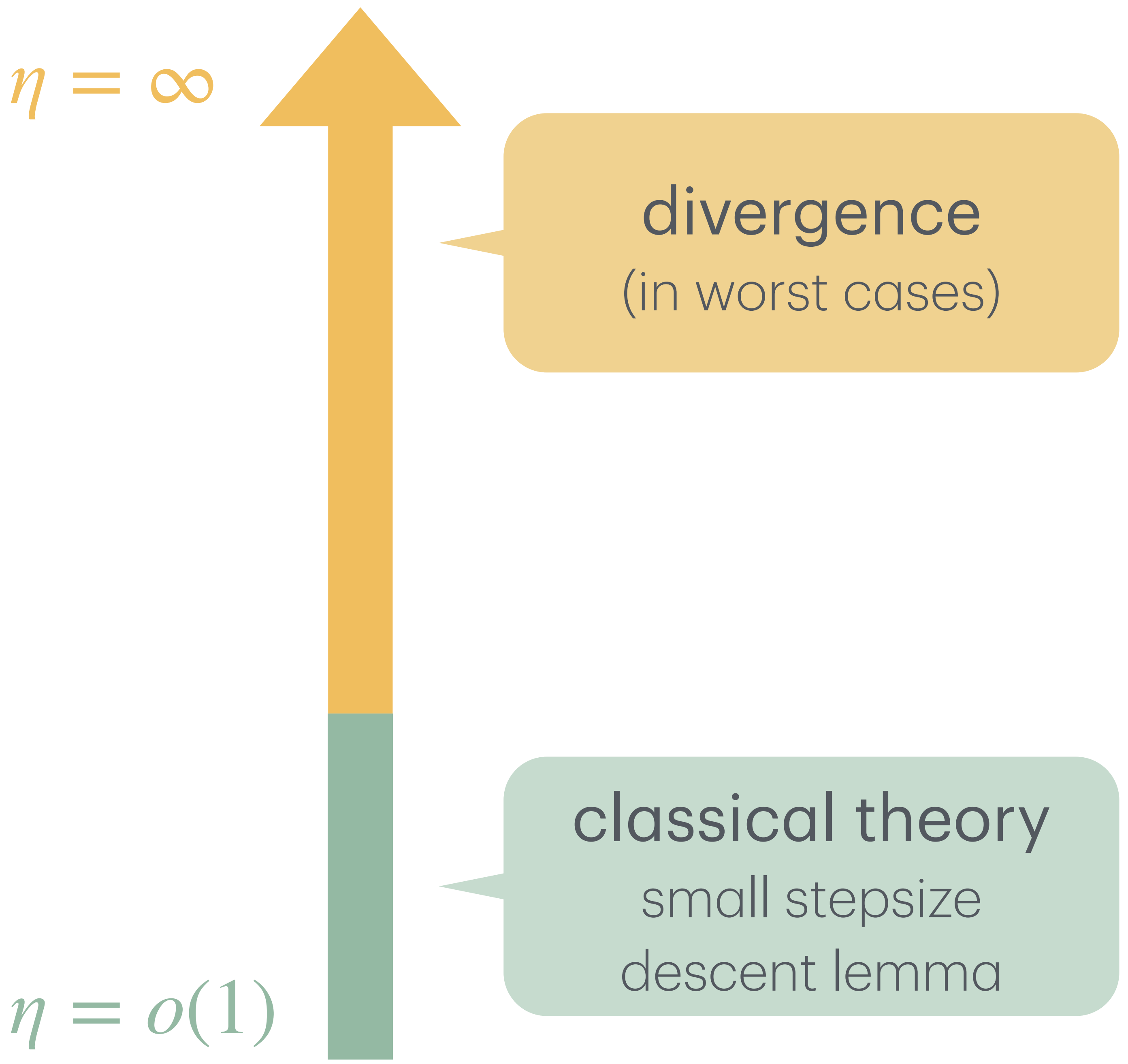
Rates. GD with $\eta = 1$ achieves

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

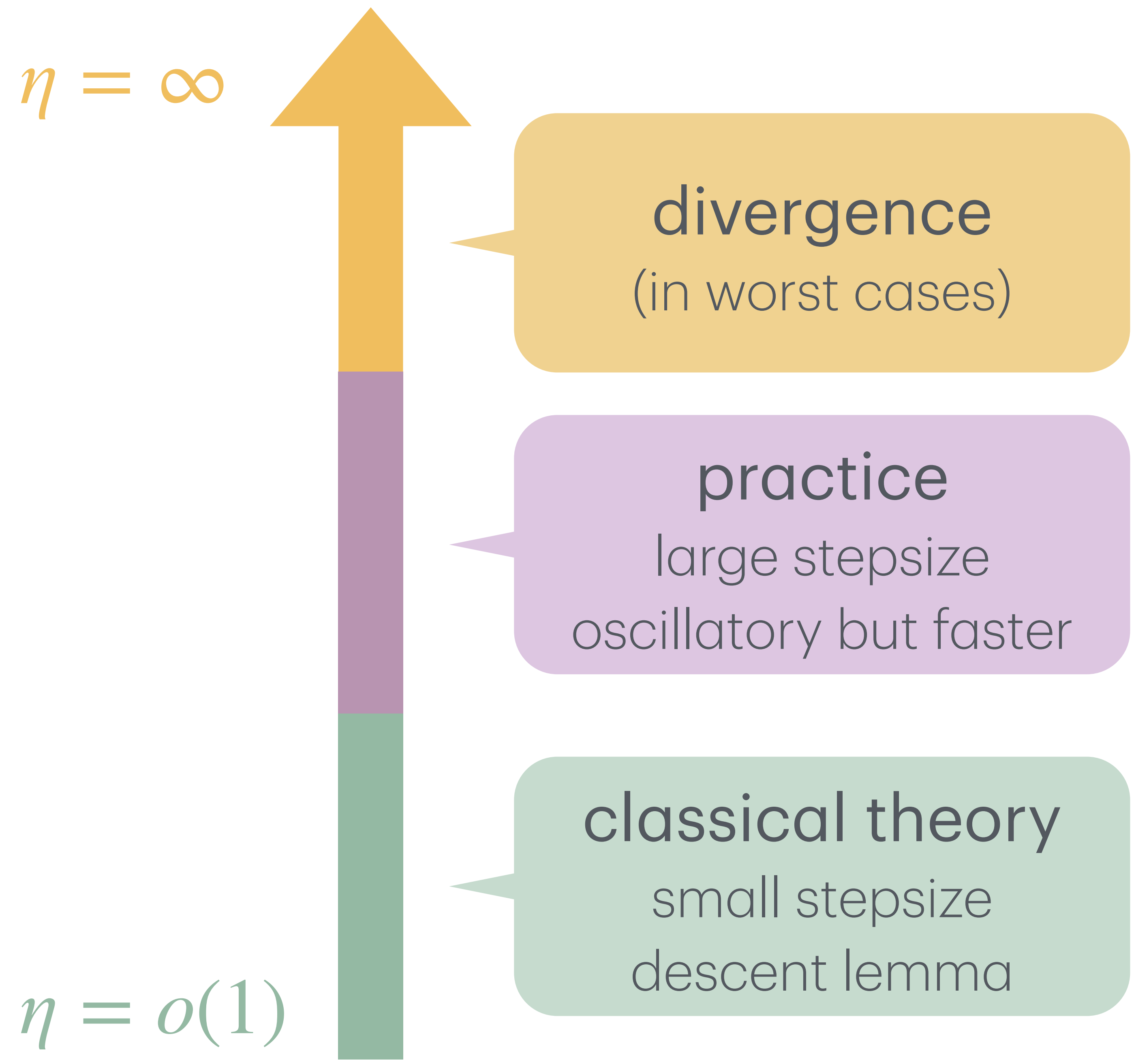
condition number
$\kappa = 1/\lambda \gg 1$

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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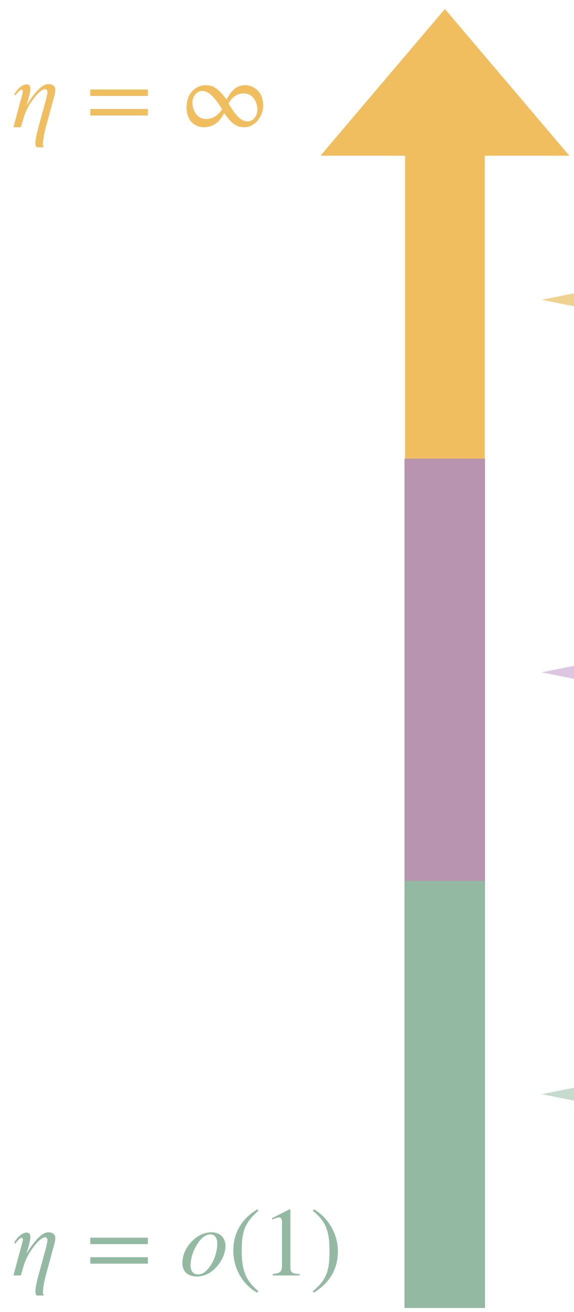

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as mental picture

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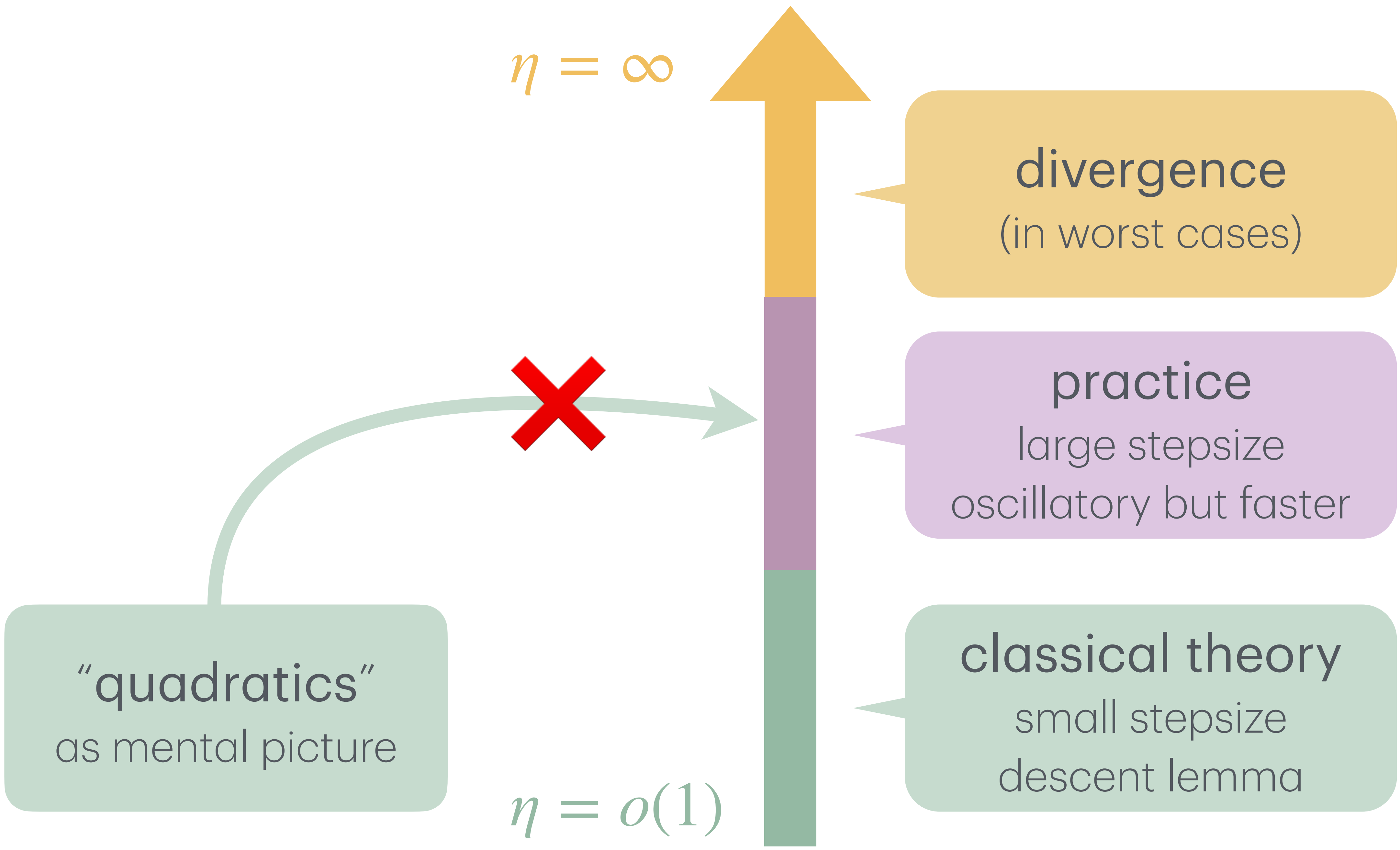

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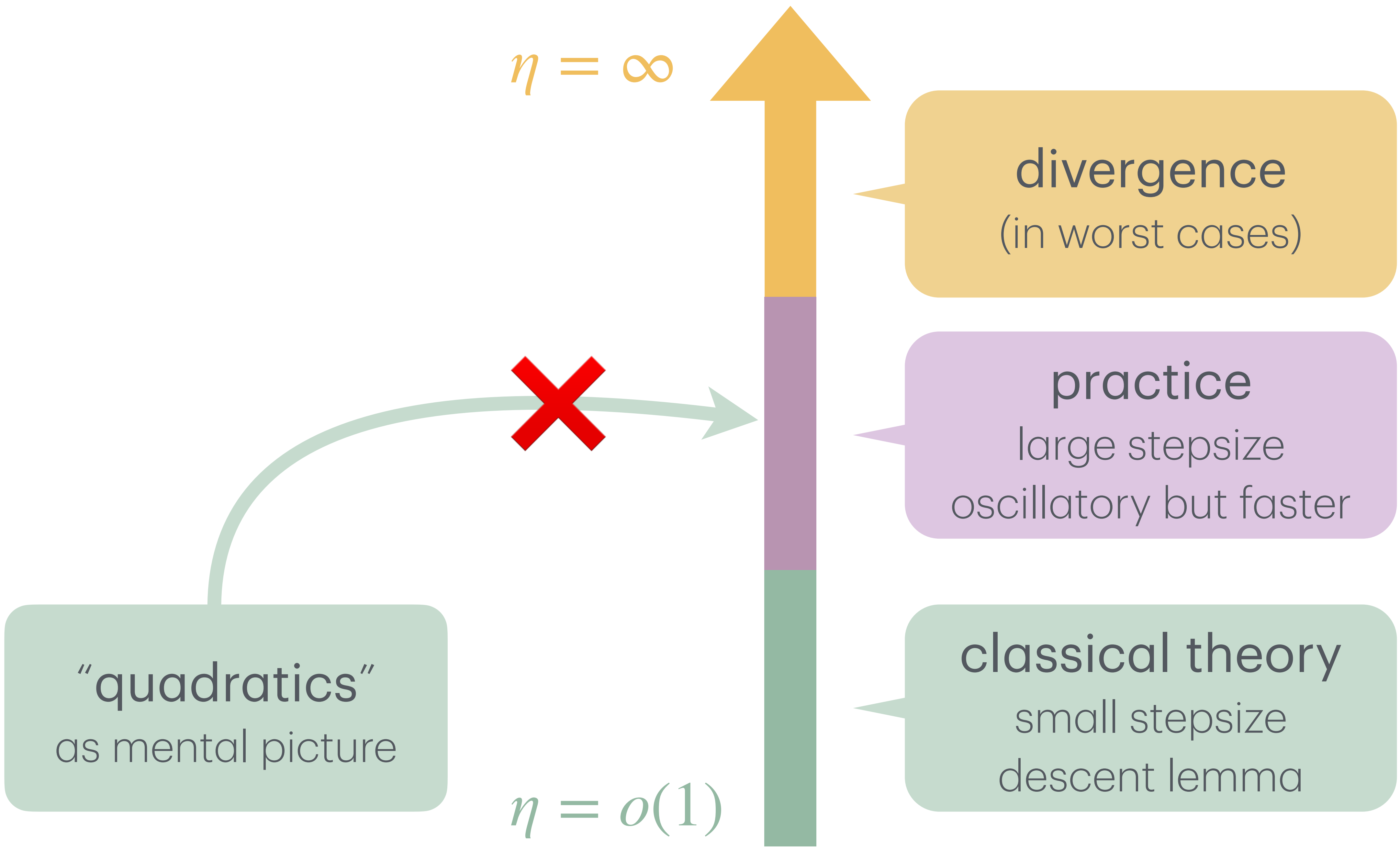

Related works

- Altschuler, Parrilo. "Acceleration by stepsize hedging I: multi-step descent and the silver stepsize schedule." Journal of the ACM 2024
- Davis, Drusvyatskiy, Jiang. "Gradient descent with adaptive stepsize converges (nearly) linearly under fourth-order growth" Mathematical Programming 2025

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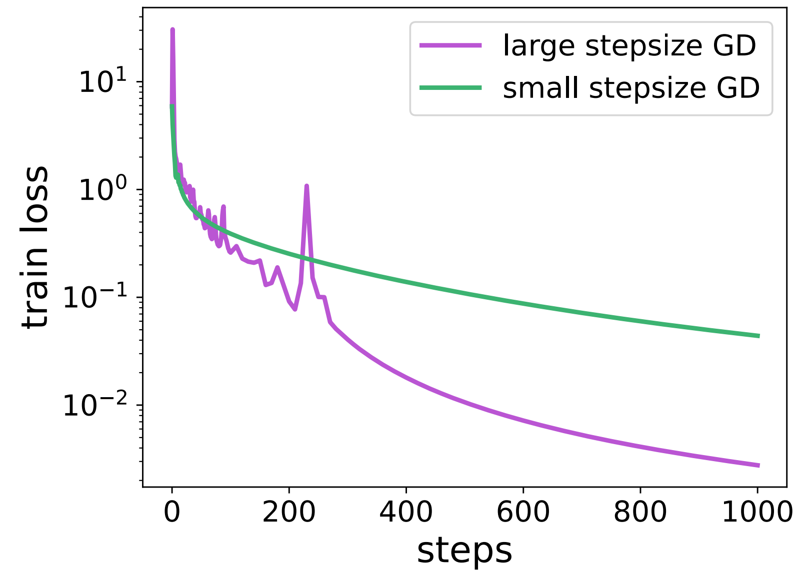
Seeking simplest sandbox

……

deep learning

unstable optimization observed



Seeking simplest sandbox

linear regression

......

deep learning

unstable optimization impossible

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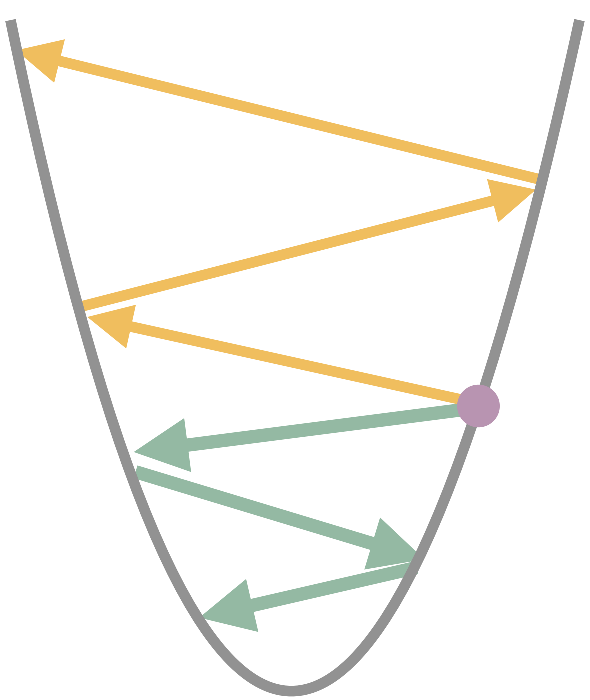

