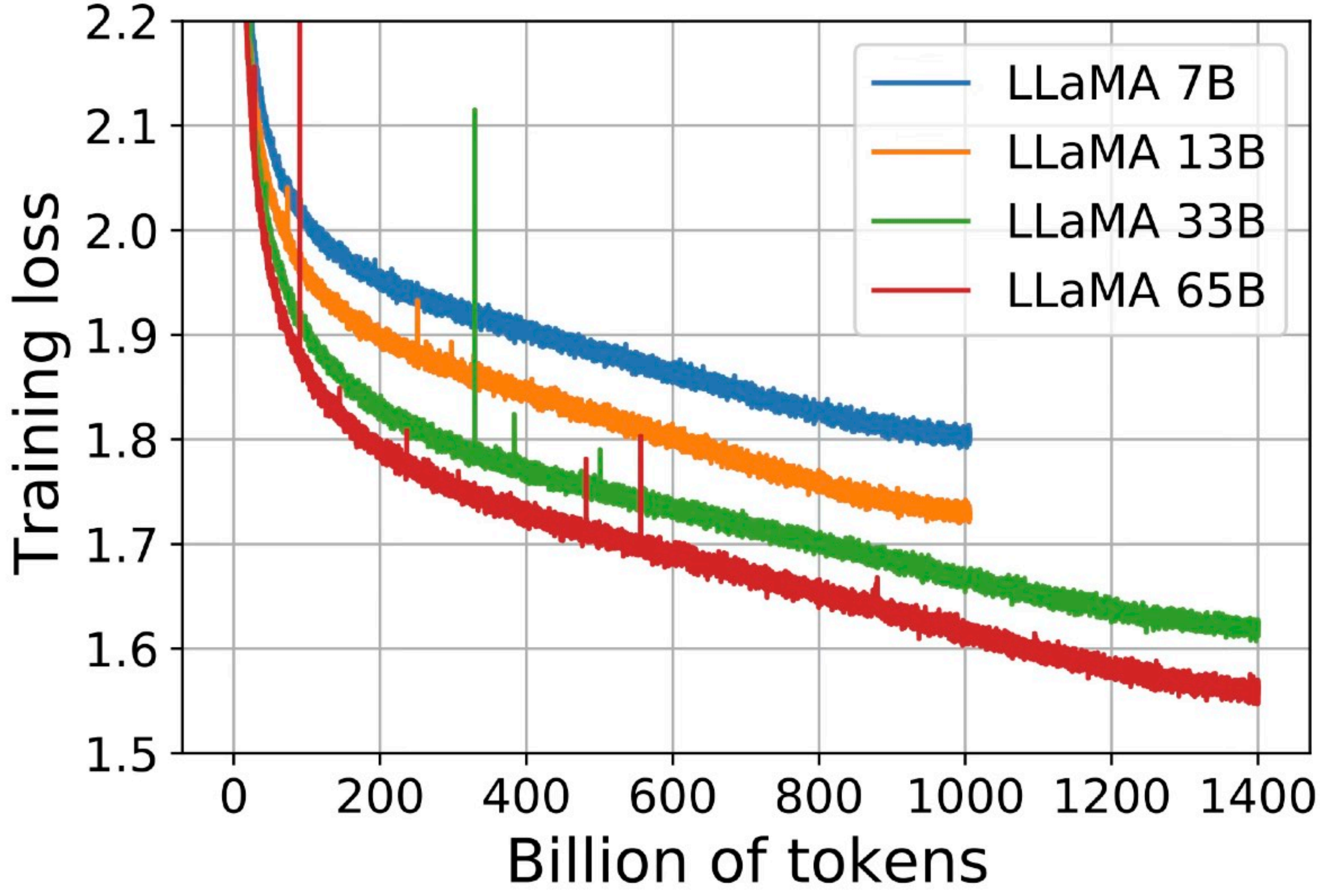
Theoretical Insights on Training Instability in Deep Learning

NeurIPS 2025 Tutorial

Jingfeng Wu UC Berkeley
Yu-Xiang Wang UC San Diego
Maryam Fazel University of Washington

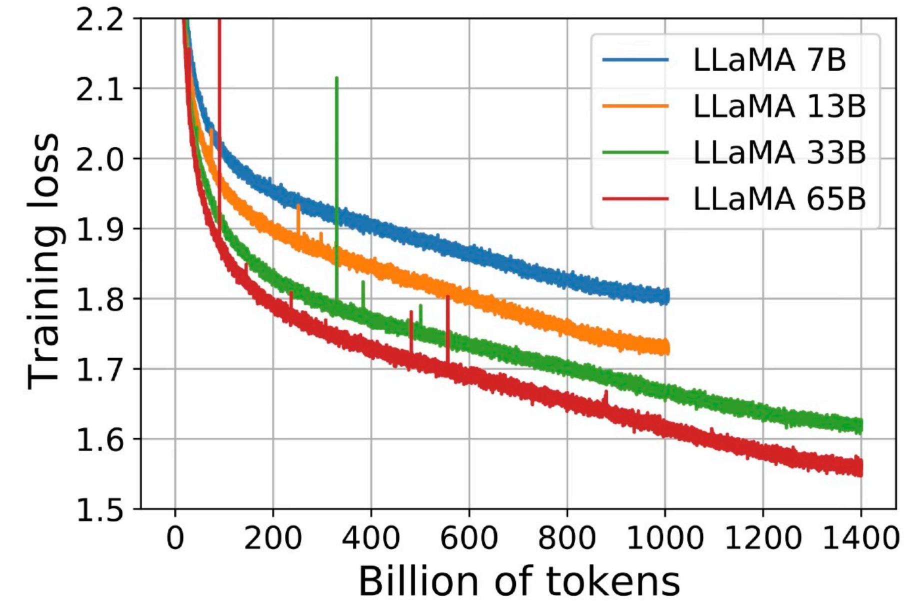
NEURAL INFORMATION PROCESSING SYSTEMS

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
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[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.

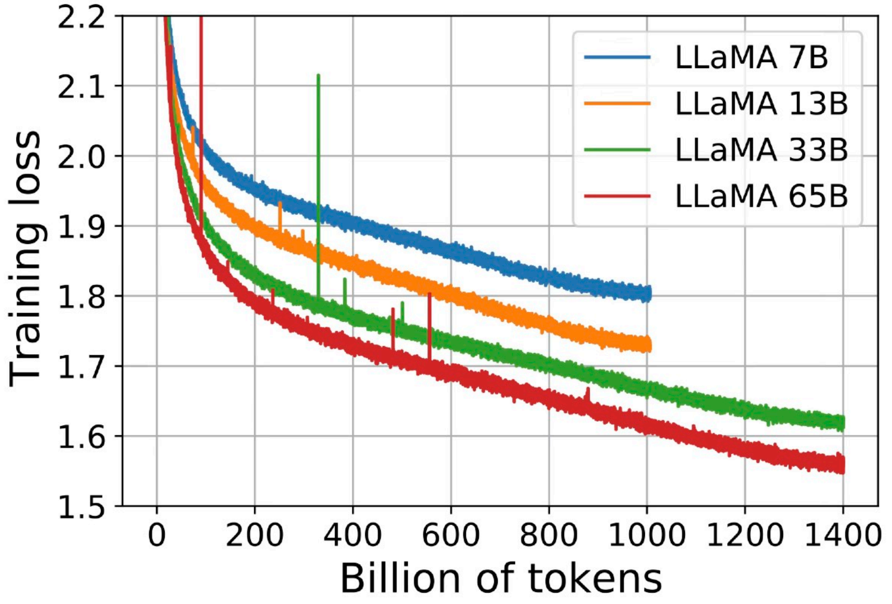
Do you have any insight or references to better understand this phenomenon?

62 20 Share

yes, we do!

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

Why loss spikes



$\theta_+ = \theta -$ stepsize $\times$ "gradient"

data randomness ← unlucky mini-batch

numerical overflow ← insufficient precision

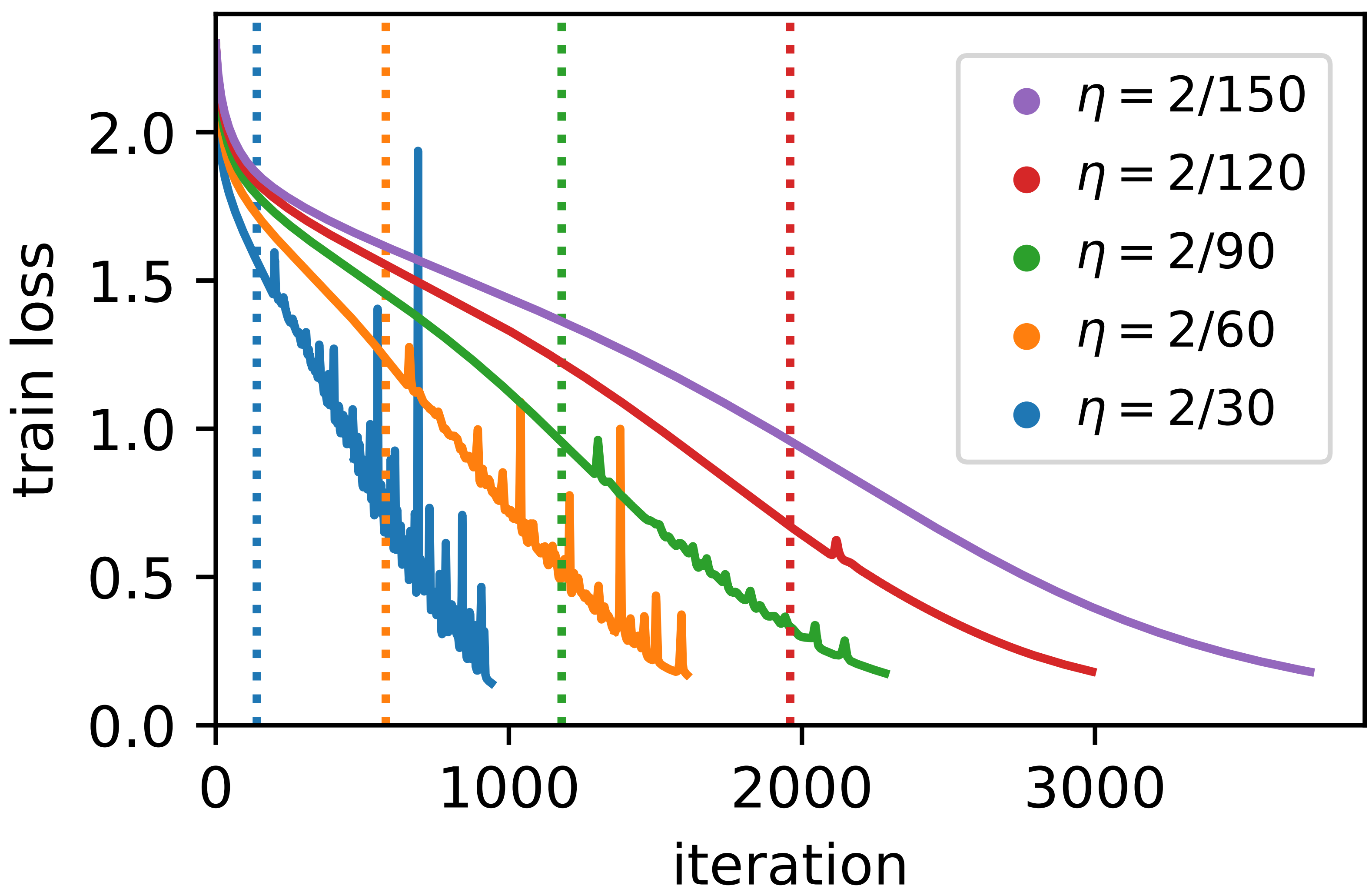
loss landscape ← varying layer-wise curvature

....

inherent instability ← **stepsize / learning rate**

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

Sandbox: GD + MLP



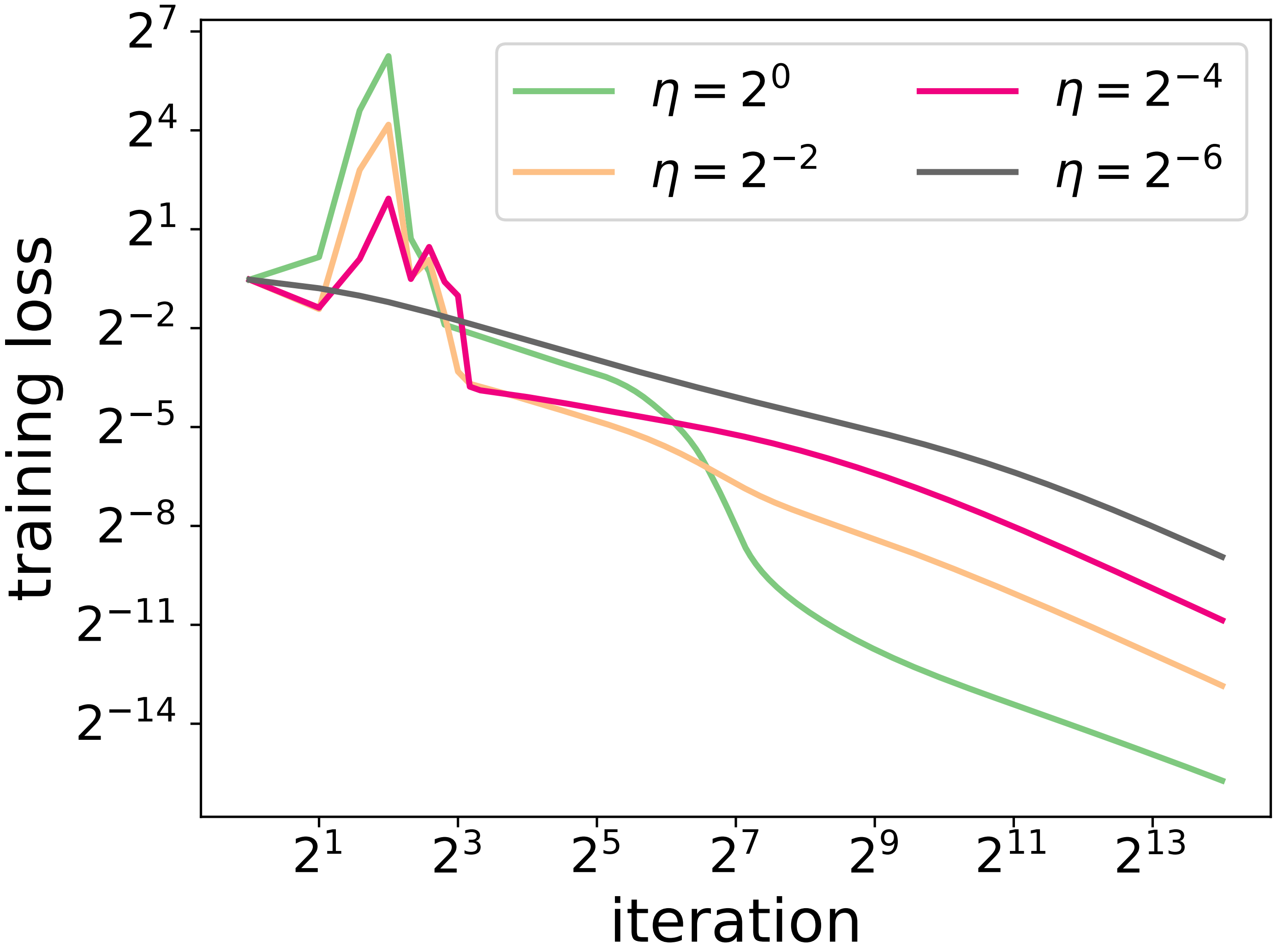
- no randomness
- mild overflow
- OK landscape

but still unstable (in efficient runs)