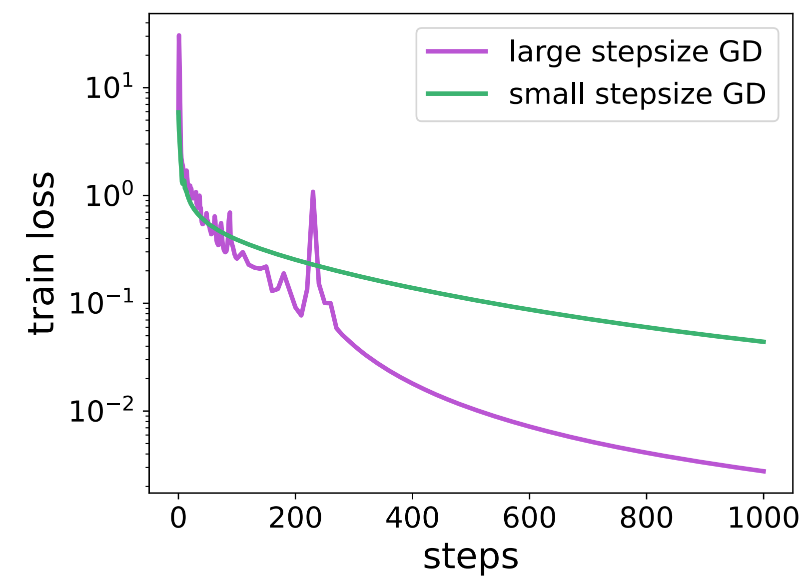

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logistic regression

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observable & provable

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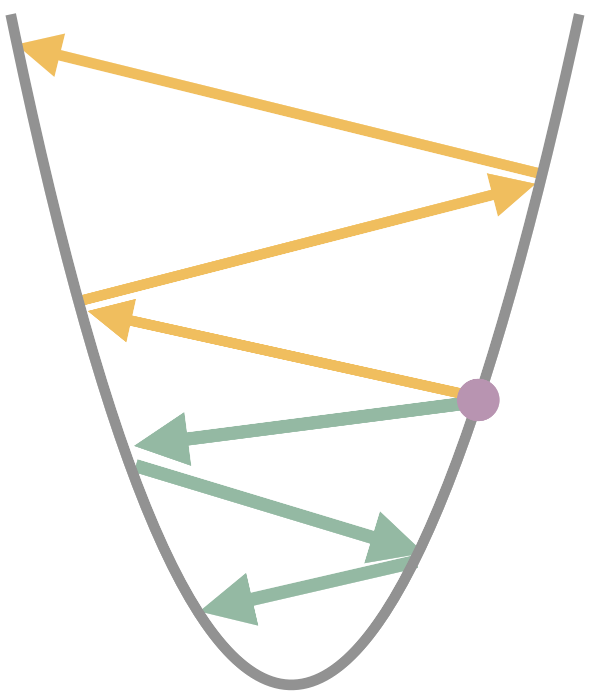

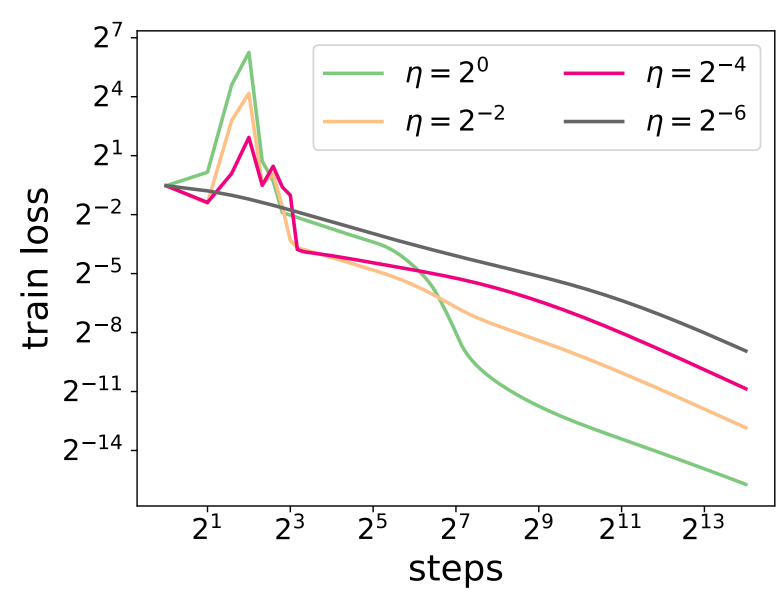

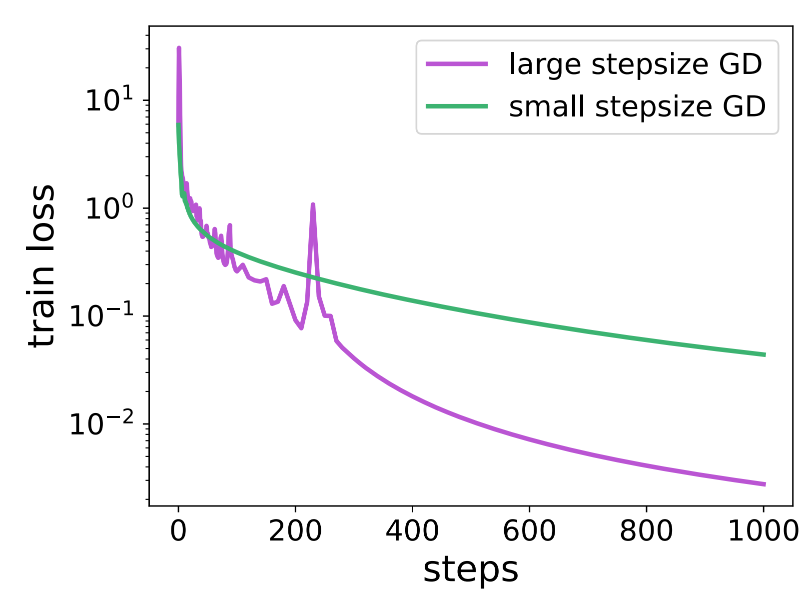

Logistic regression

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

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

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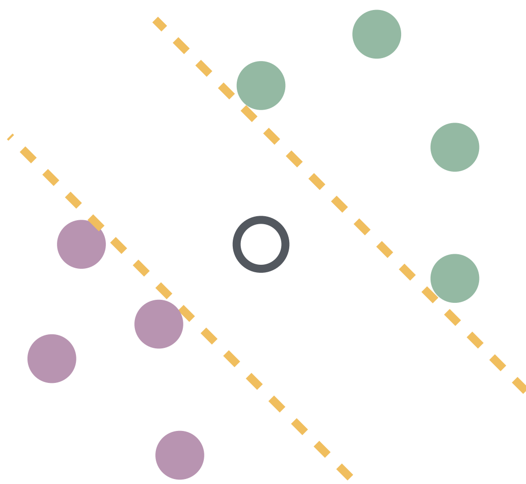

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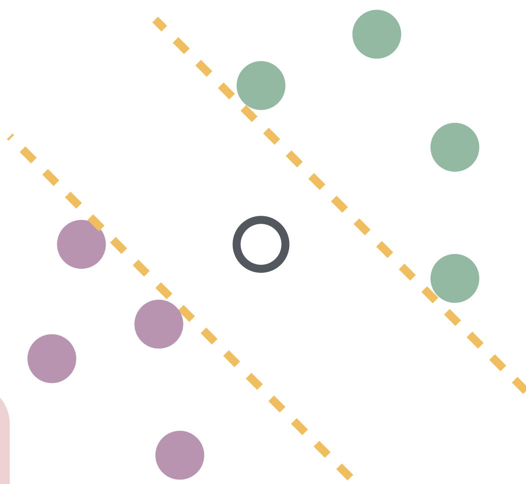
implied by overparameterization



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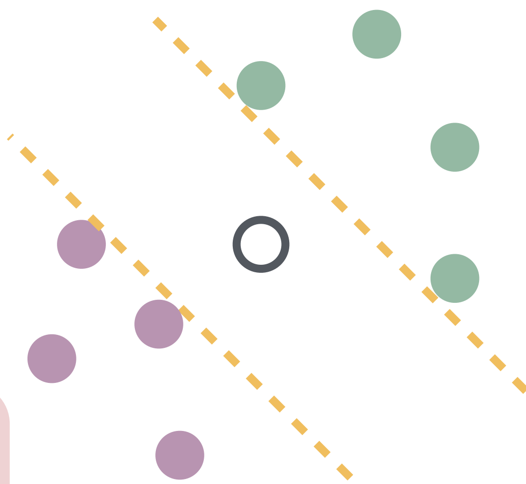

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smooth, convex
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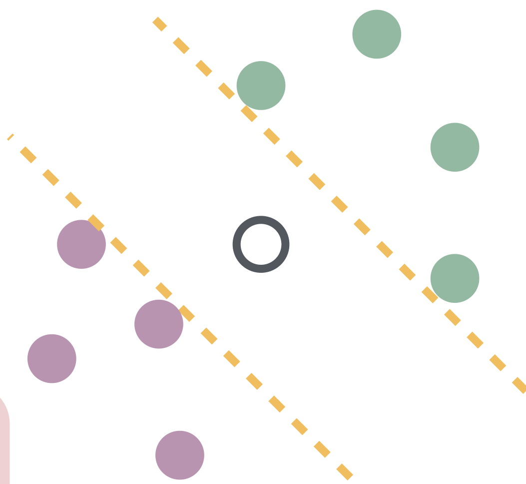

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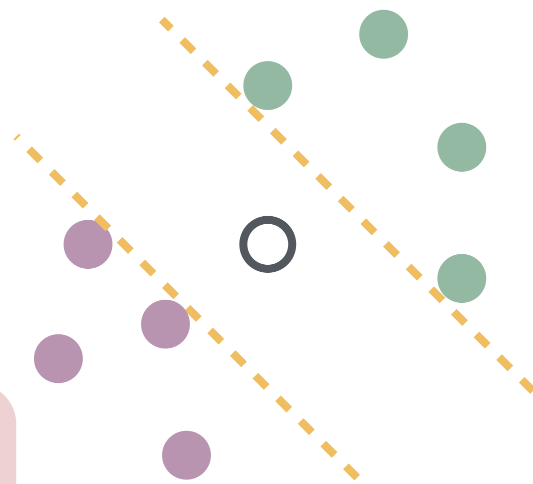

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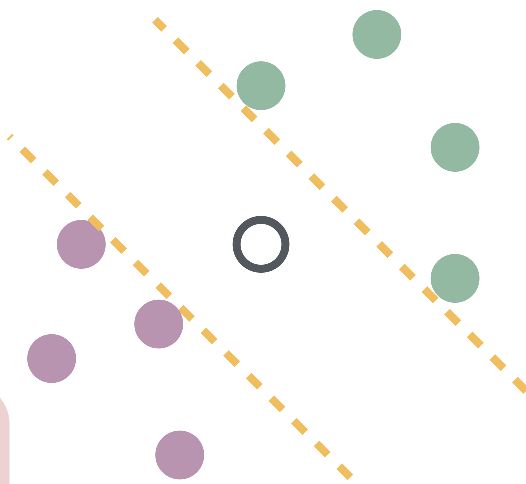

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improved to $\tilde{O}(1/t^2)$ by Nesterov

Large stepsize accelerates GD

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

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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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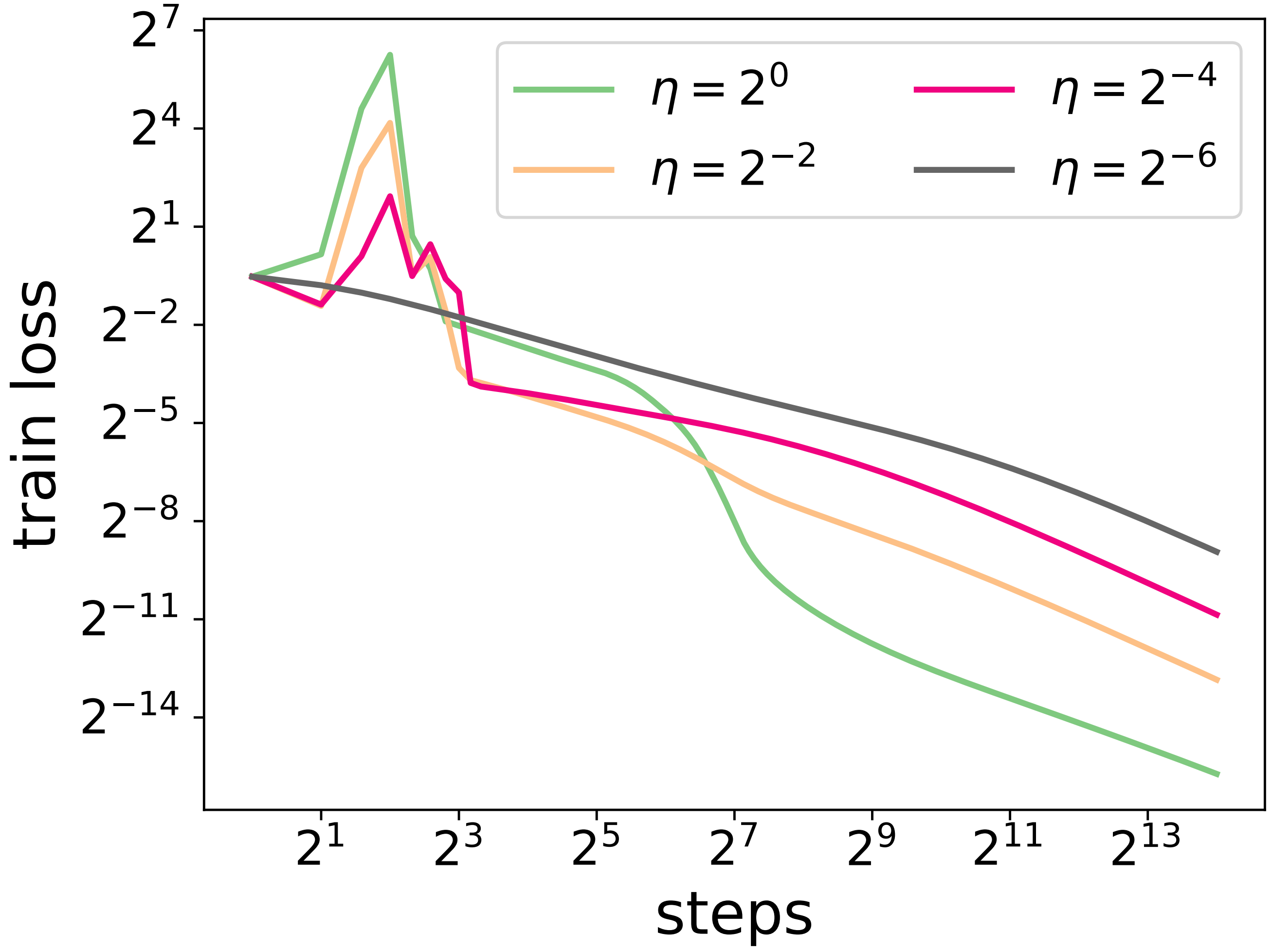

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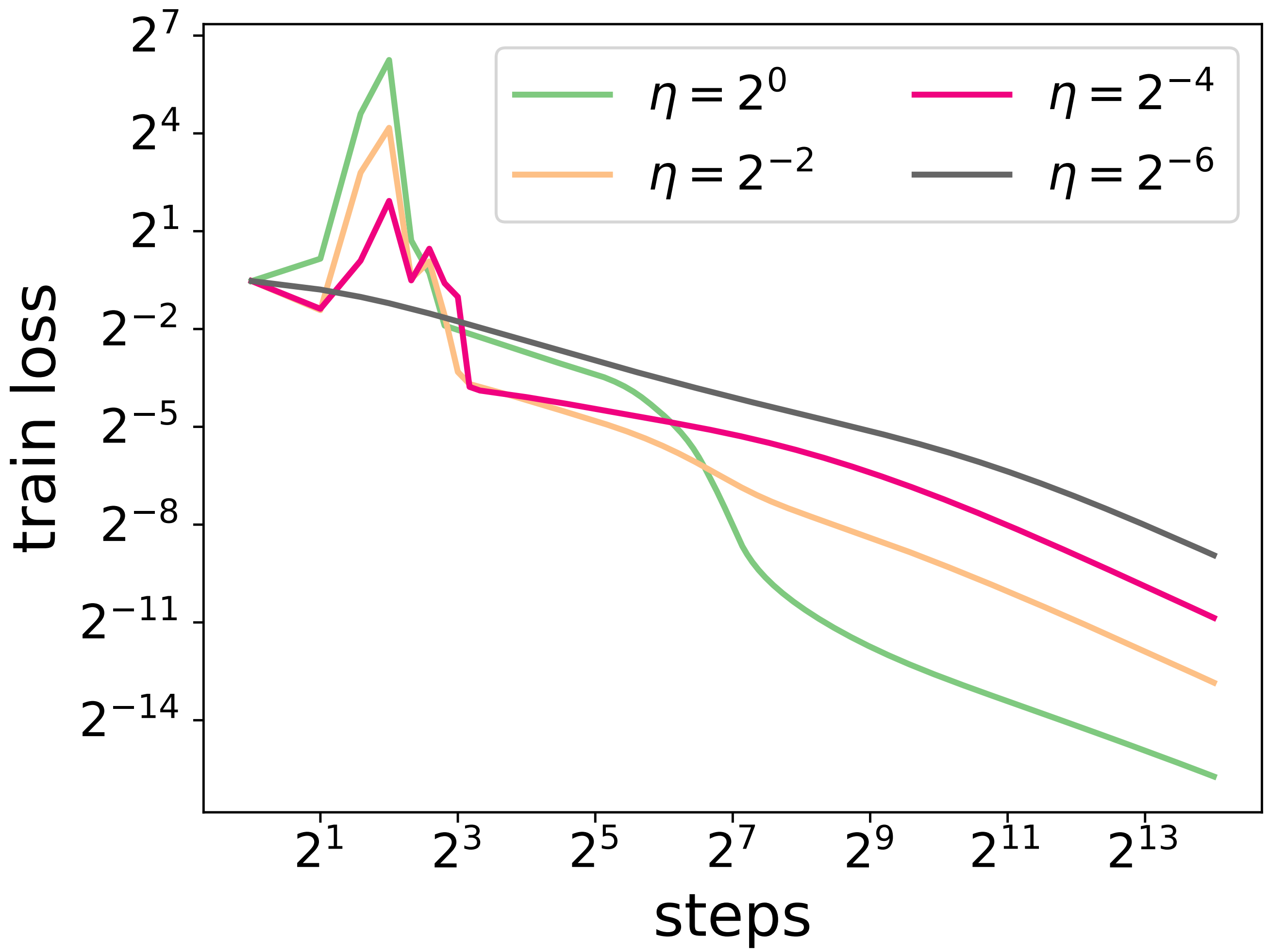