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

Cohen, Kaur, Li, Kolter, Talwalkar. "Gradient descent on neural networks typically occurs at the edge of stability." ICLR 2021

Sandbox²: GD + linear model



- no randomness
- no overflow
- convex landscape

but still unstable
(in efficient runs)

🙀 — me in 2023

GD, 1k subset of MNIST "0" vs "8", logistic regression

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

Infinitesimal stepsize is stable

gradient descent $\theta_+ = \theta - \eta \nabla L(\theta)$

$\eta \downarrow 0_+$

gradient flow $\mathrm{d}\theta = -\nabla L(\theta)\mathrm{d}t$

chain rule $\Rightarrow \ \mathrm{d}L(\theta) = \nabla L(\theta)^\top \mathrm{d}\theta$

$$= -\|\nabla L(\theta)\|^2 \mathrm{d}t$$

$$\leq 0$$

integration $\Rightarrow \ L(\theta) \downarrow$

GD with infinitesimal stepsize is stable

Infinitesimal stepsize is stable

GD → gradient flow

✅ **momentum.** GD with momentum → second order ODE

✅ **mini batch.** SGD → gradient flow + o(1) diffusion (SDE)

these ODE/SDEs minimize certain potential

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

Su, Boyd, Candes. "A differential equation for modeling Nesterov's accelerated gradient method: theory and insights." JMLR 2016

Li, Tai, E. "Stochastic modified equations and dynamics of stochastic gradient algorithms I: mathematical foundations." JMLR 2019

From infinitesimal to small stepsize

Descent lemma. For GD, $L(w_t)$ decreases monotonically if

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

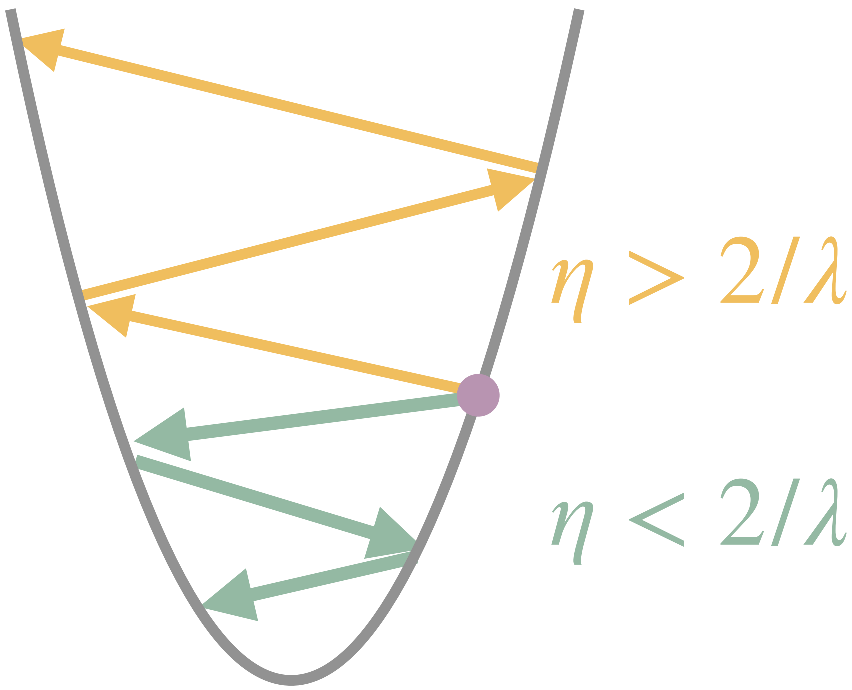
small stepsize implies descent

cornerstone of optimization theory

quadratics $\quad L(\theta) = \frac{1}{2}\lambda\theta^2$

Hessian $\quad \nabla^2 L(\theta) = \lambda$

GD $\quad \theta_+ = \theta - \eta \nabla L(\theta) = (1 - \lambda\eta)\theta$



From small to large stepsize

Large stepsize. A stepsize η is large for GD if

$$L(\theta_t) \text{ does not decrease monotonically}$$

Dynamical stability. If GD with large η converges to stationary point (why?), then in "regular" cases

$$\|\nabla^2 L(\theta_\infty)\| < \frac{2}{\eta}$$

sharpness penalty

Intuition. Descent lemma is tight for quadratics

alternative names: linear stability, Lyapunov stability...

Wu, Ma, E. "How SGD selects the global minima in over-parameterized learning: a dynamical stability perspective." NeurIPS 2018.

From small to large stepsize

Sharpness penalty. If label-noise* SGD converges, under suitable assumptions,

$$\mathrm{tr}(\nabla^2 L(\theta_\infty)) < O(1/\eta)$$

*for general SGD, the penalty also depends on noise covariance

training instability: $L(\theta_t)$ oscillates for $t = 1,2,\ldots$

minimizer flatness: $|L(\theta_\infty + \epsilon) - L(\theta_\infty)|$ is small

large stepsize: less stable training, but flatter minima

convergence? generalization?

Damian, Ma, Lee. "Label noise SGD provably prefers flat global minimizers." NeurIPS 2021

Li, Wang, Arora. "What happens after SGD reaches zero loss?—A mathematical framework." ICLR 2022

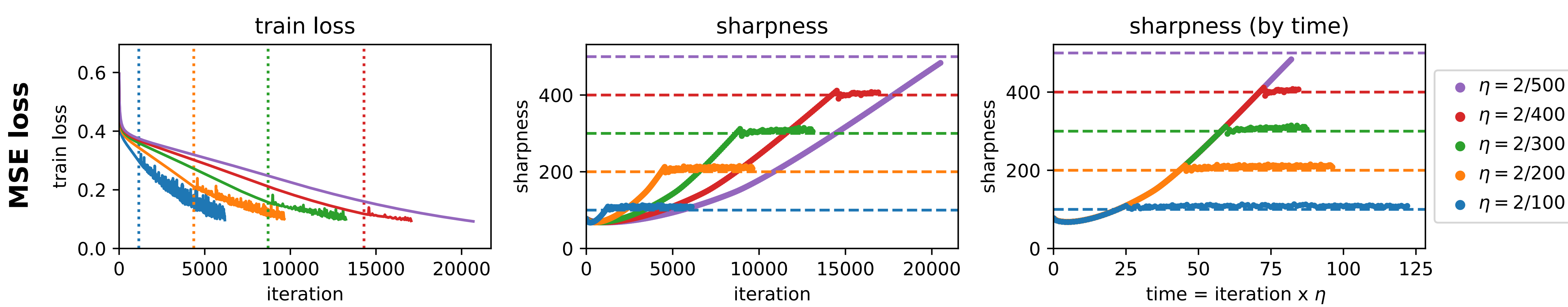
From small to large stepsize

progressive sharpening

even starting satisfying descent lemma, sharpness increases along GD path until hitting $2/\eta$

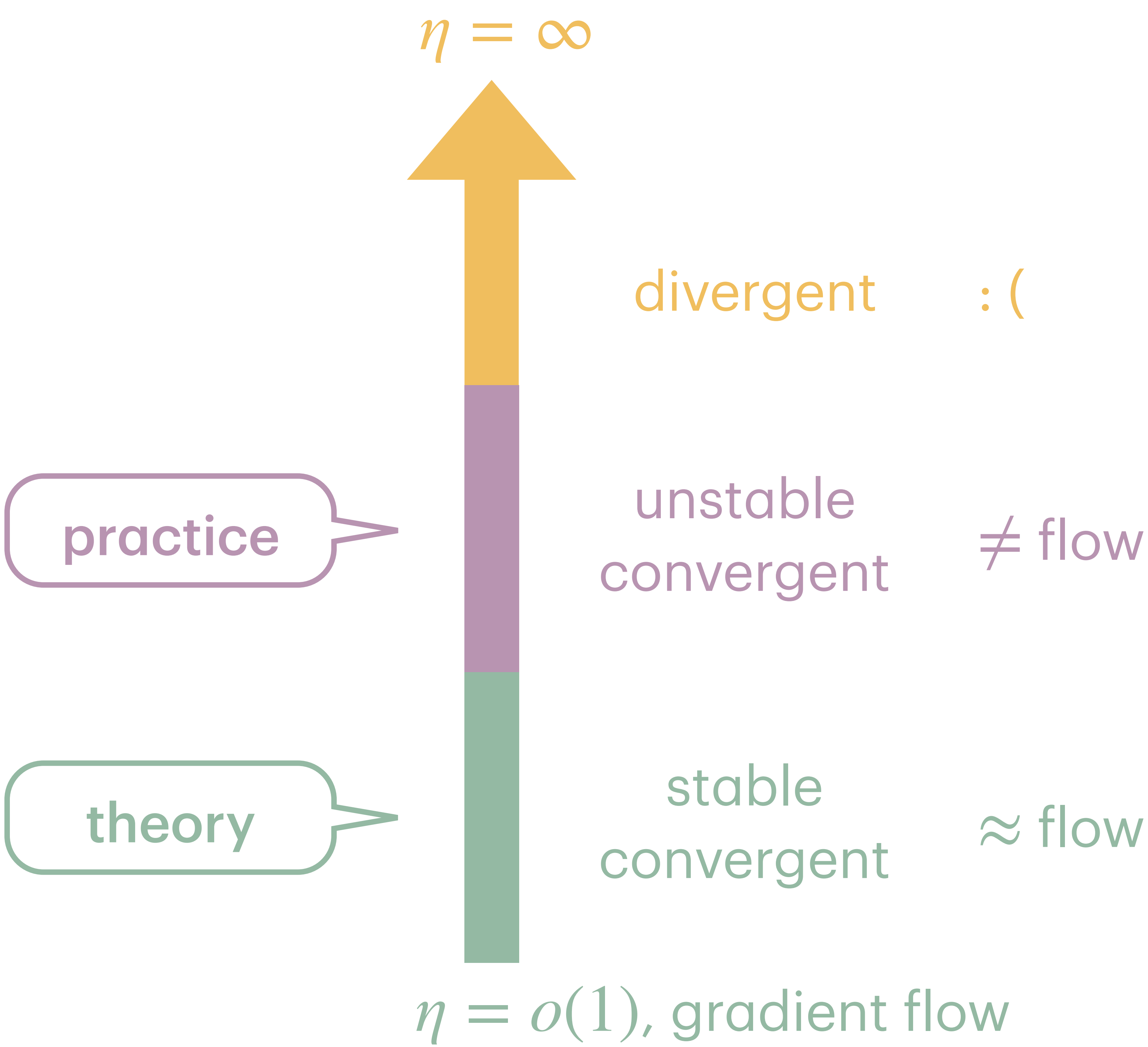
edge of stability

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



Cohen, Kaur, Li, Kolter, Talwalkar. "Gradient descent on neural networks typically occurs at the edge of stability." ICLR 2021

From small to large stepsize



We will cover

Part 1: large stepsizes accelerate optimization

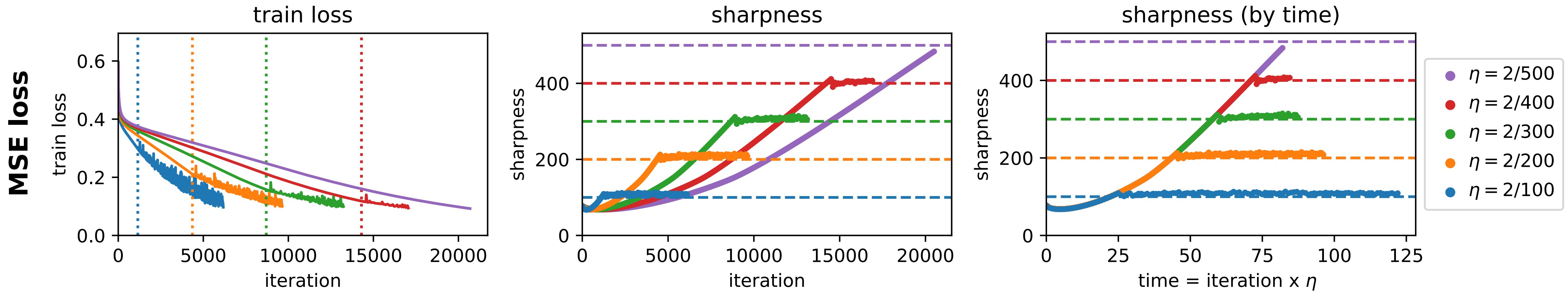
Part 2: large stepsizes prevent overfitting