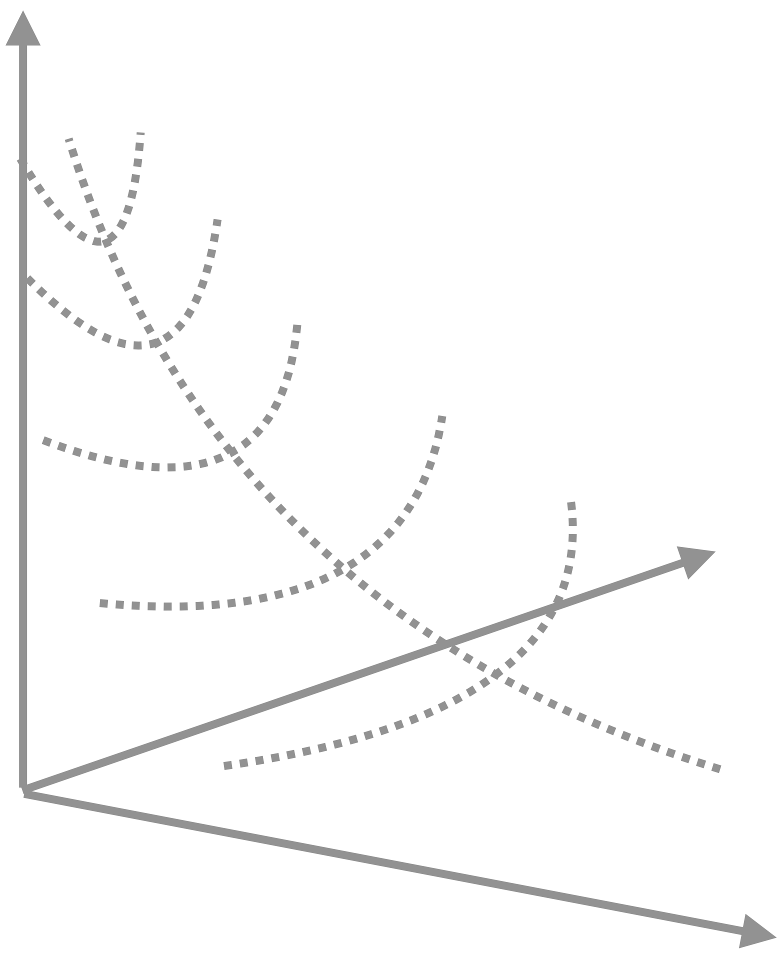

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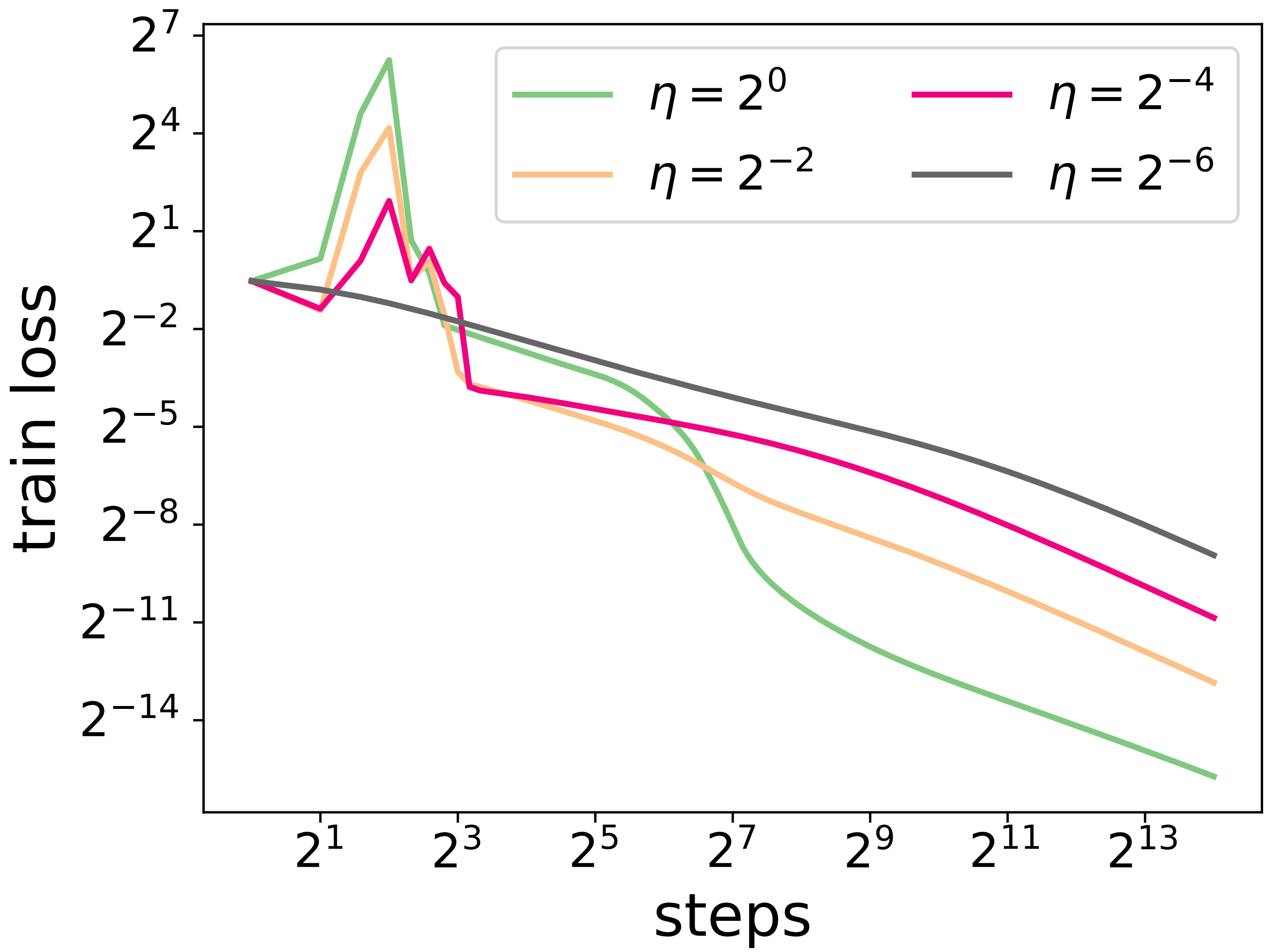

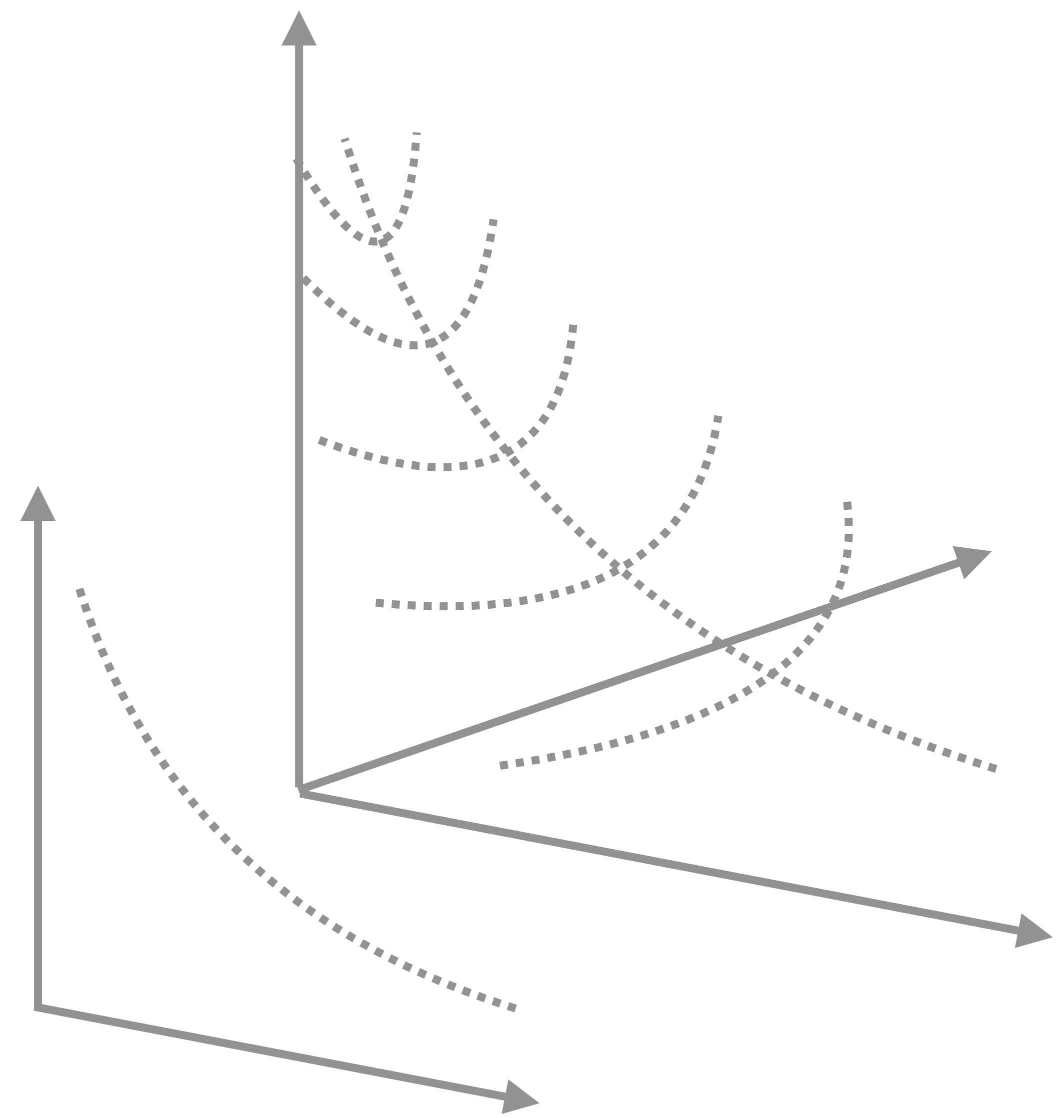

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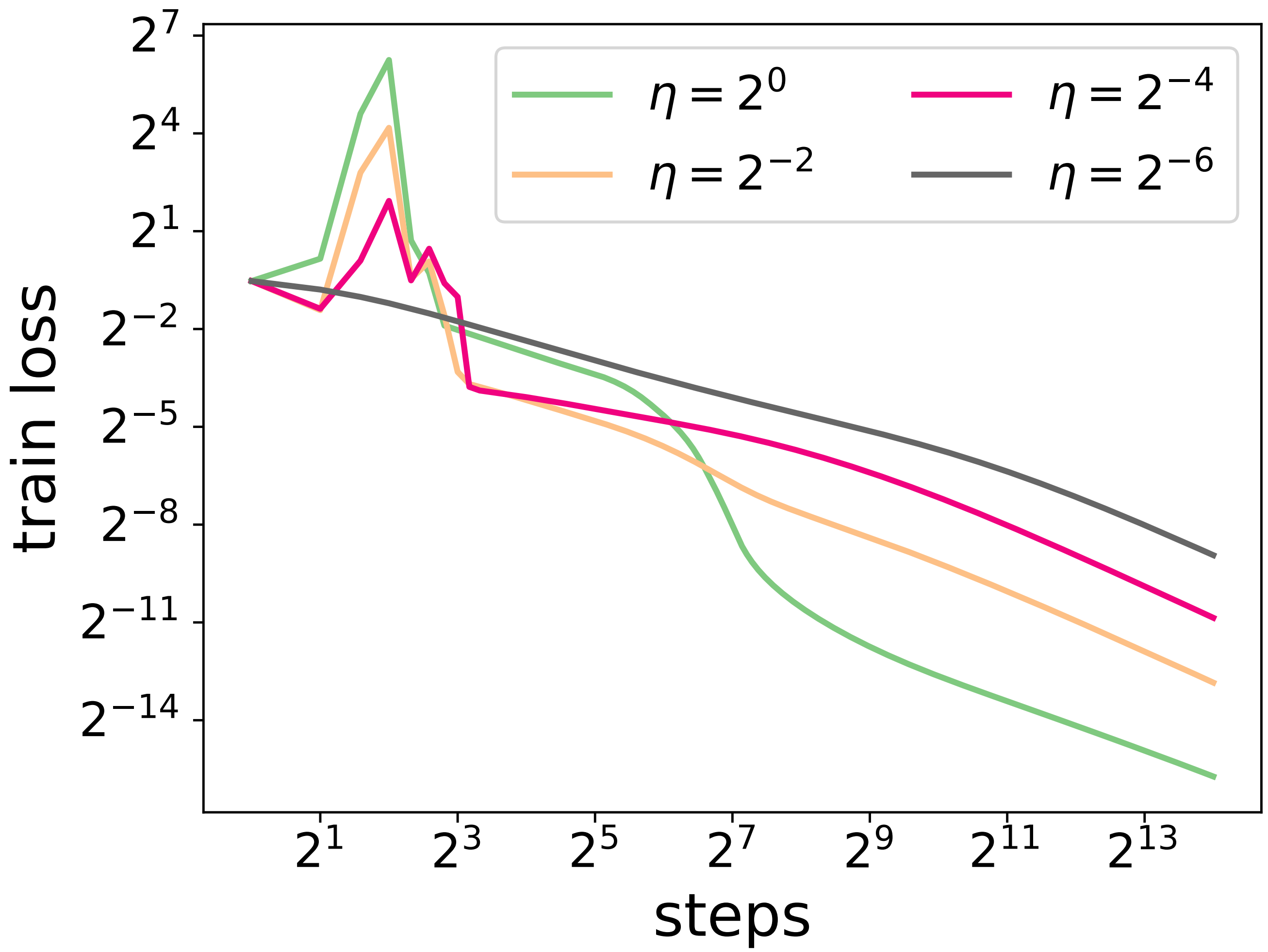

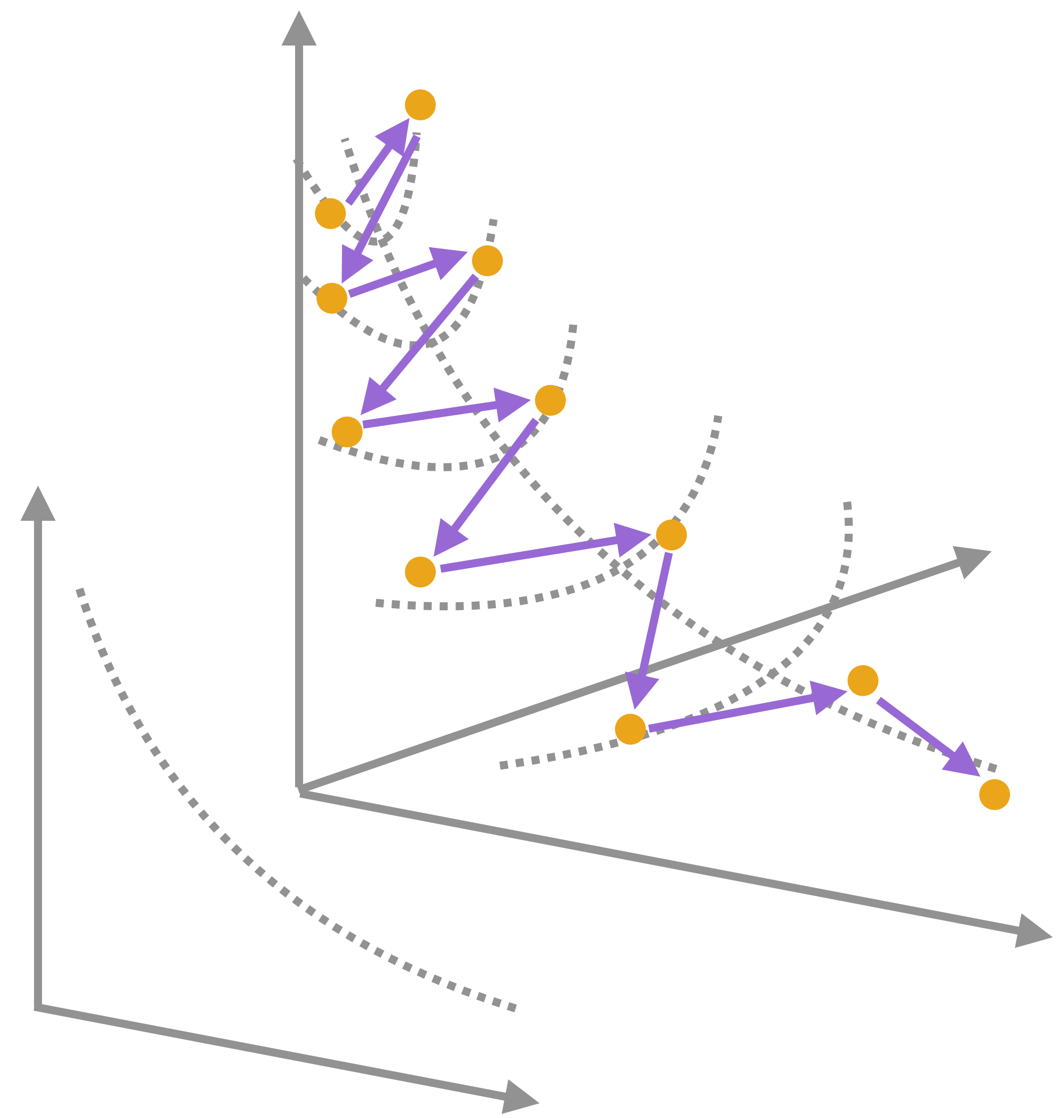

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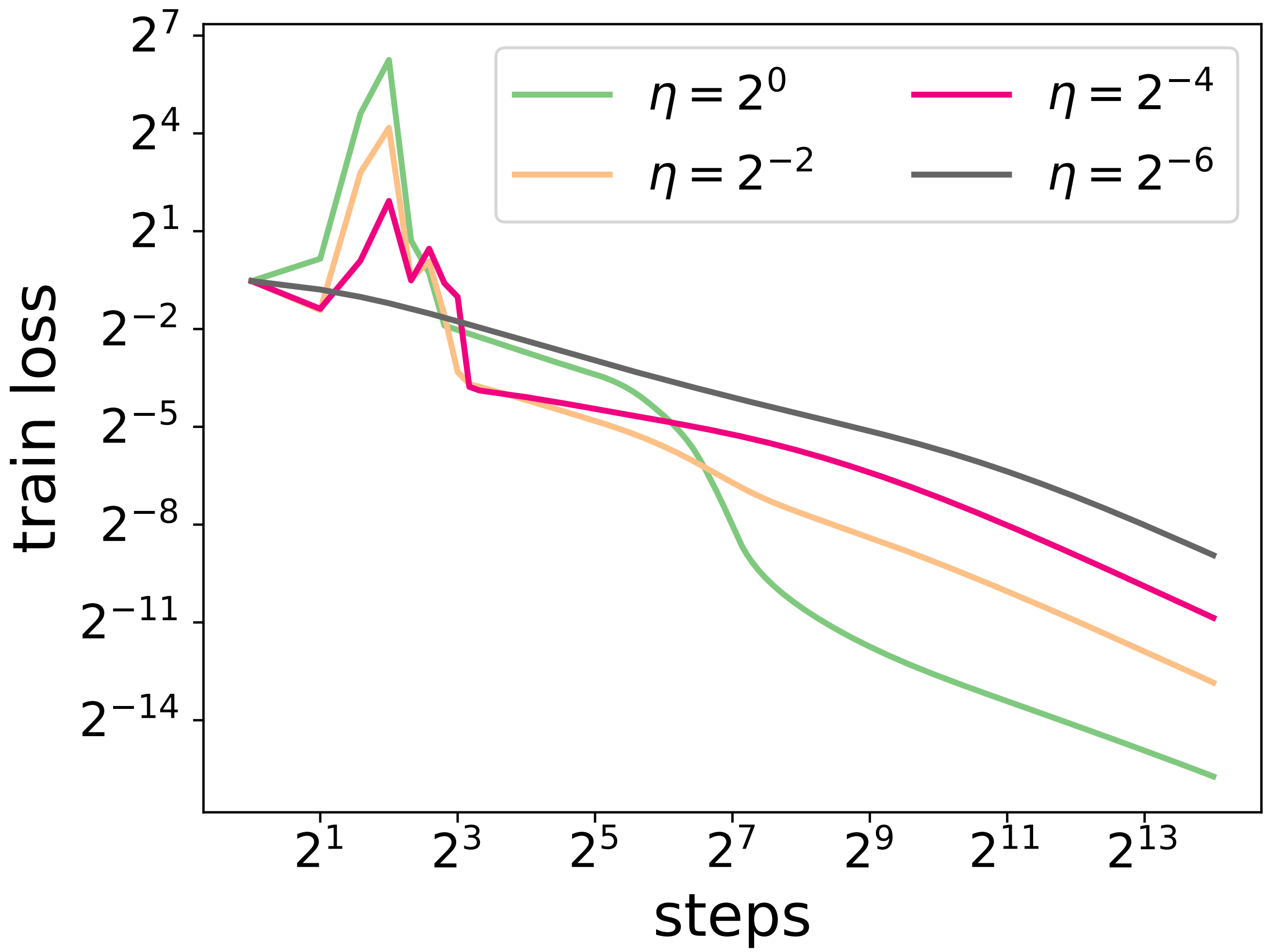