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

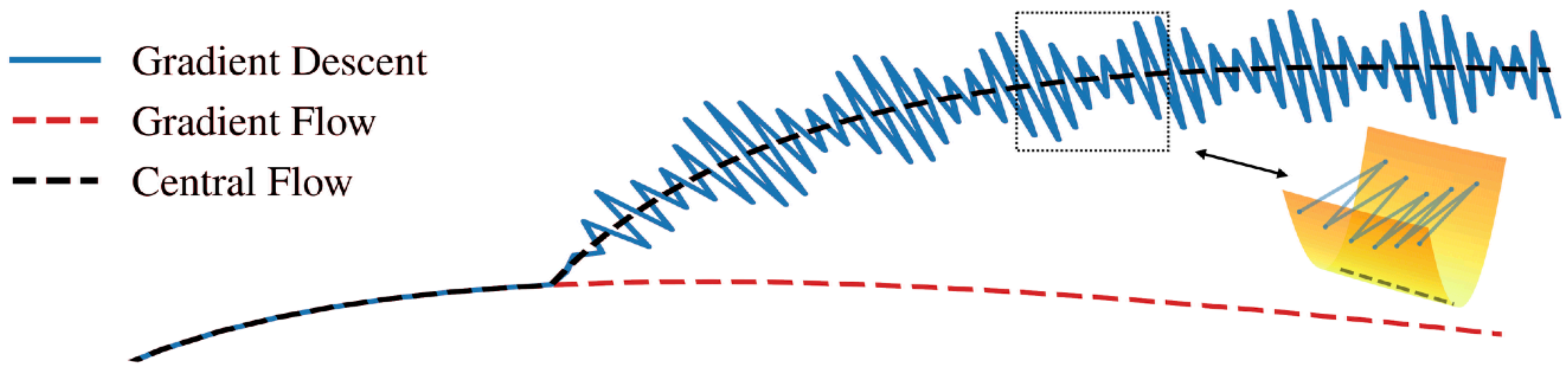
We won't cover but worth checking

(1/many) experimental science of large stepsize

📋 progressive sharpening & edge of stability



📋 central flow: an approximation of the trajectory



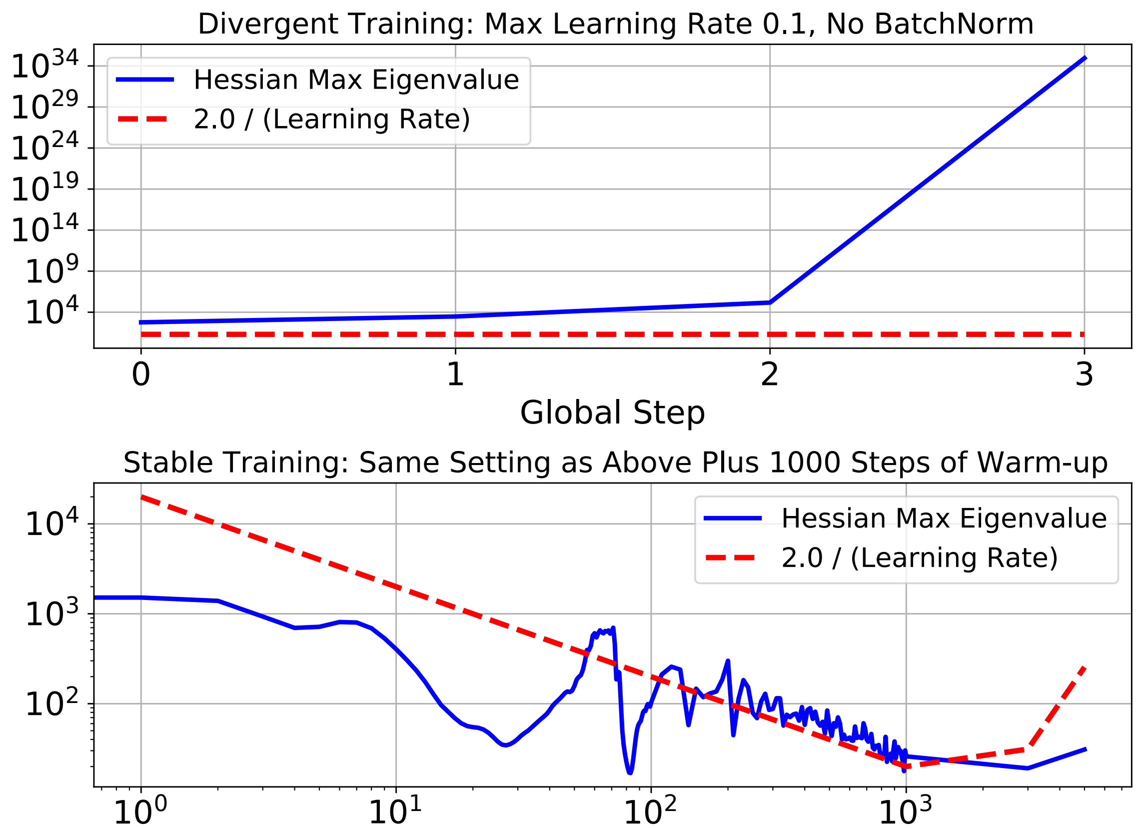
*check our website for more references

Cohen, Damian, Talwalkar, Kolter, Lee. "Understanding optimization in deep learning with central flows." ICLR 2025

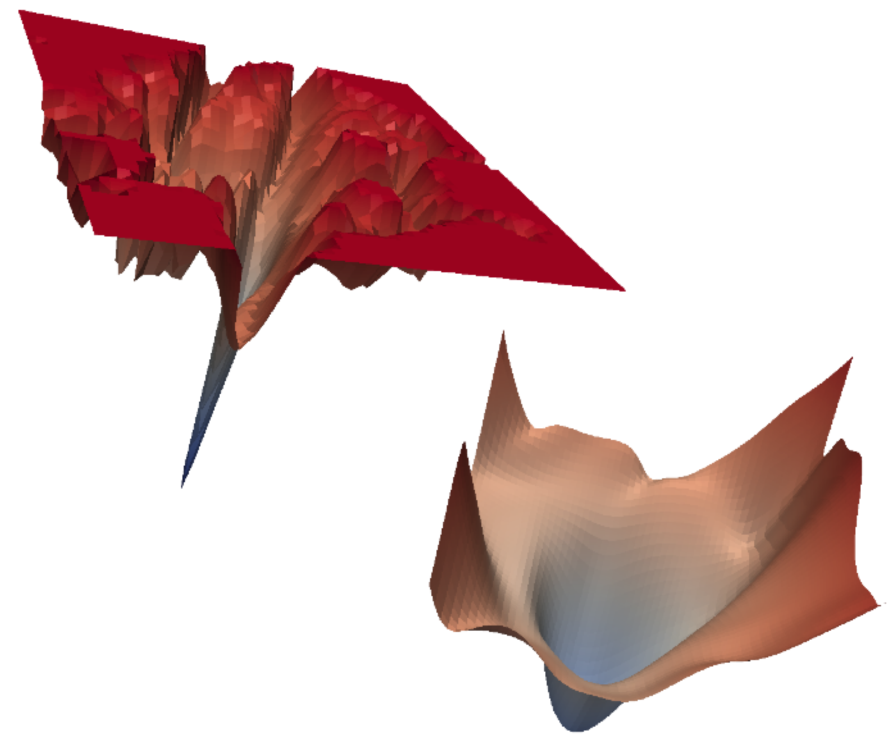
We won’t cover but worth checking

(2/many) optimizer-landscape codesign

📋 learning rate warmup navigates to flatter region



📋 sharpness-aware minimization



*check our website for more references

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

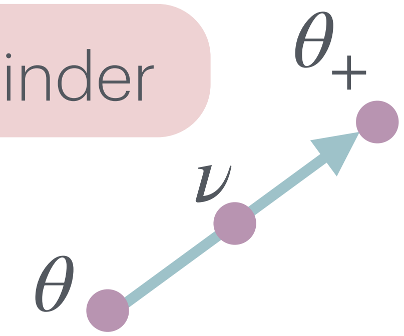
$$\eta < \frac{2}{\sup \|\nabla^2 L(\,\cdot\,)\|}$$

Proof.

$$L(\theta_+) = L(\theta - \eta \nabla L(\theta))$$

GD step

Taylor remainder



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

$$\leq L(\theta) - \eta \|\nabla L(\theta)\|^2 \left(1 - \frac{\eta}{2} \|\nabla^2 L(\nu)\|\right)$$

operator norm

$$\leq L(\theta)$$

small stepsize

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 $L(\theta_t) \downarrow$

convexity $L(\theta_t) - \min L \leq \dfrac{\|\theta_0 - \theta^*\|^2}{2t}$

α**-strong convexity** $L(\theta_t) - \min L \leq e^{-\alpha t}(L(\theta_0) - \min L)$

number of steps to get ϵ-error:

$O\big(1/\epsilon\big)$ and $O\big(\kappa \log(1/\epsilon)\big)$

$\kappa = 1/\alpha$, 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

$$L(\theta_t) - L(\nu) \le \frac{\|\theta_0 - \nu\|^2}{2t} \quad \text{for all } \nu$$

Proof.

step 1:

chain rule — gradient flow — convexity

$$\mathrm{d}\frac{1}{2}\|\theta_t - \nu\|^2 = \langle \theta_t - \nu, \mathrm{d}\theta_t \rangle = \langle \theta_t - \nu, -\nabla L(\theta_t) \rangle \mathrm{d}t \le L(\nu) - L(\theta_t)$$

step 2:

integration — descent lemma

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

step 3: rearranging terms

for small stepsize, discretize this => GD analysis

Review: acceleration

number of steps to get ϵ-error

GD

$$\theta_+ = \theta - \eta \nabla L(\theta)$$

$$O\big(1/\epsilon\big) \ \& \ O\big(\kappa \log(1/\epsilon)\big)$$

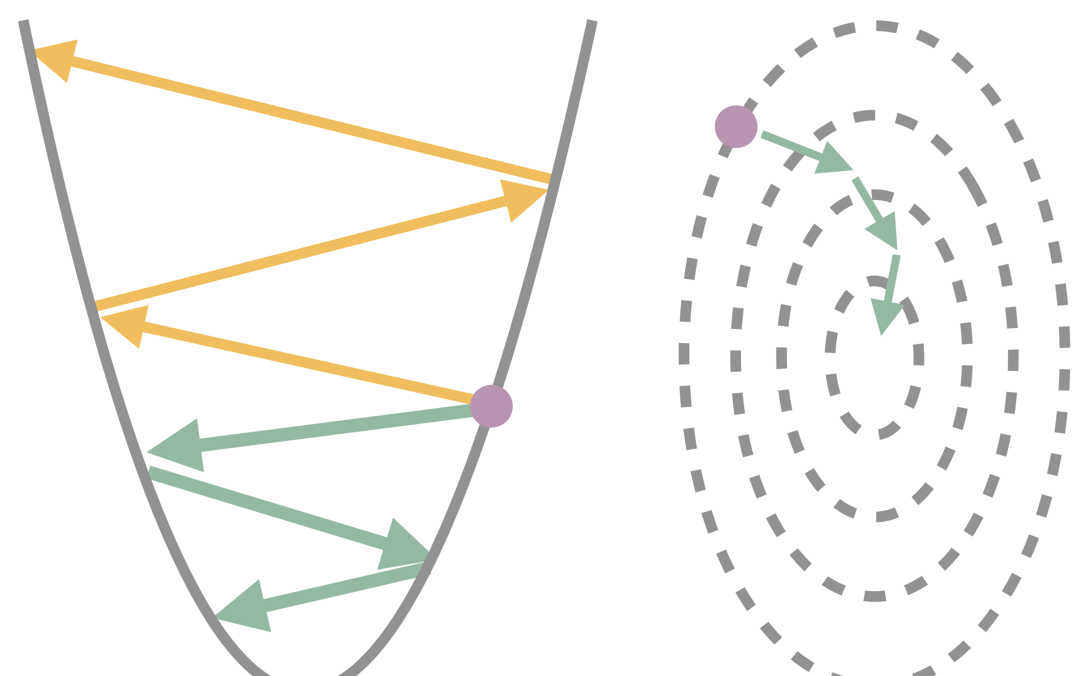
Nesterov's momentum

$$\theta_+ = \nu - \eta \nabla L(\nu)$$
$$\nu_+ = \theta_+ + \beta(\theta_+ - \theta)$$