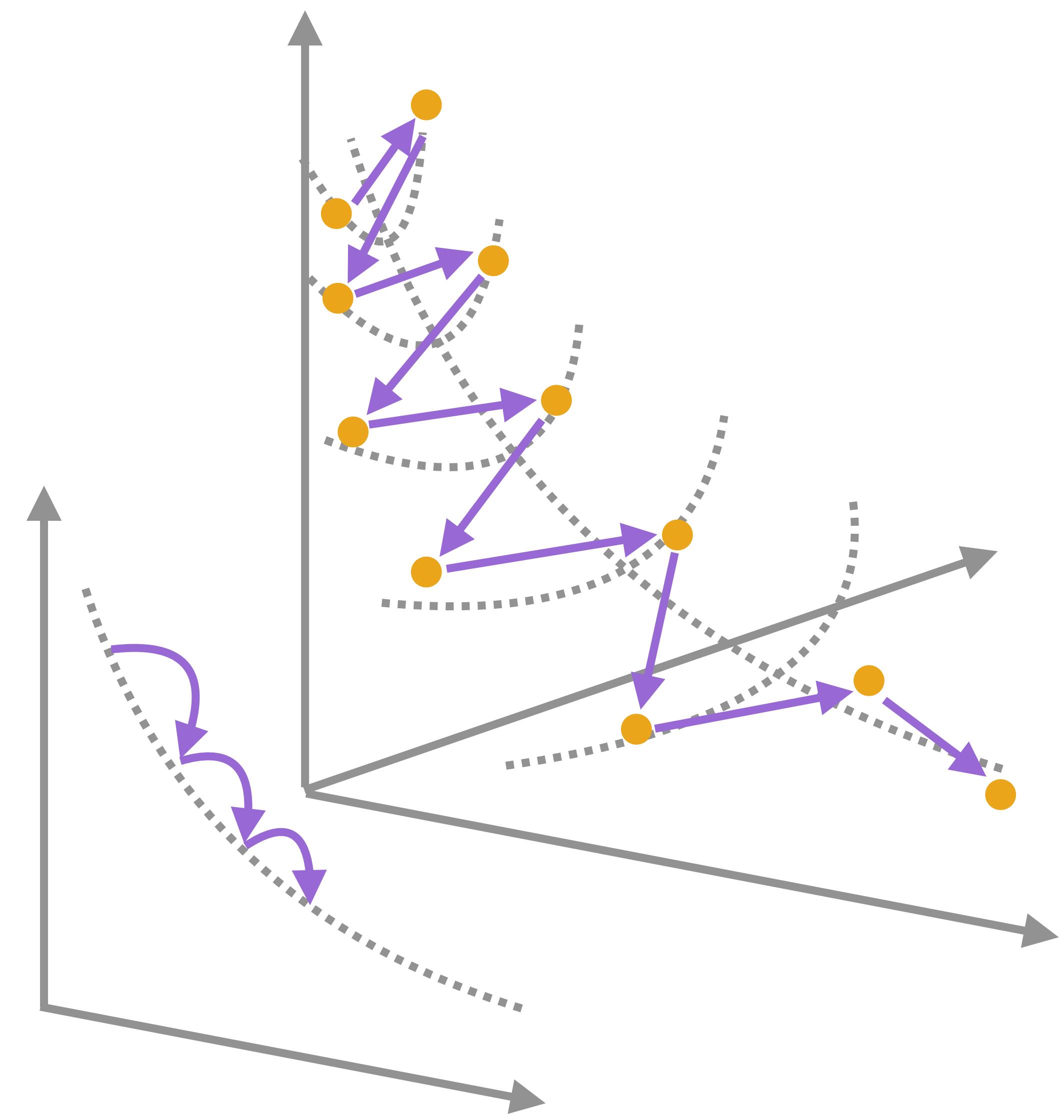

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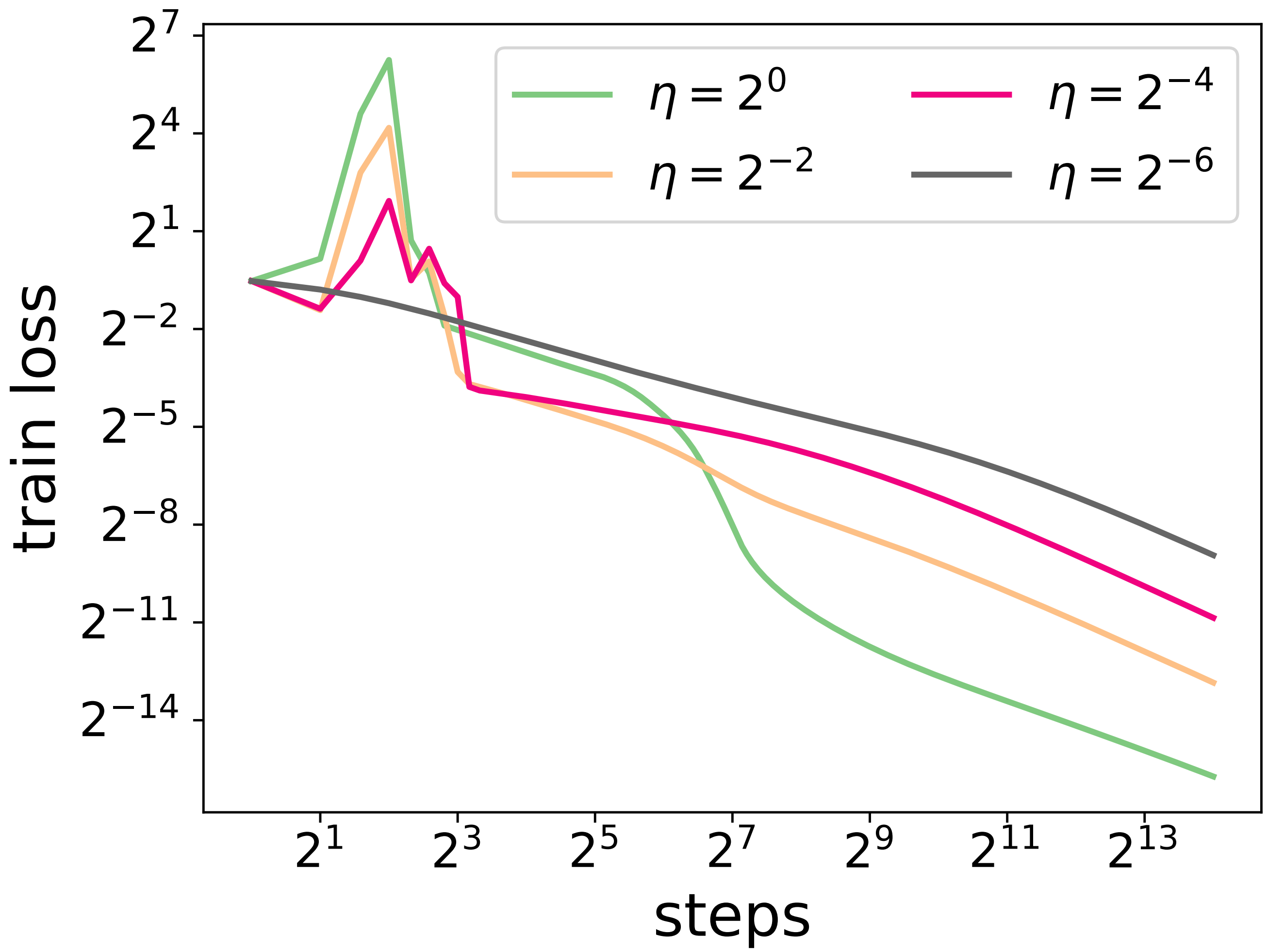
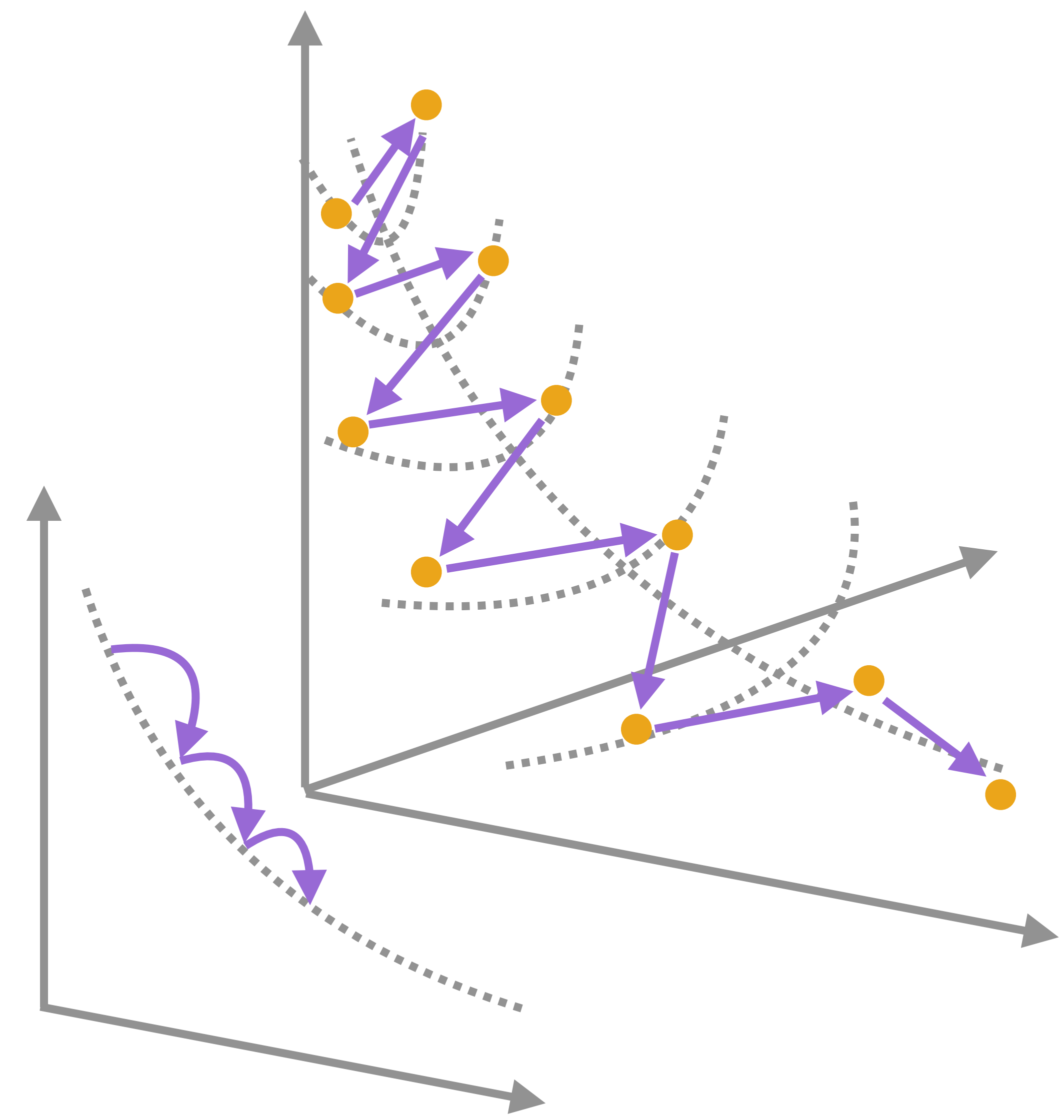
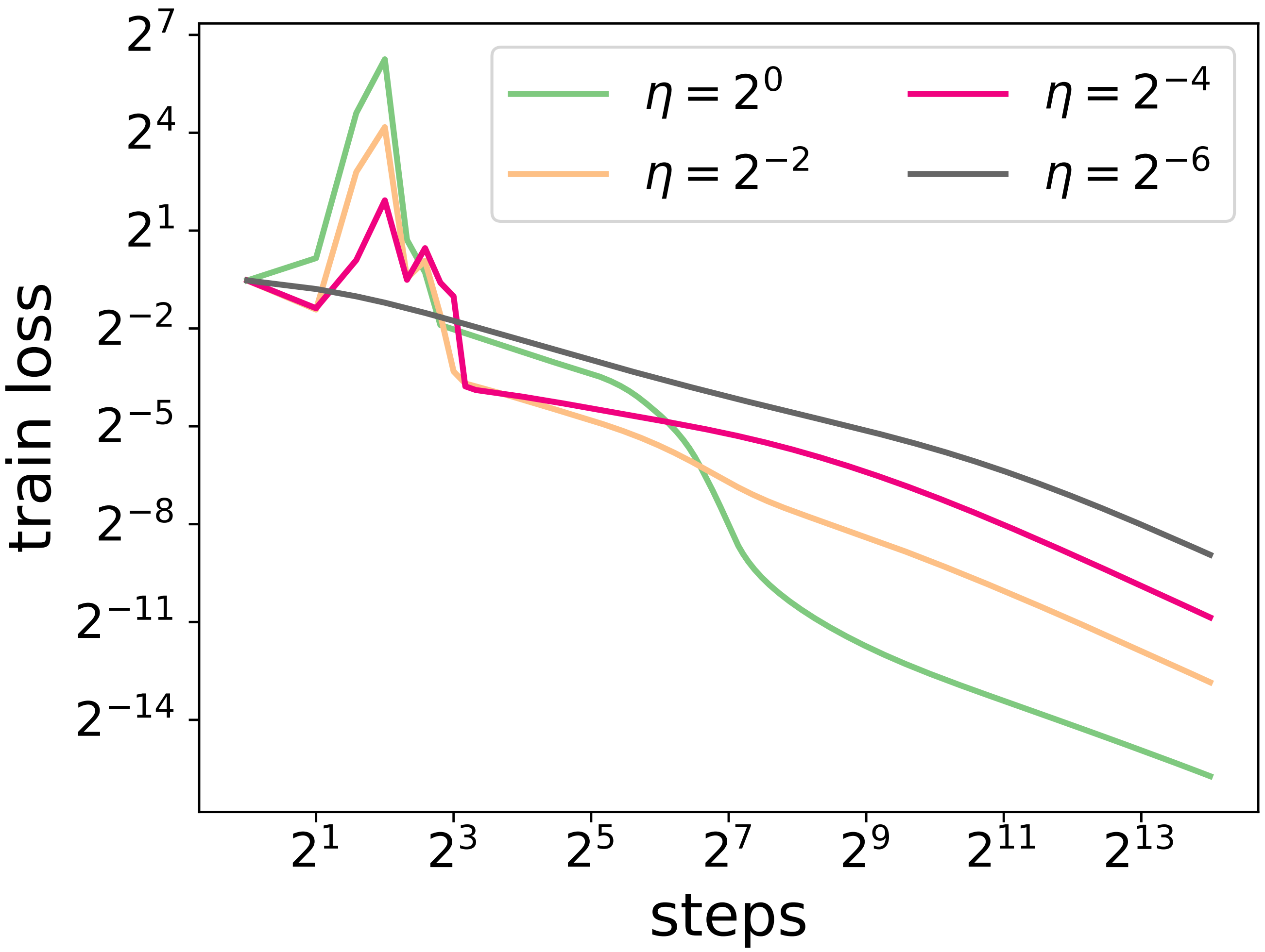




"open valley" as mental picture

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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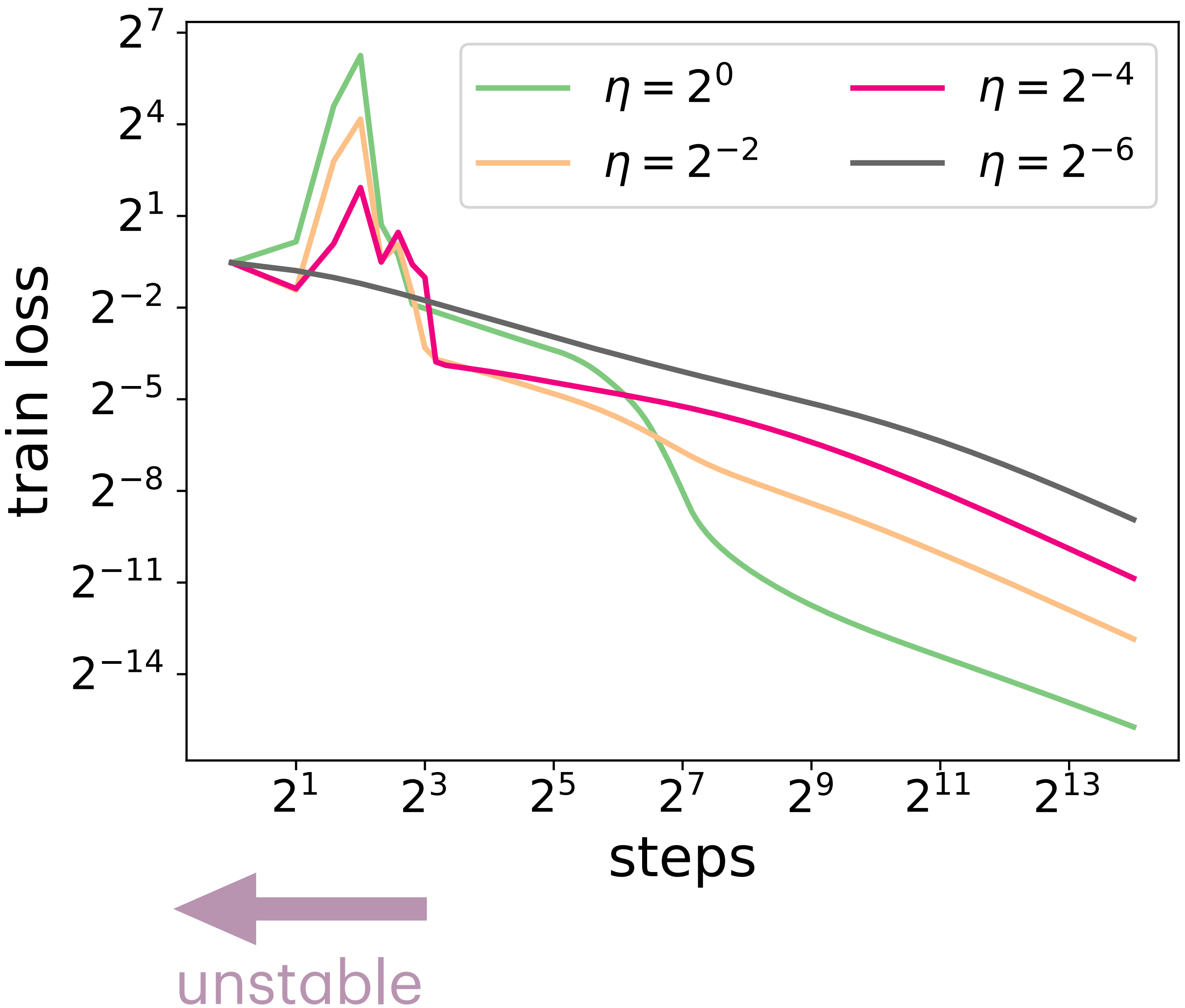

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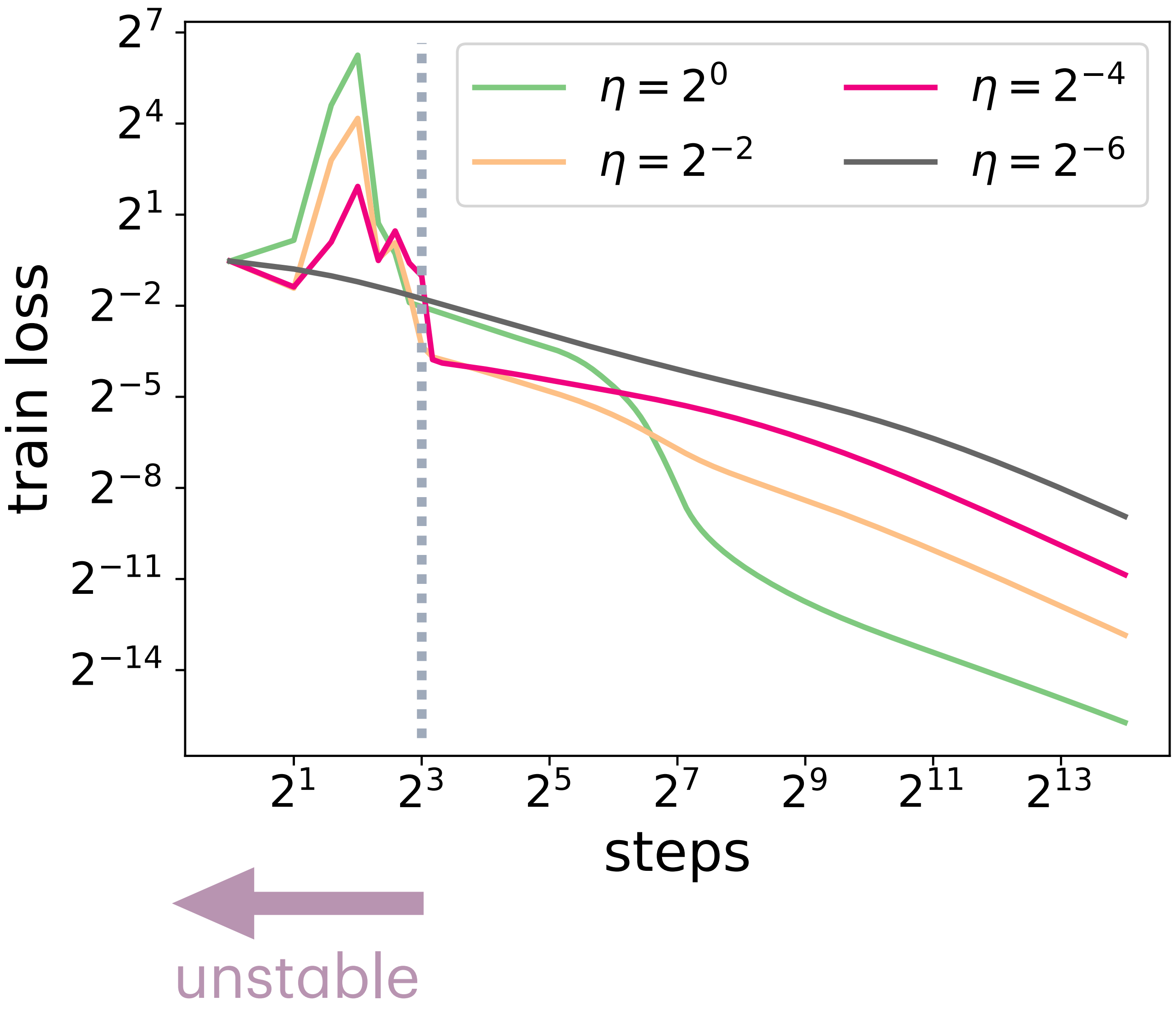

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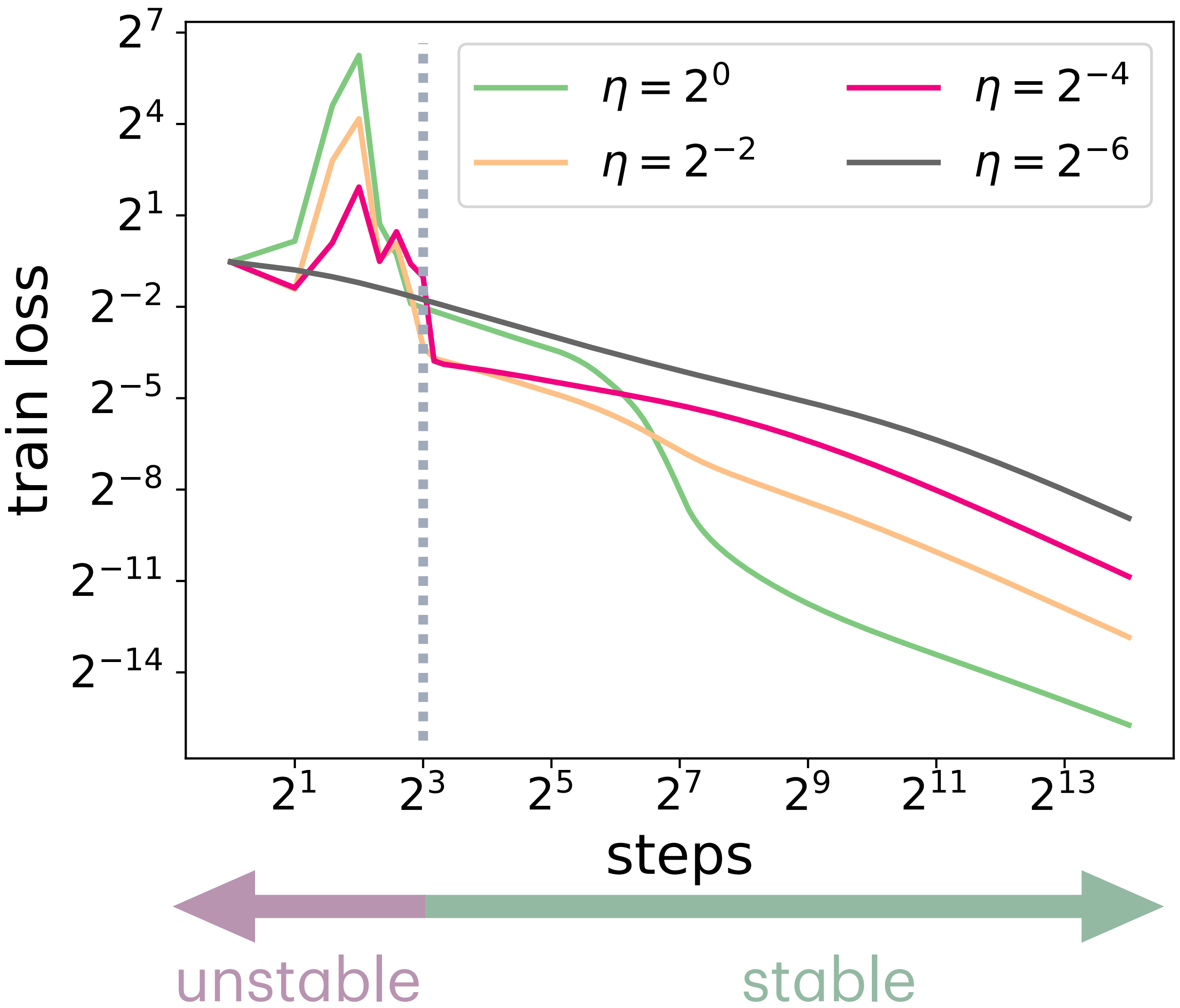

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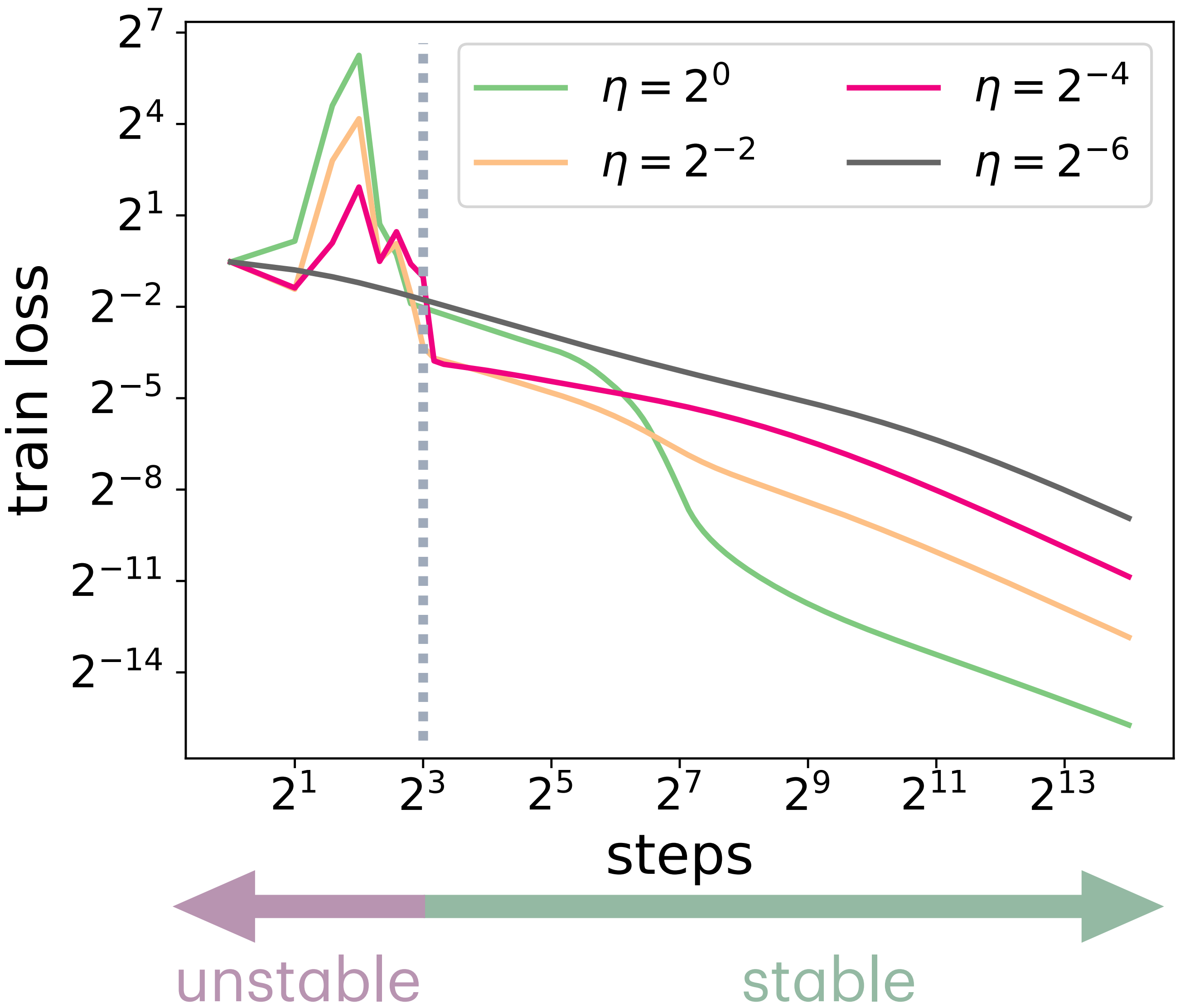

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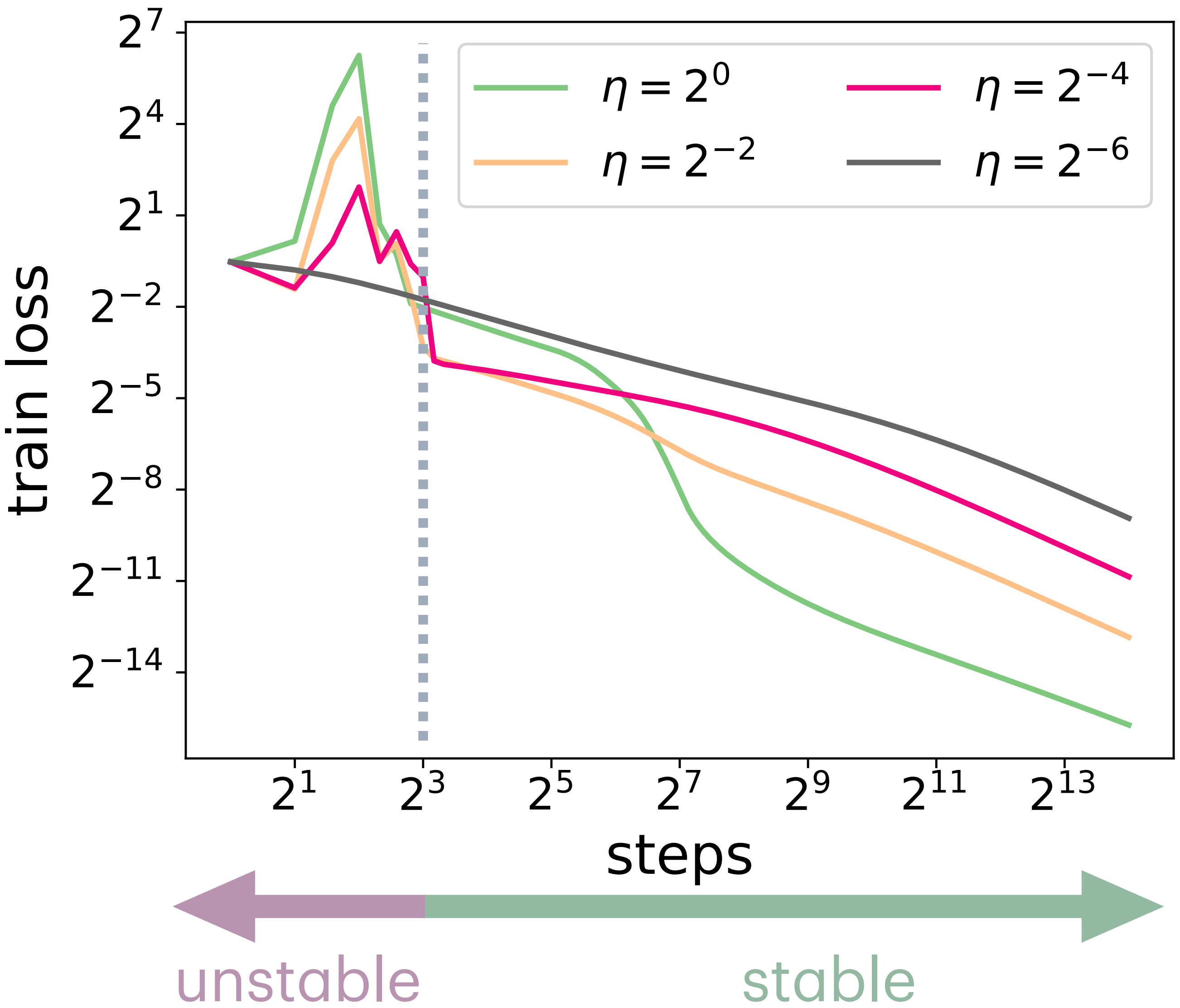

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Regularized logistic regression

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

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

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

$\tilde{L}(\theta_t) - \min \tilde{L} \leq \epsilon$ for $t = O\big(\sqrt{\kappa} \ln(1/\epsilon)\big)$

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

$$\tilde{L}(\theta_t) - \min \tilde{L} \le \epsilon \text{ for } t = O\big(\kappa \ln(1/\epsilon)\big)$$

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match Nesterov
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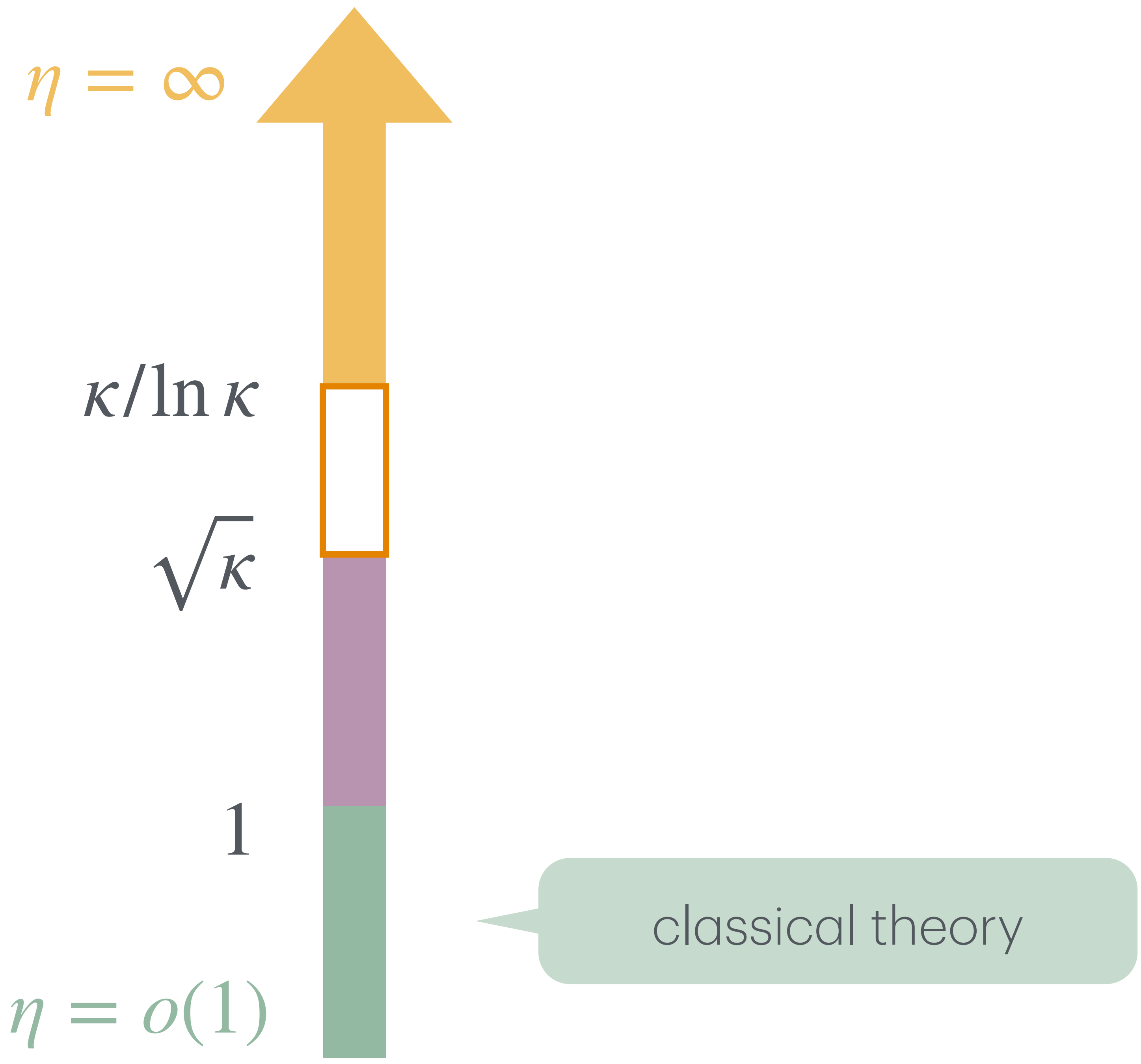
Stepsize diagram revisited



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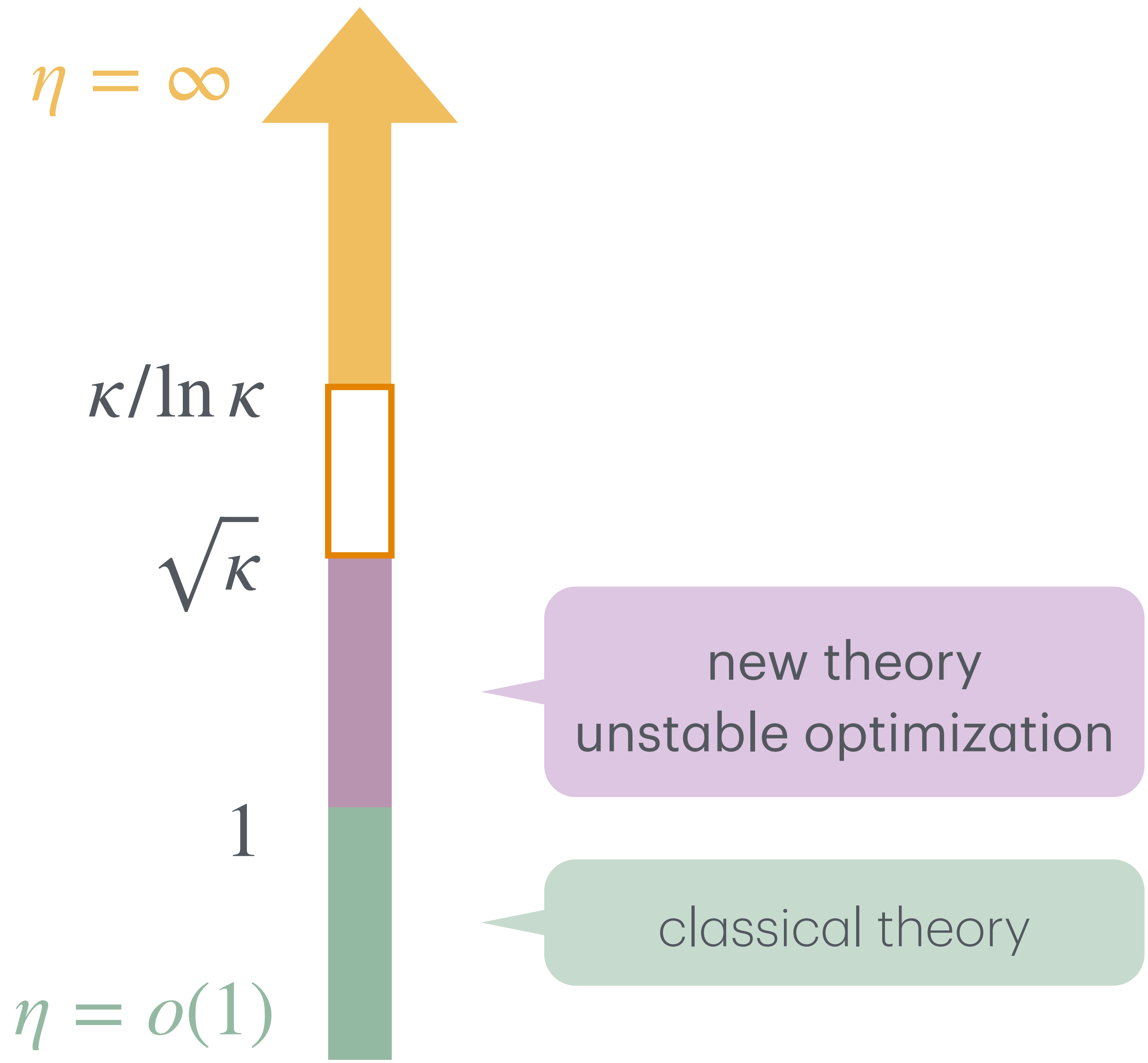