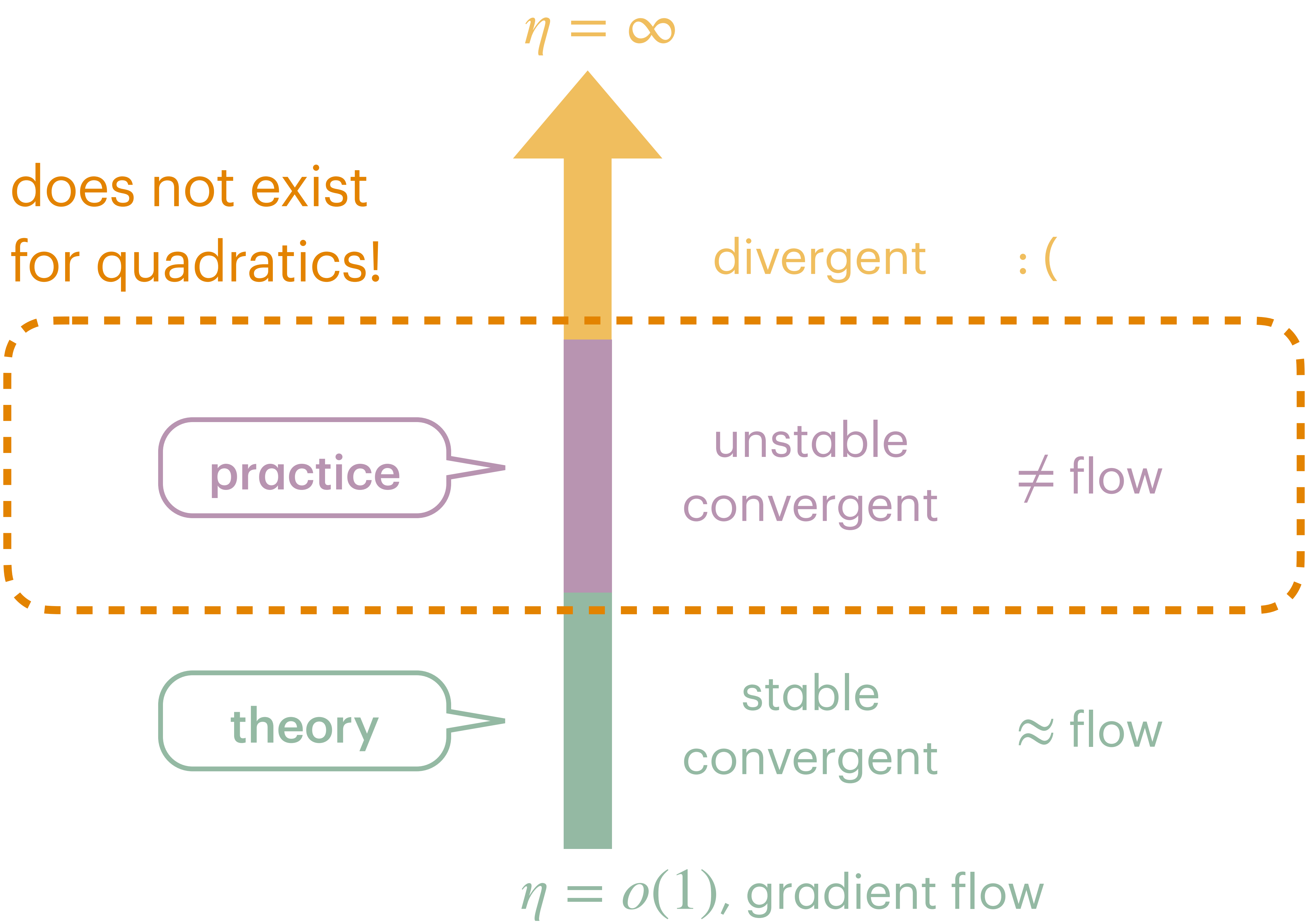
$$O\big(1/\sqrt{\epsilon}\big) \ \& \ O\big(\sqrt{\kappa} \log(1/\epsilon)\big)$$

these rates are optimal

hard case: quadratics in high-dim



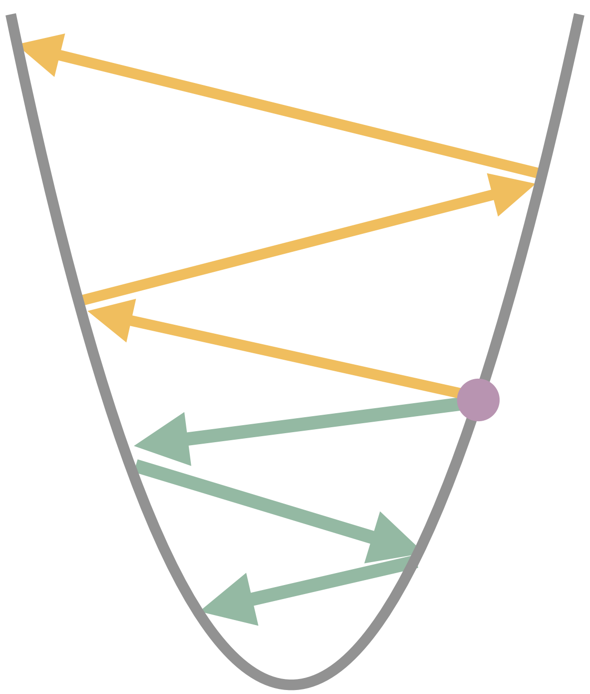
From small to large stepsize

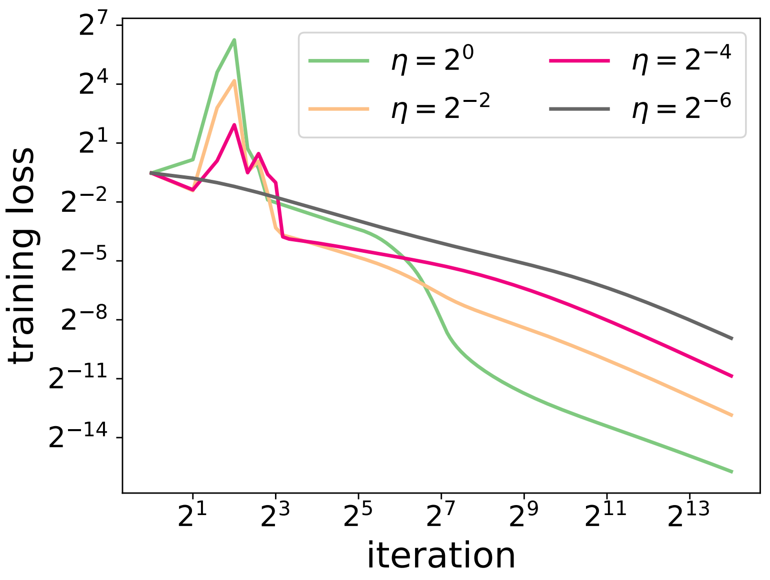


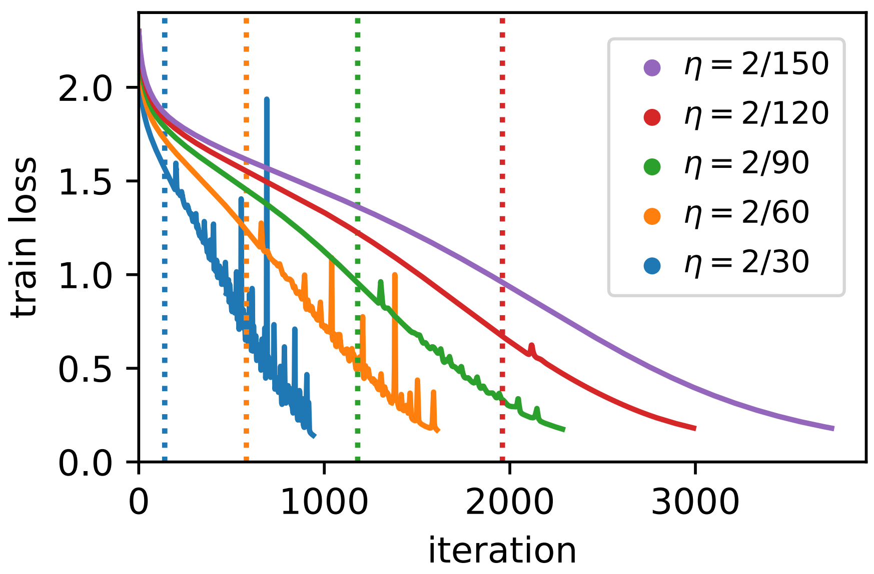
Alternative mental model

linear regression | logistic regression | ...... | deep learning

unstable convergence impossible | observable & provable | | unstable convergence observed







(1/3) Logistic regression

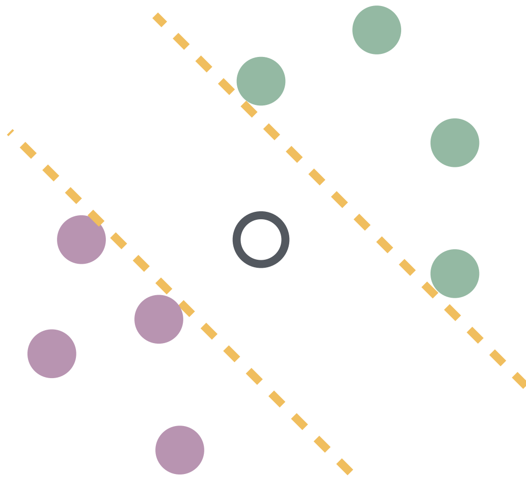
$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ln\left(1 + \exp(-y_i x_i^\top \theta)\right)$$

smooth, convex
non-strongly convex

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

Assumption (bounded + separable)

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



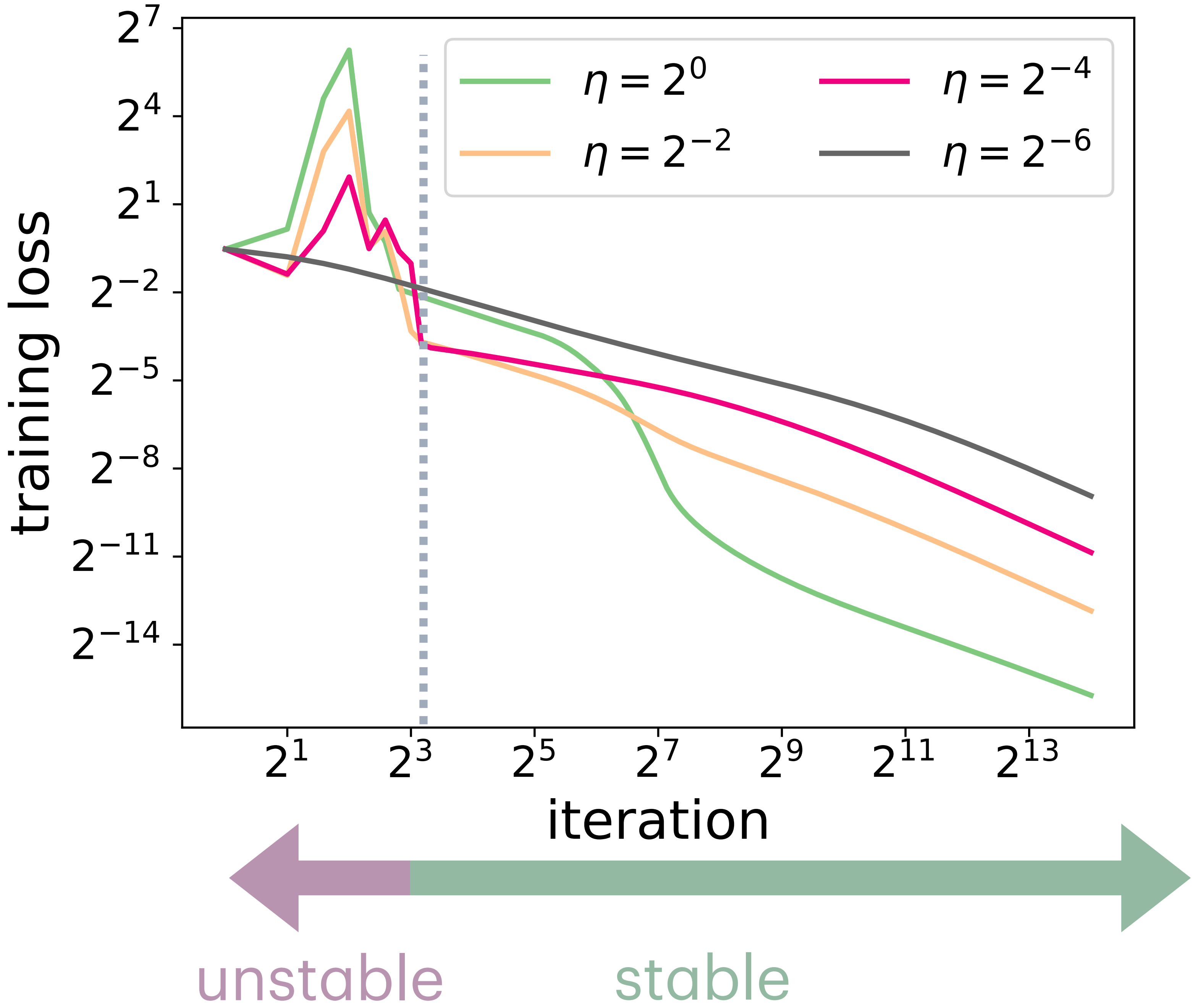
"almost surely" if overparameterized

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



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.

tendency to decrease

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

Phase transition.

GD exits unstable phase in τ steps for

$\tau = \Theta(\eta)$

$$\tau = \Theta\big(\max\{\eta,\ n,\ n/\eta \ln(n/\eta)\}\big)$$

Stable phase.

$$L(\theta_{\tau+t}) \downarrow \text{ and } L(\theta_{\tau+t}) = \tilde{O}\left(\frac{1}{\eta t}\right)$$

"flow rate"

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

(1/3) Effects of large stepsize

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

2. Phase transition in $\Theta(\eta)$ steps $\Rightarrow$ longer unstable phase

3. Given #steps $T \geq \Theta(n)$, if choose $\eta = \Theta(T)$, then

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

A lower bound. There exists a separable dataset, if η is such that $L(\theta_t) \downarrow$ for all t, then

$$L(\theta_t) = \Omega(1/t)$$

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^*, $\min_i y_i x_i^\top \theta^* > \gamma > 0$