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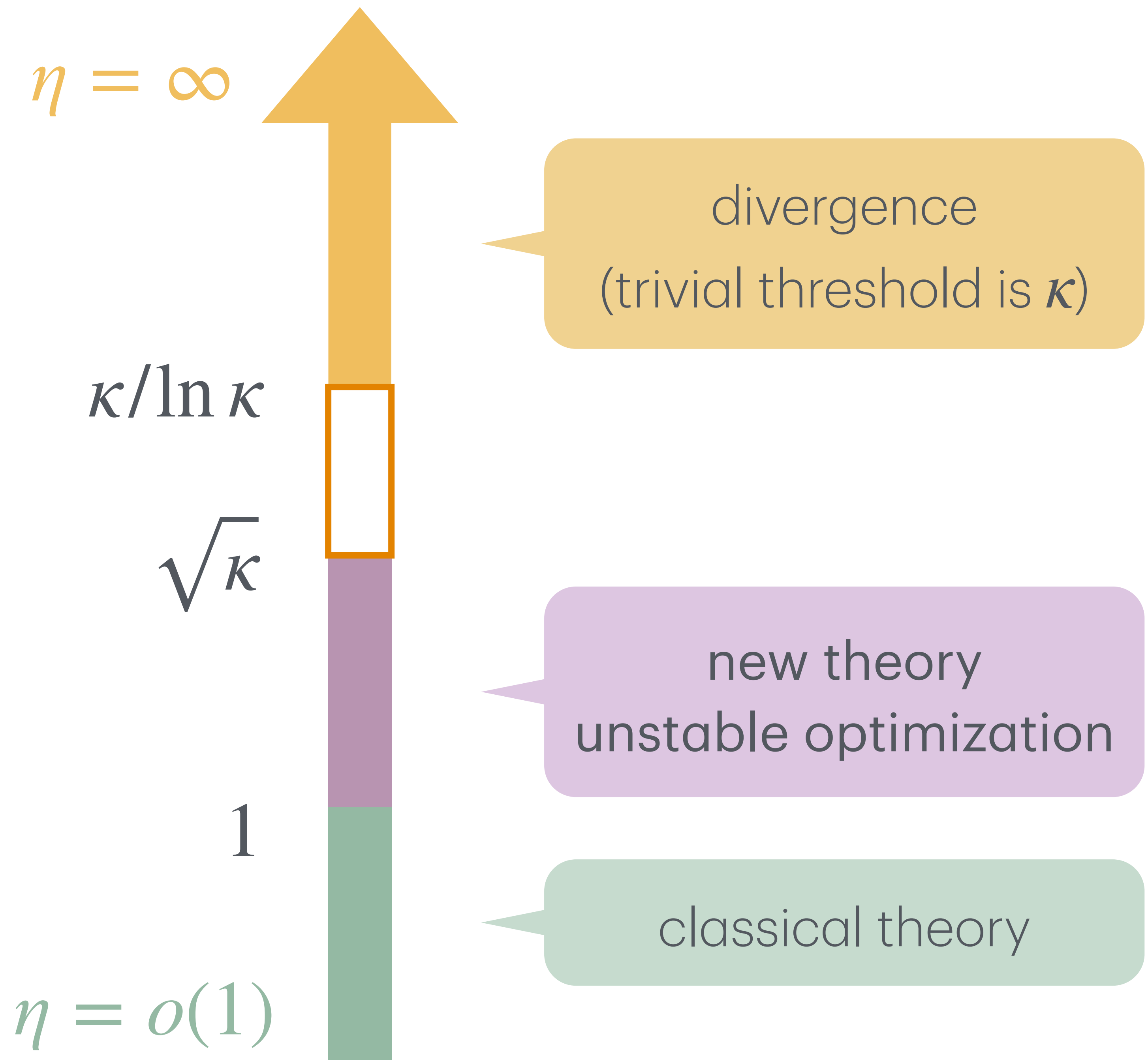

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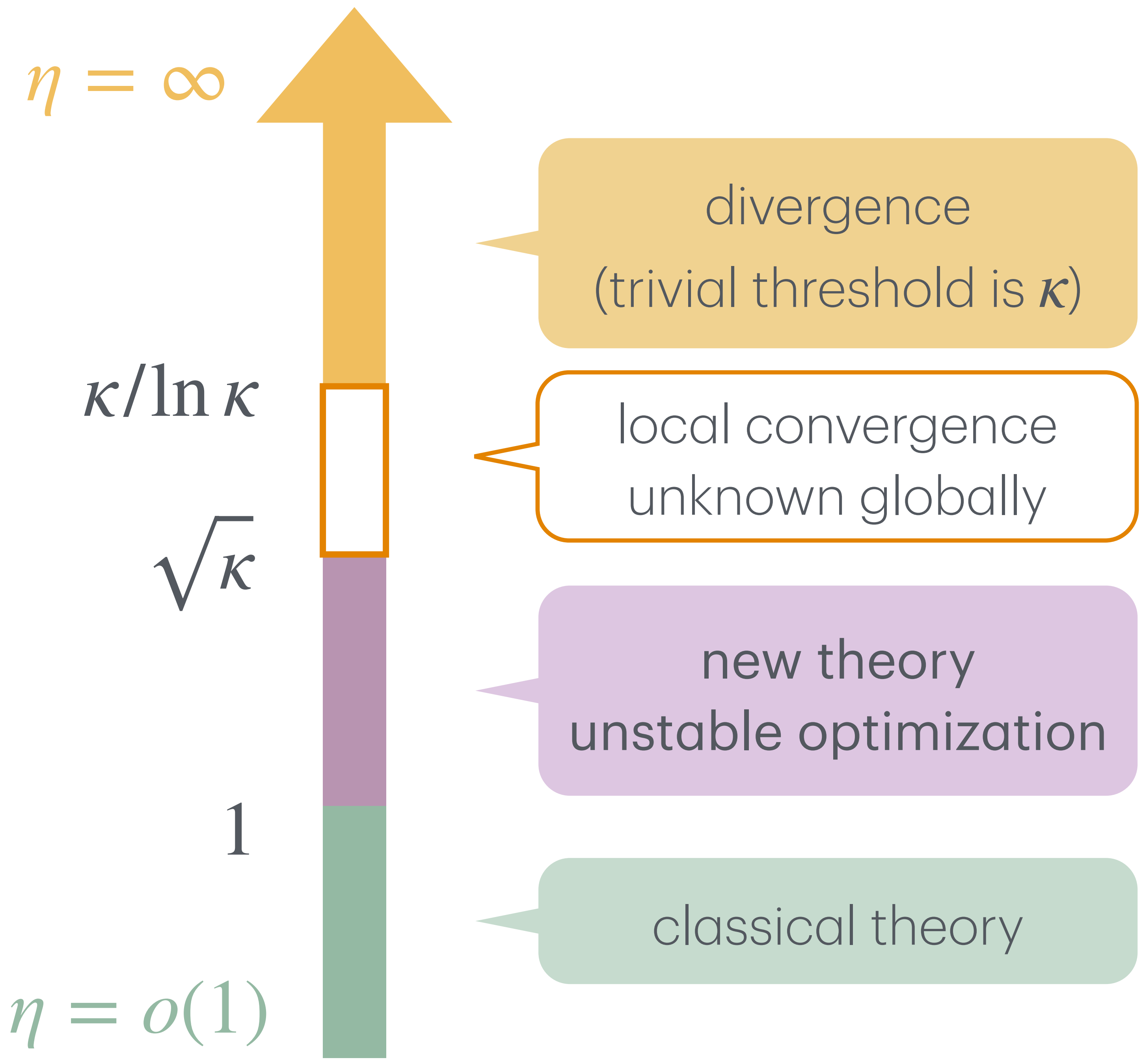

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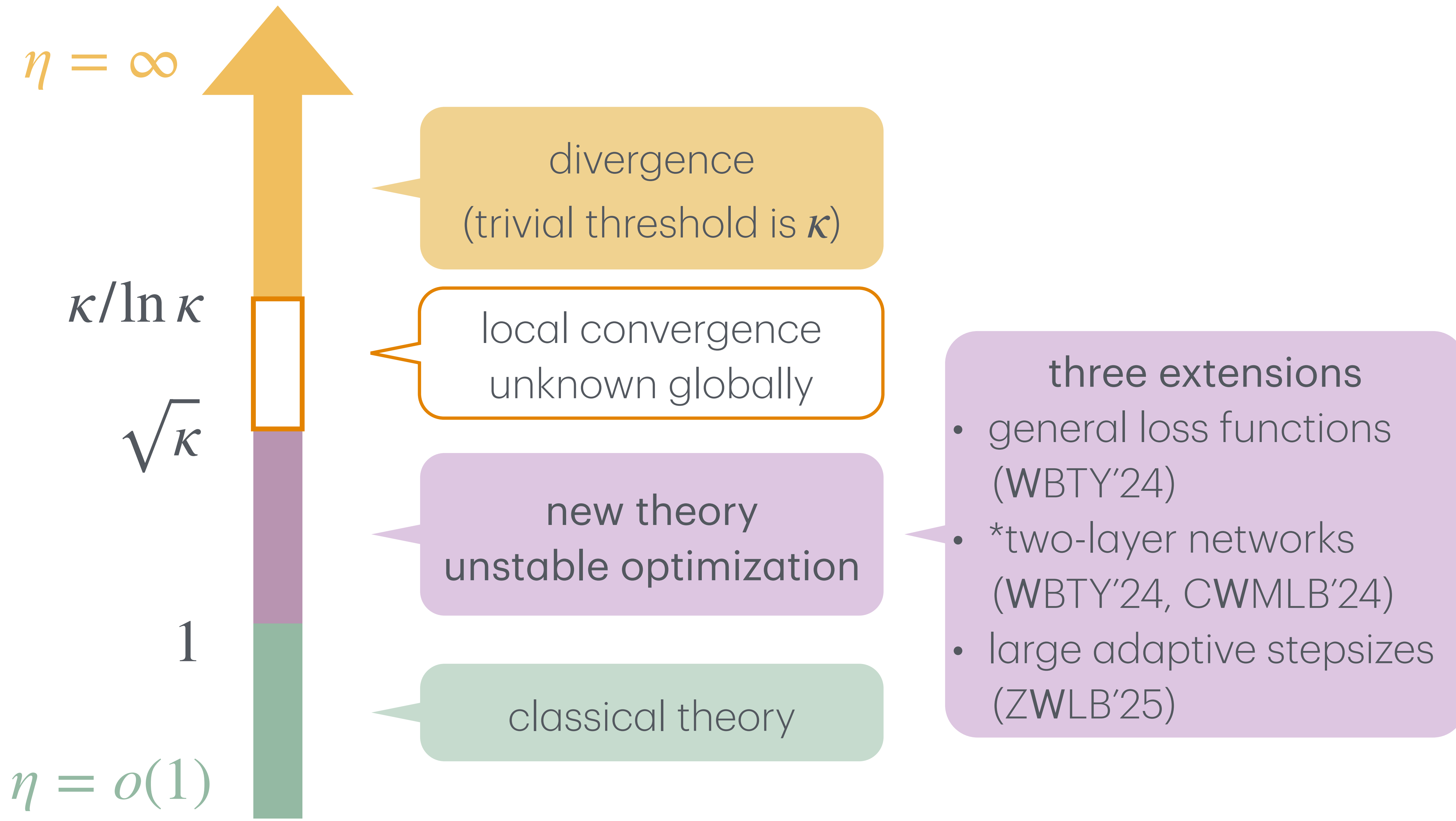

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Cai, **Wu**, Mei, Lindsey, Bartlett. "Large stepsize GD for non-homogeneous two-layer networks: margin improvement and fast optimization." NeurIPS 2024
Zhang, **Wu**, Lin, Bartlett. "Minimax optimal convergence of gradient descent in logistic regression 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

$$\text{test error} \leq \text{training error} + \sqrt{\frac{\text{complexity}}{n}}$$

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Sandbox:
linear regression

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Implicit dominates explicit regularization

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

early-stopped GD is

- always no worse
- sometimes much better

than ℓ_2-regularization (ridge regression)

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(excess) test error / prediction risk

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

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

- $\hat{\theta}_t^{\text{gd}} = \theta_t$

GD dominates ridge

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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$$\hat{\theta}_\lambda^{\text{ridge}} = g(X^\top X)X^\top Y \qquad \hat{\theta}_t^{\text{gd}} = h(X^\top X)X^\top Y$$

Tsigler & Bartlett. “Benign overfitting in ridge regression.” JMLR 2023

Approach

"dominance": always no worse, sometimes much better

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

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$$g : z \mapsto \frac{1}{z + n\lambda}$$

more effective when θ^* decays fast

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GD is inadmissible

Theorem. In linear regression, GD dominates ridge;

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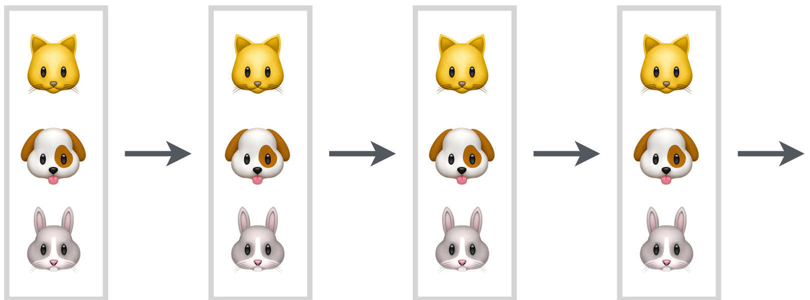

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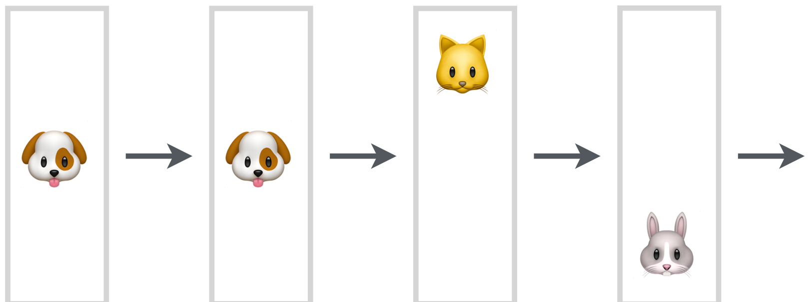

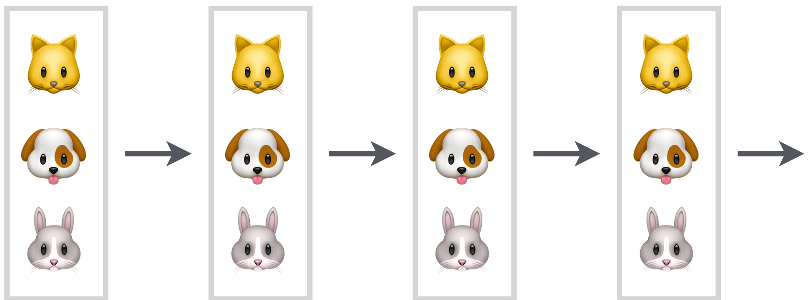

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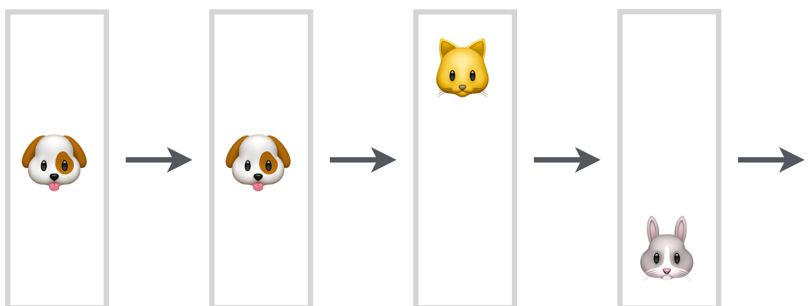

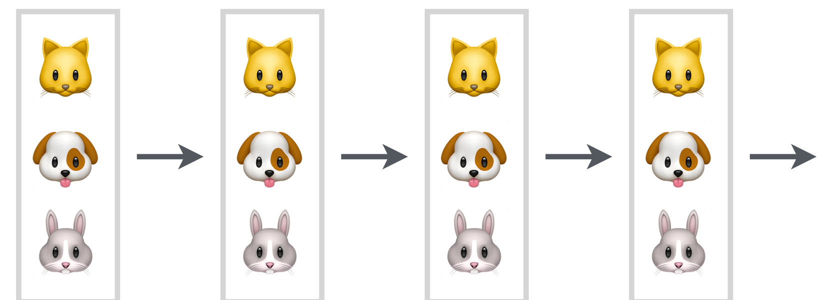

online SGD $\lesseqgtr$ GD

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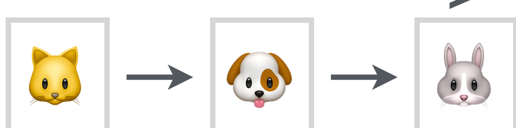

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high-dim; related to benign overfitting

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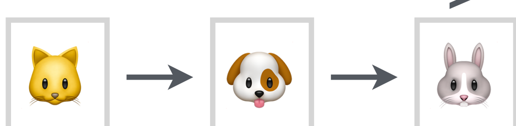

multi-epoch SGD (without replacement) **dominates GD**

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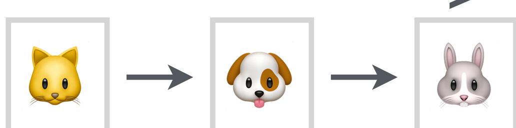

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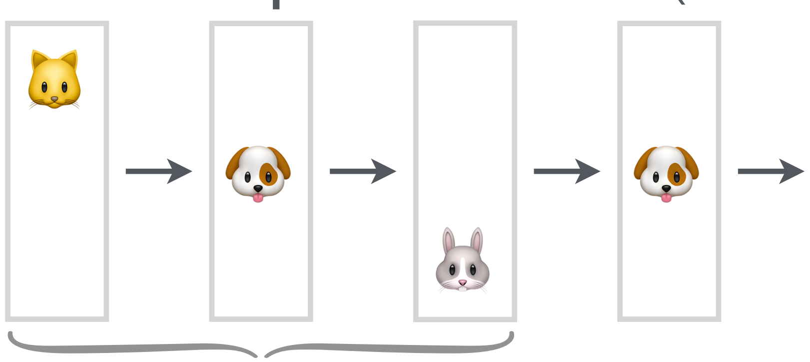

epoch 1

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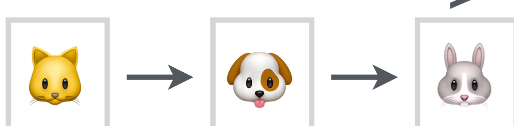

≥ max{online SGD, GD}

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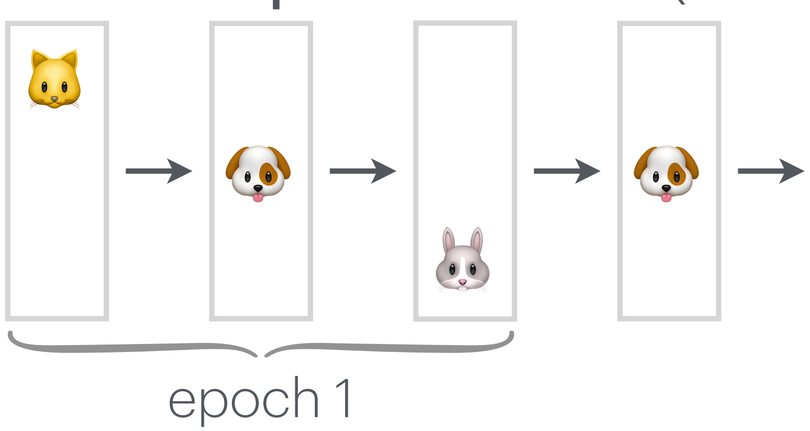

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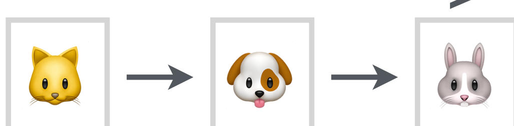

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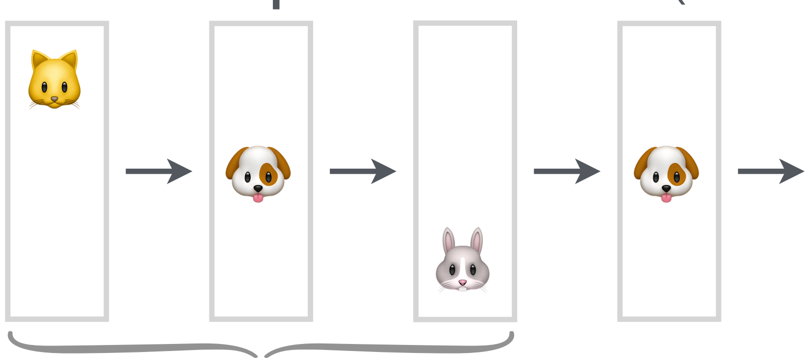

epoch 1

the SGD variant
used in deep learning

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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

Language Model (LM) training

Practice. LM training is "online": #data $\propto$ #flops

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

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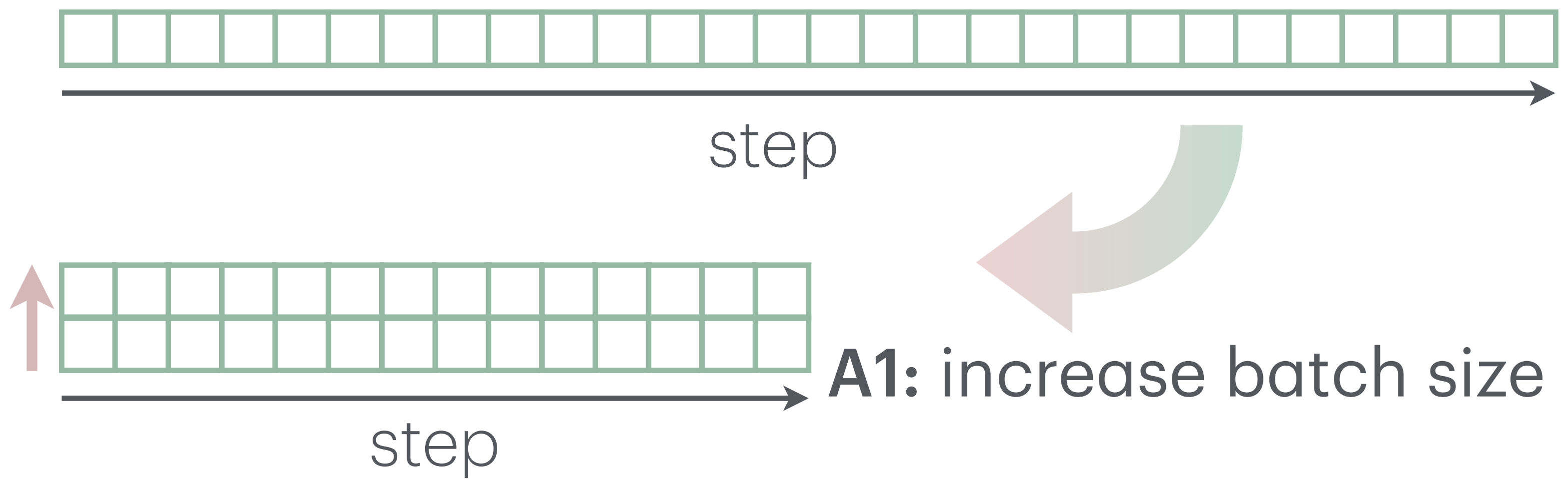

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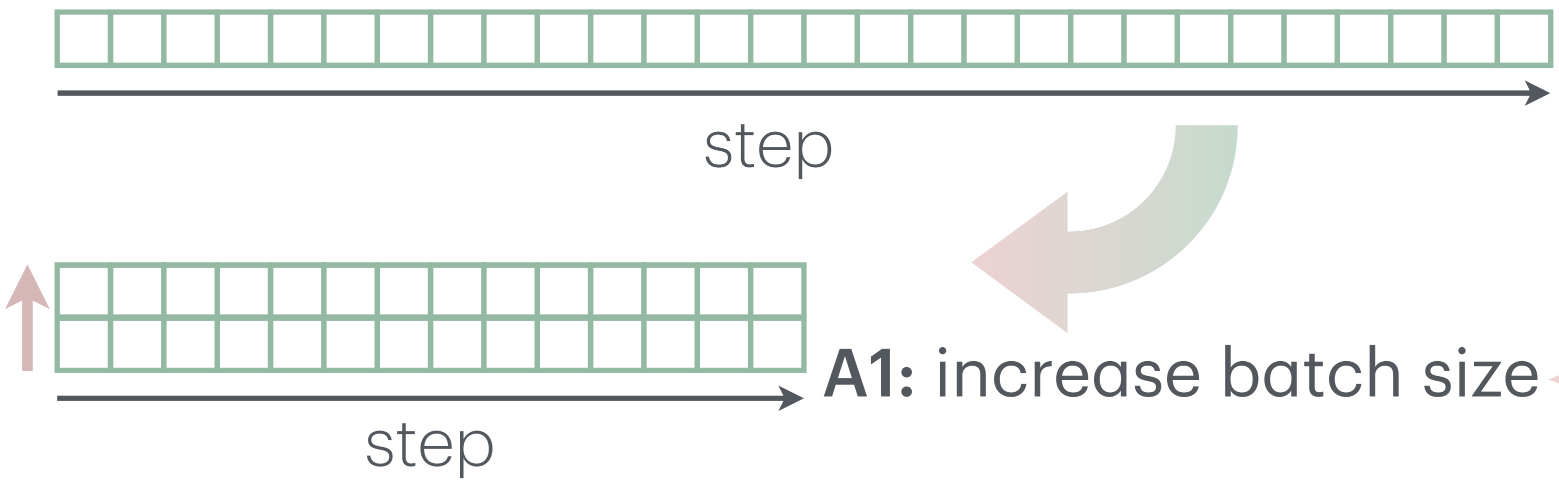

cannot exceed
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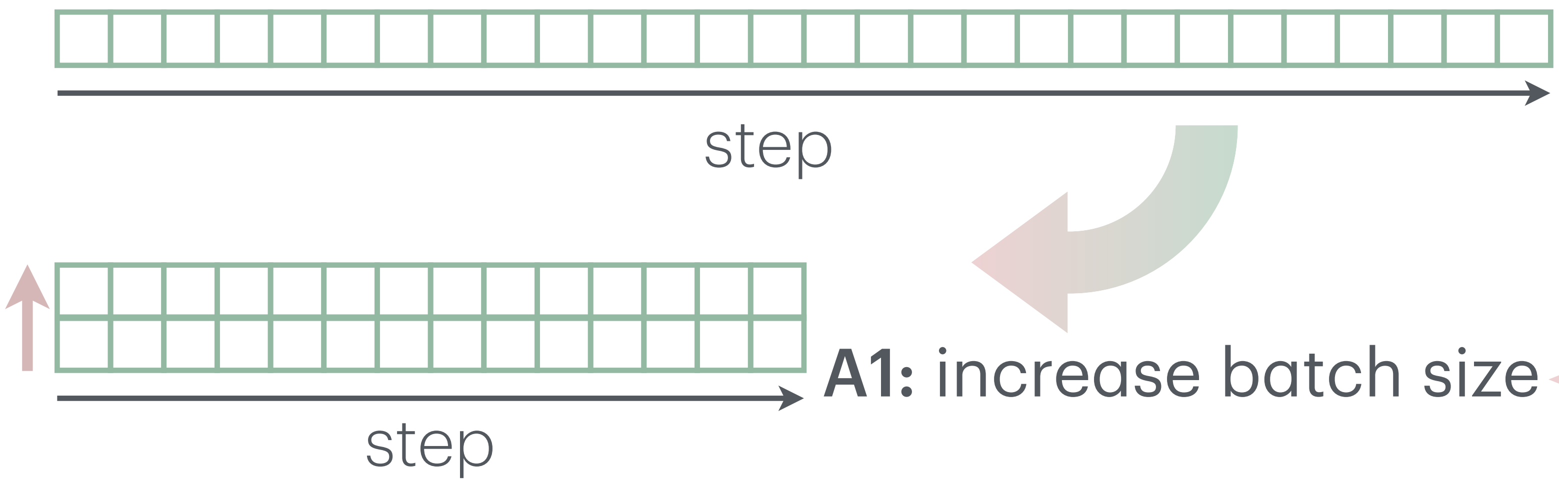

A1: increase batch size

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1. known in literature pre-LM

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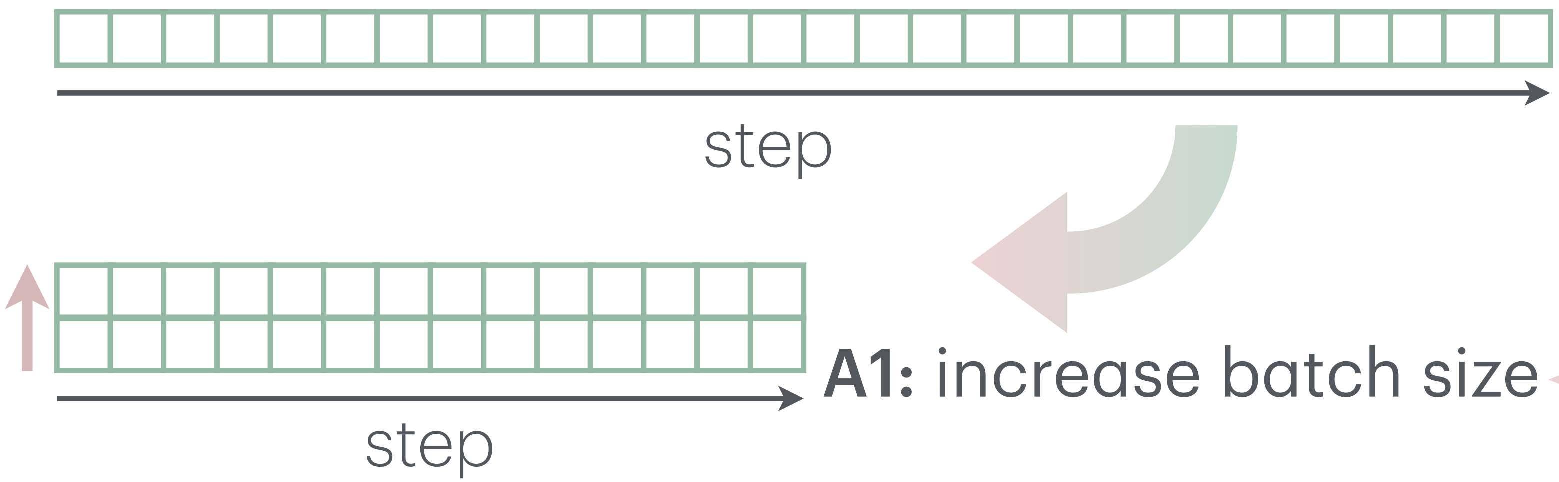

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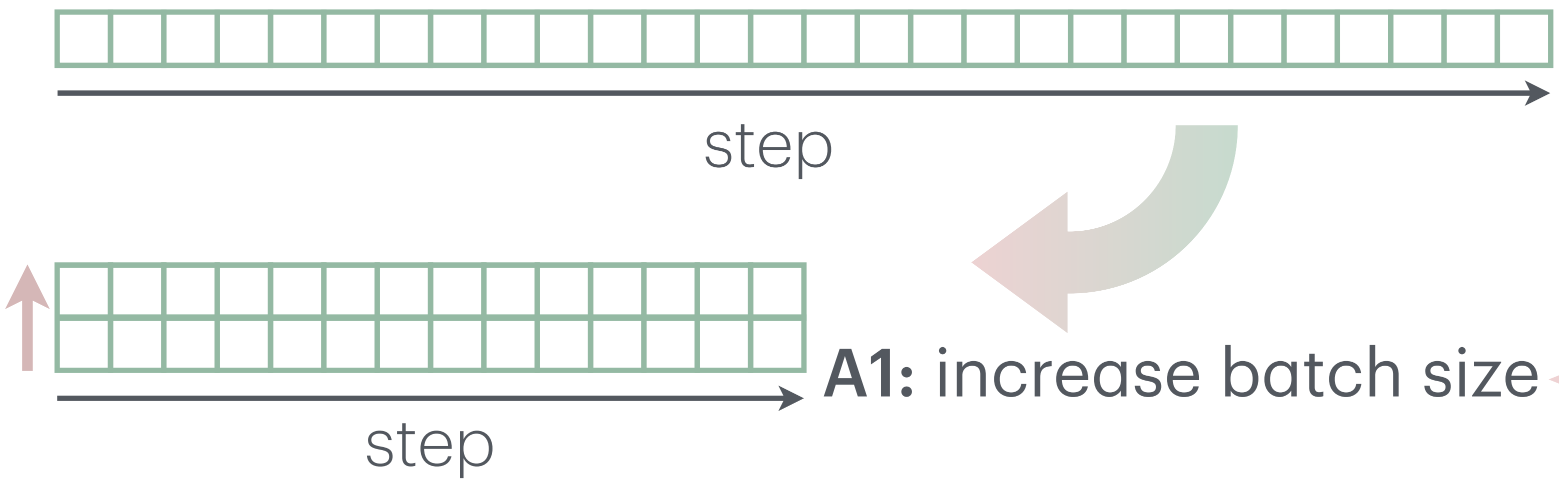

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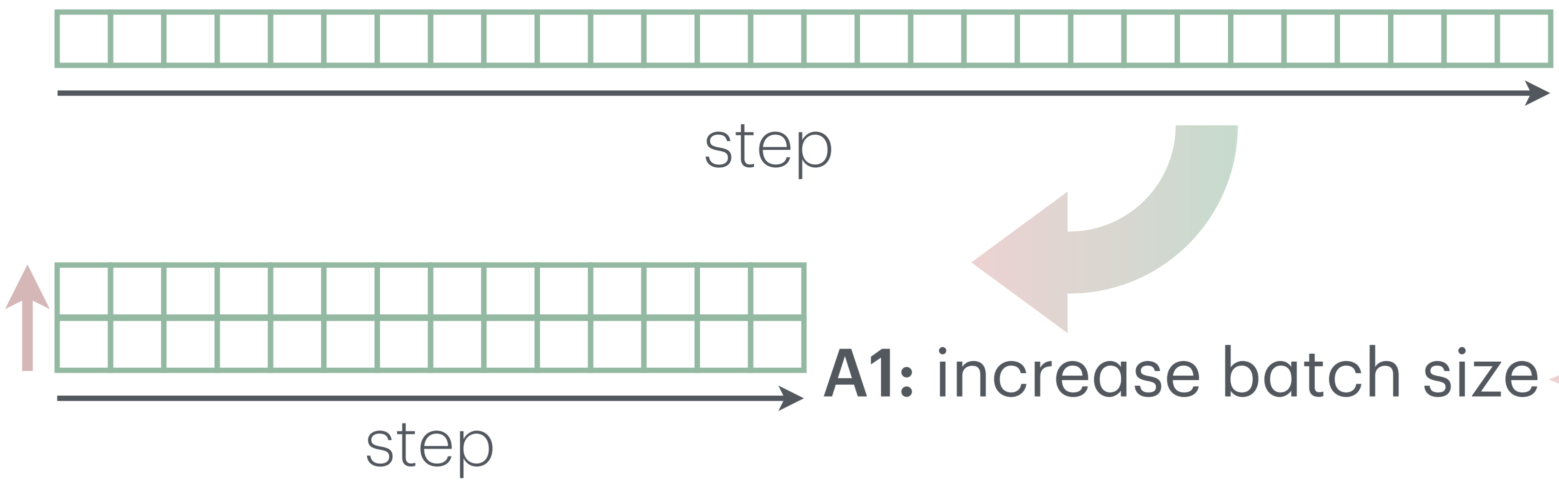

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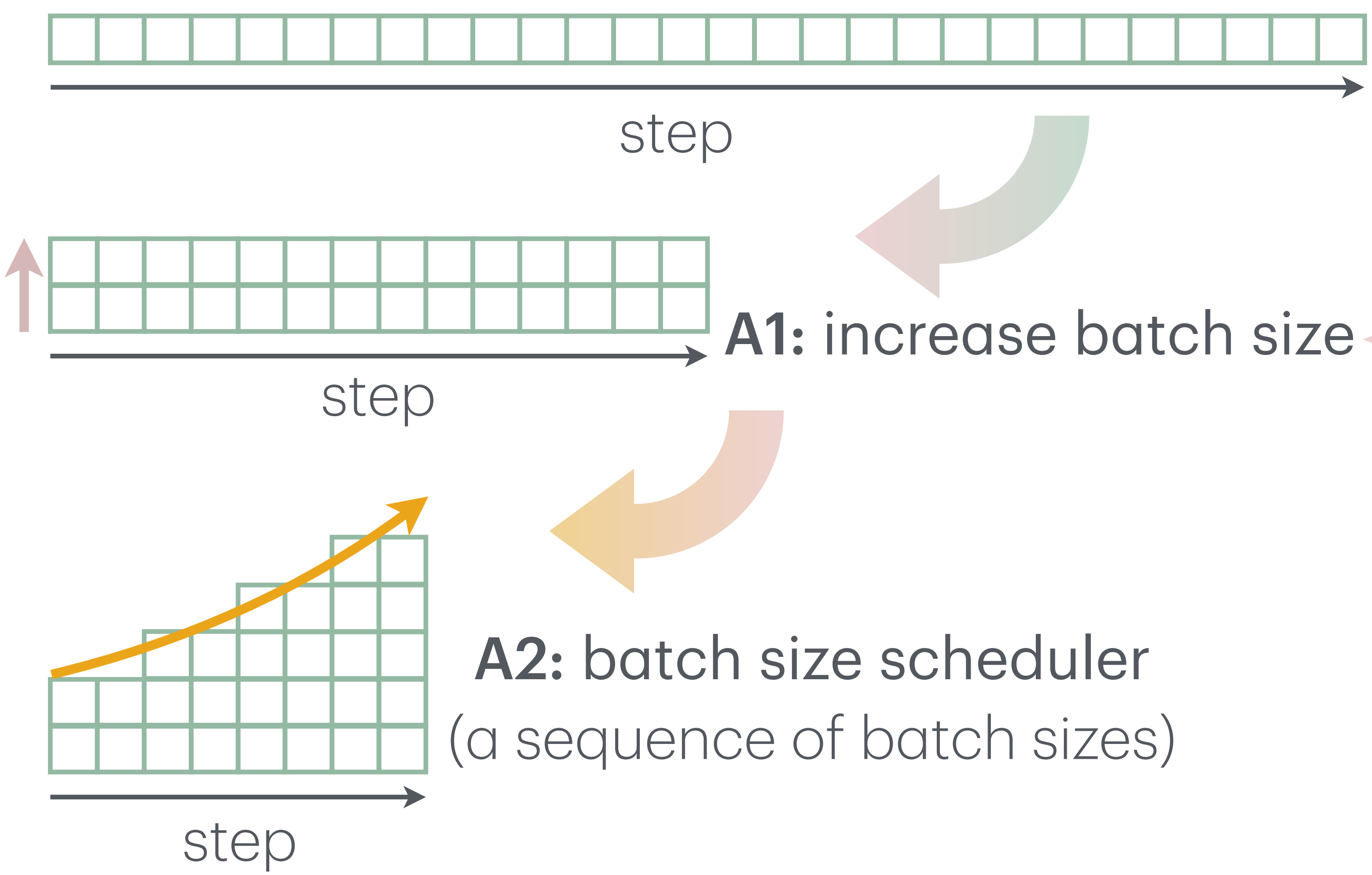

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Seesaw — a principled batch size scheduler

batch size scheduler — same test error with fewer steps?

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works with language models | **sandbox:** linear regression

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

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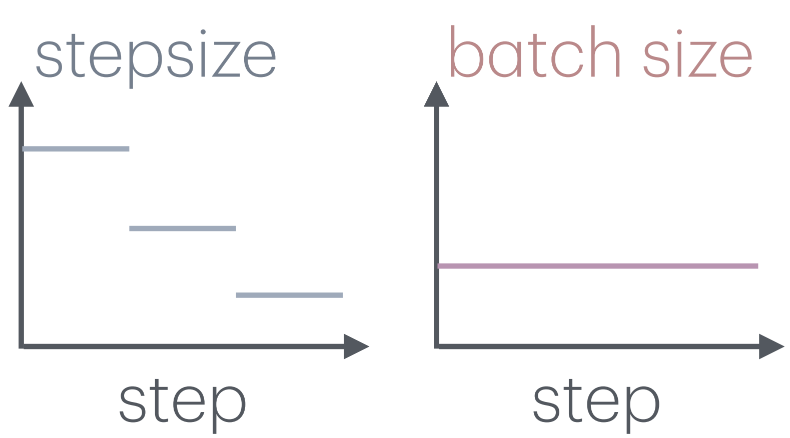
default: stepsize scheduler
$\eta \to \eta/1.1$, B fixed



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default: stepsize scheduler
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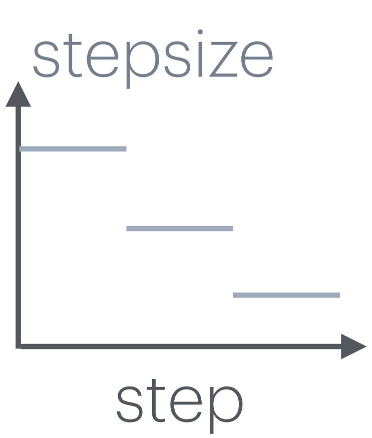
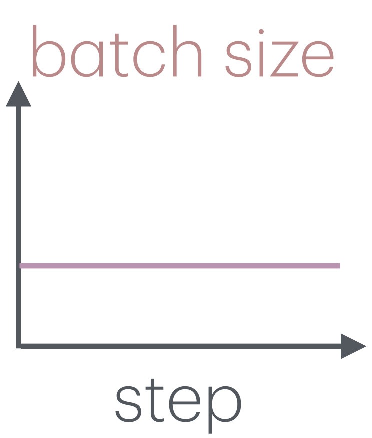
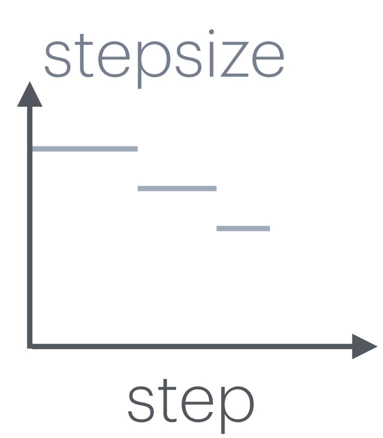
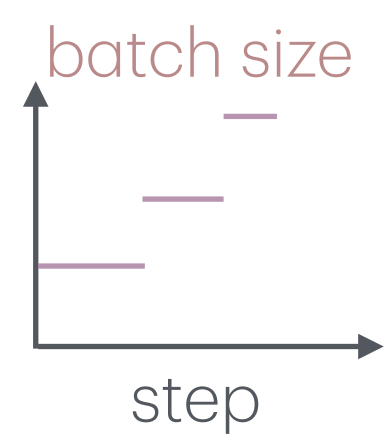
Seesaw: joint scheduler
$\eta \to \eta/\sqrt{1.1}$, $B \to 1.1B$



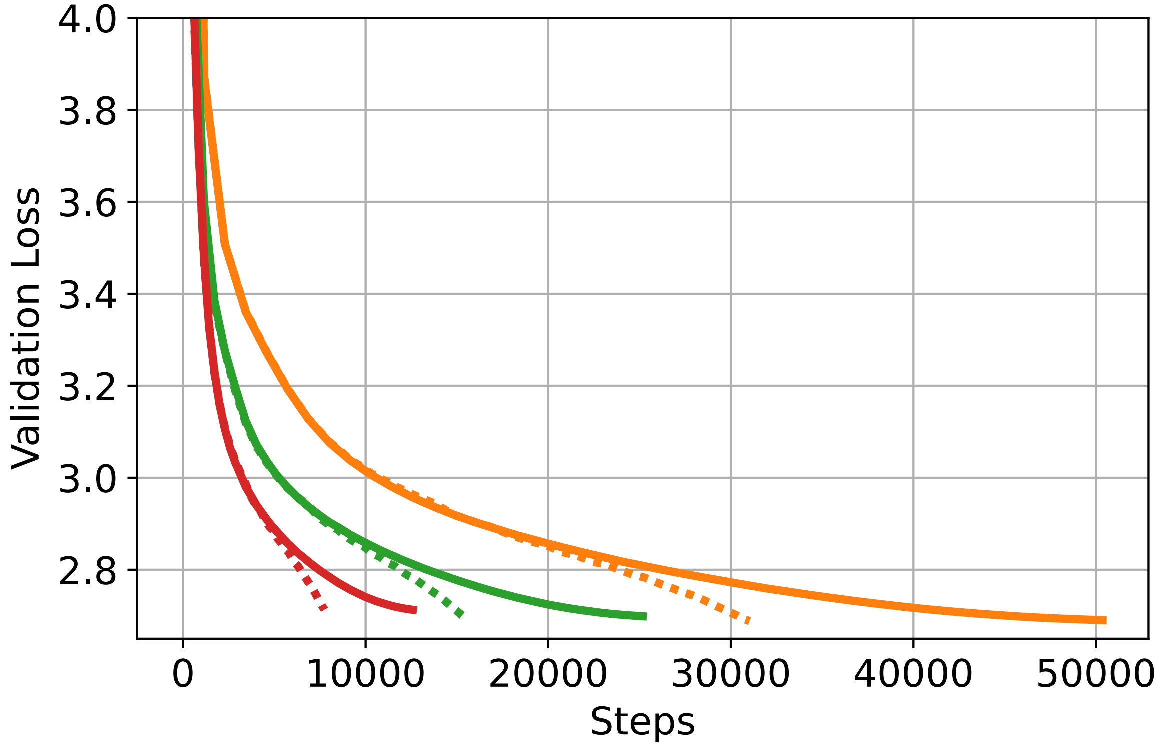






Meterez, Morwani, **Wu**, Oncescu, Pehlevan, Kakade. "*Seesaw*: accelerating training by balancing learning rate and batch size scheduling." ICLR 2026

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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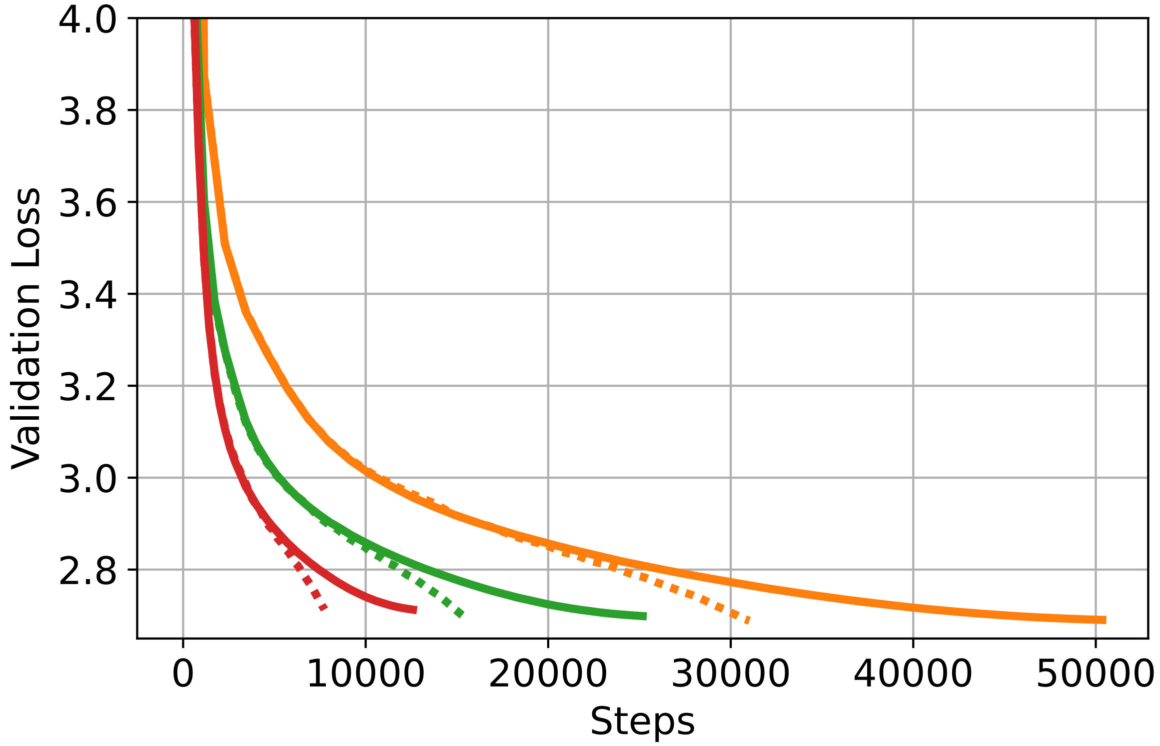

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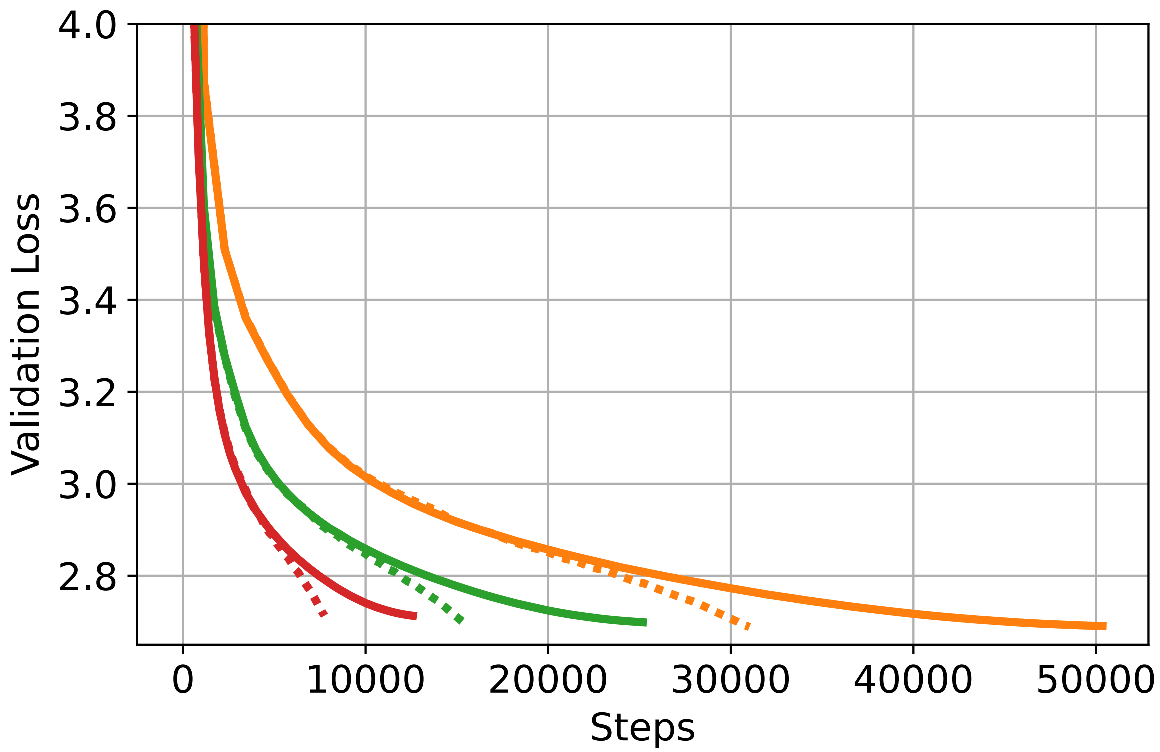

transformer (600M), Adam, C4

Seesaw

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

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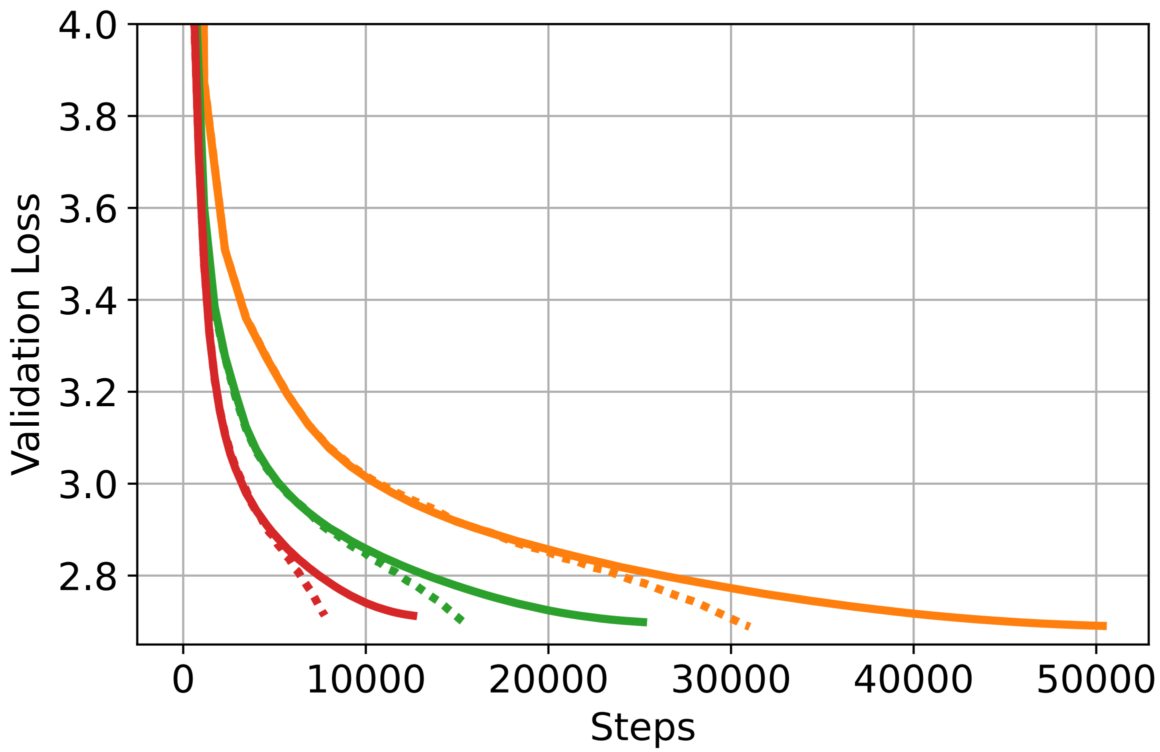

transformer (600M), Adam, C4

Seesaw

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simple, meaningful sandbox can be predictive!

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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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

✨✨✨

Contribution 1: unstable optimization

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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

“worst-case”, “stable”, ...

optimization | statistics

Summary

my aim: theory that is explanatory, predictive, inspirational

my research: less conservative

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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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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

Going forward

my aim: theory that is explanatory, predictive, inspirational

1. embrace *instability* in optimization theory
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instability

new technique?
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stats → opt

new criterion
hyperparameter?
data reuse?

opt → stats

opt algorithm as estimator?

Going forward

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stats → opt

new criterion

hyperparameter?

data reuse?

opt → stats

opt algorithm as estimator?

practice

testbed

new question?

new sandbox?

other domain?

Going forward

my aim: theory that is explanatory, predictive, inspirational

1. embrace *instability* in optimization theory
2. explore *synergies* between statistics & optimization
3. connect theory with *practice*

my research: less conservative

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

optimization x statistics

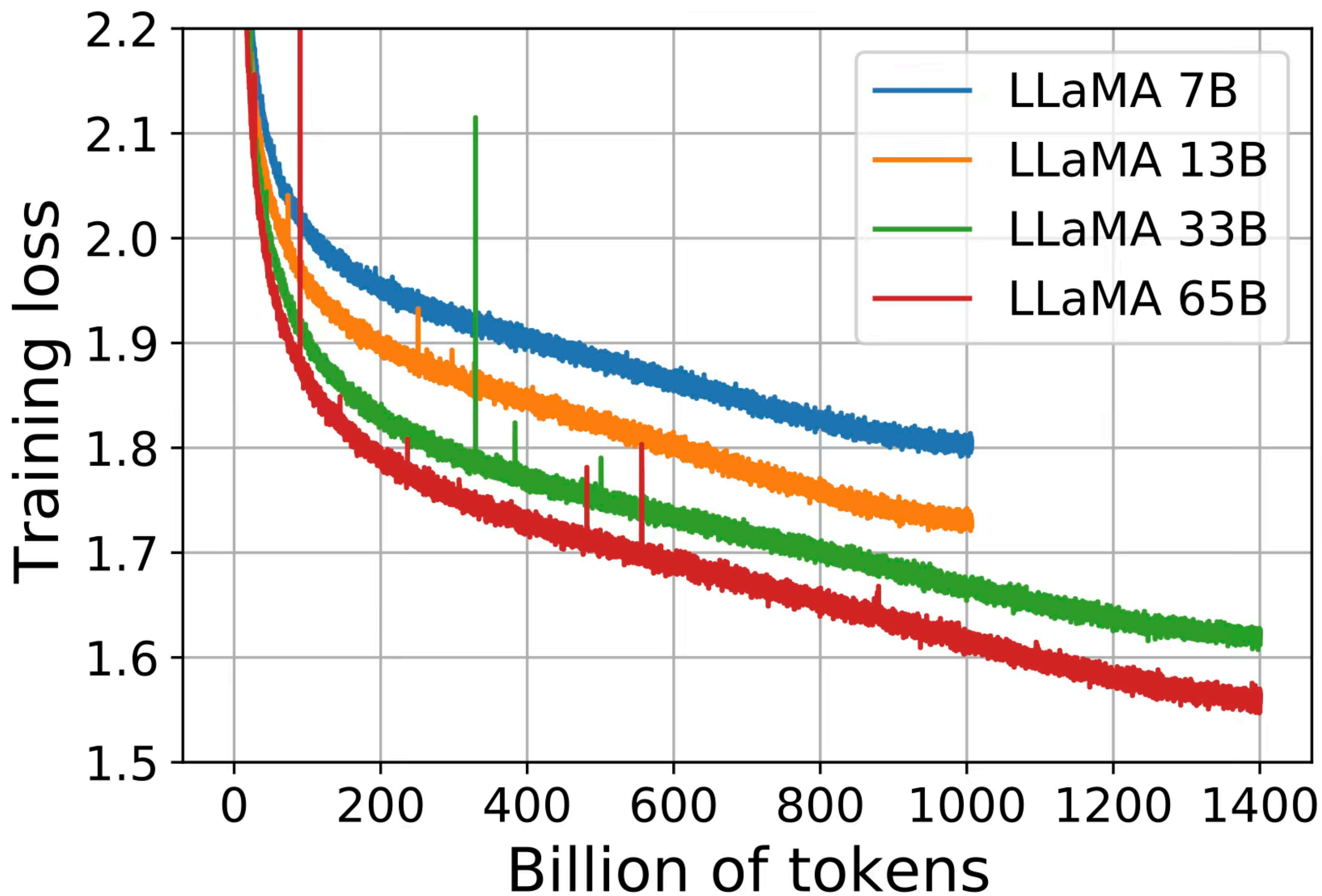
classical theory: conservative

"worst-case", "stable", ...

optimization | statistics

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

$$\theta_{t+1} = \theta_t - \eta\Big((-\ell^{-1})' \circ L(\theta_t)\Big)\,\nabla L(\theta_t) \approx \theta_t - \frac{\eta}{L(\theta_t)}\nabla L(\theta_t)$$

$$\ell(t) = \ln\big(1 + \exp(-t)\big)$$

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

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

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

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

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matching "Perceptron"
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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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$\theta_t \in \theta_0 + \text{span}\{\nabla L(\theta_0), \ldots, \nabla L(\theta_{t-1})\}$
where $L(\theta) = \hat{\mathbb{E}}\ell(yx^\top\theta)$ for any ℓ

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