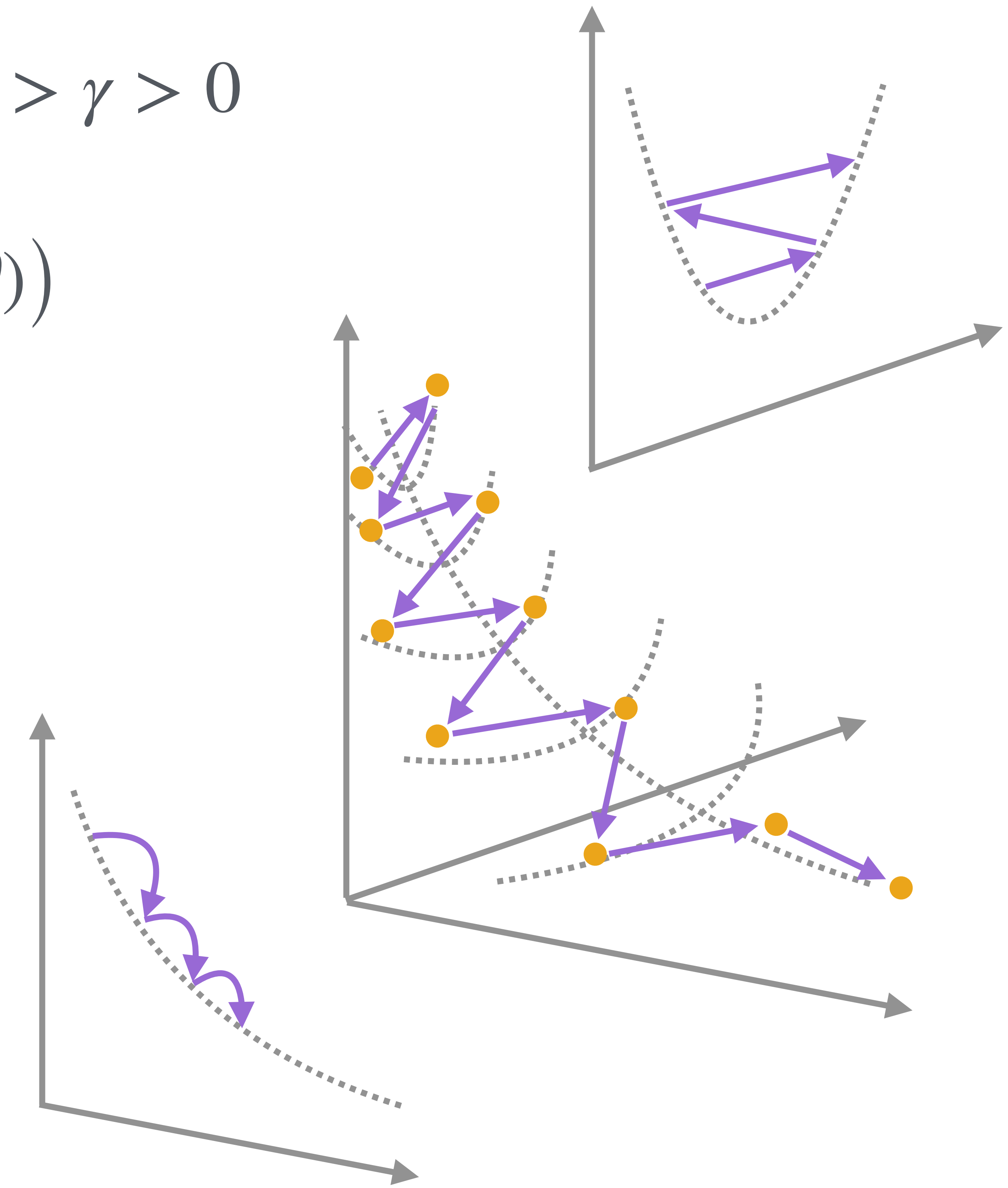
$L(\theta) = \hat{\mathbb{E}} \ln\big(1 + \exp(-y x^\top \theta)\big)$

minimizer at ∞

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

self-bounded

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



Two extensions

minimizer at ∞

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

finite minimizer →

e.g. regularization

unstable convergence under finite minimizer

self-bounded

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

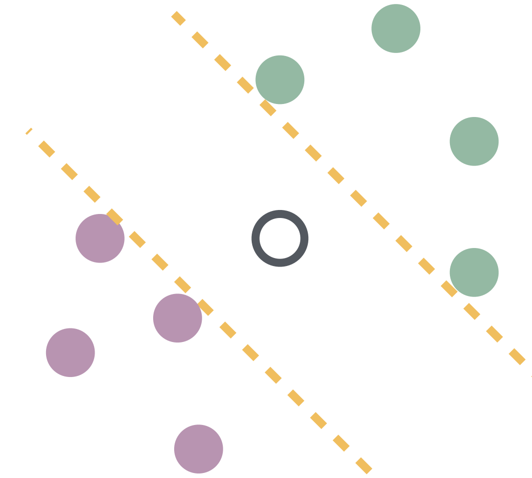
enabling "tricks" →

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

large stepsizes for GD variants

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

(2/3) Large, adaptive stepsize



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

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

adapt to curvature

$$\approx \theta_t - \frac{\eta}{L(\theta_t)} \nabla L(\theta_t)$$

$$\theta_{t+1} = \theta_t - \eta \nabla \phi(\theta_t) \qquad \phi(\theta) = -\,\ell^{-1}(L(\theta))$$

$$\approx \ln \sum \exp(-y_i x_i^\top \theta)$$

[Ji & Telgarsky, 2021]

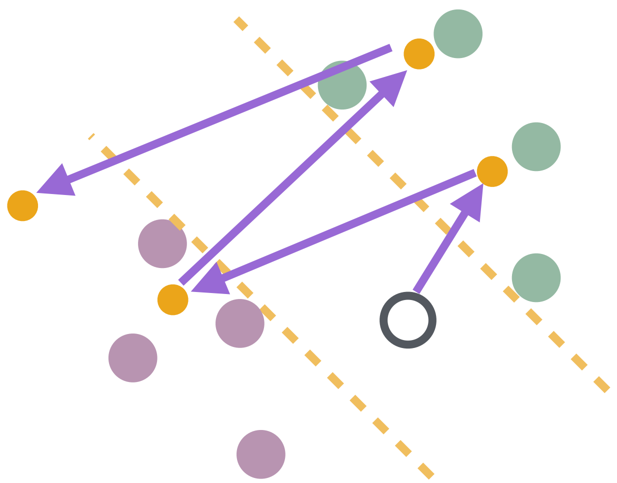
For $\eta = \Theta(1)$, $L(\theta_t) \downarrow$ and $L(\theta_t) \le \exp(-\Theta(t))$

large stepsize makes adaptive GD even faster

(2/3) Theorem

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

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



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

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

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

(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

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

first-order batch method:

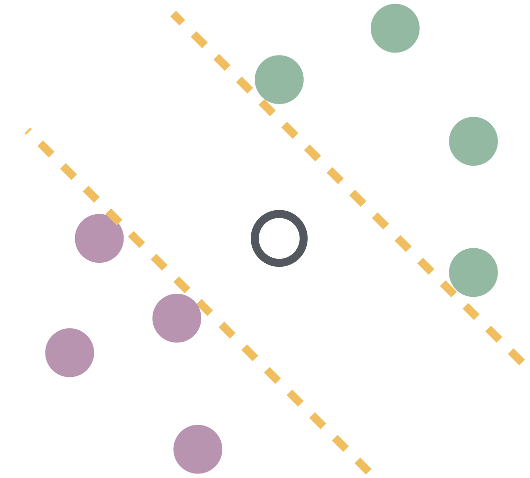
$$\theta_t \in \theta_0 + \mathsf{span}\{\nabla L(\theta_0), \ldots, \nabla L(\theta_{t-1})\}$$

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

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



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

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

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

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

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

(3/3) Theorem

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

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

$\eta_{\max} = \Theta(\sqrt{\kappa})$

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

Phase transition. GD exits unstable phase in τ steps for

$$\tau := \Theta\Big(\max\{\eta, n, n/\eta \ln(n/\eta)\}\Big)$$

$\tau = \Theta(\sqrt{\kappa})$

Stable phase. $\tilde{L}(\theta_{\tau+t}) \downarrow$ and

$t = \Theta(\sqrt{\kappa}\ln(1/\epsilon))$

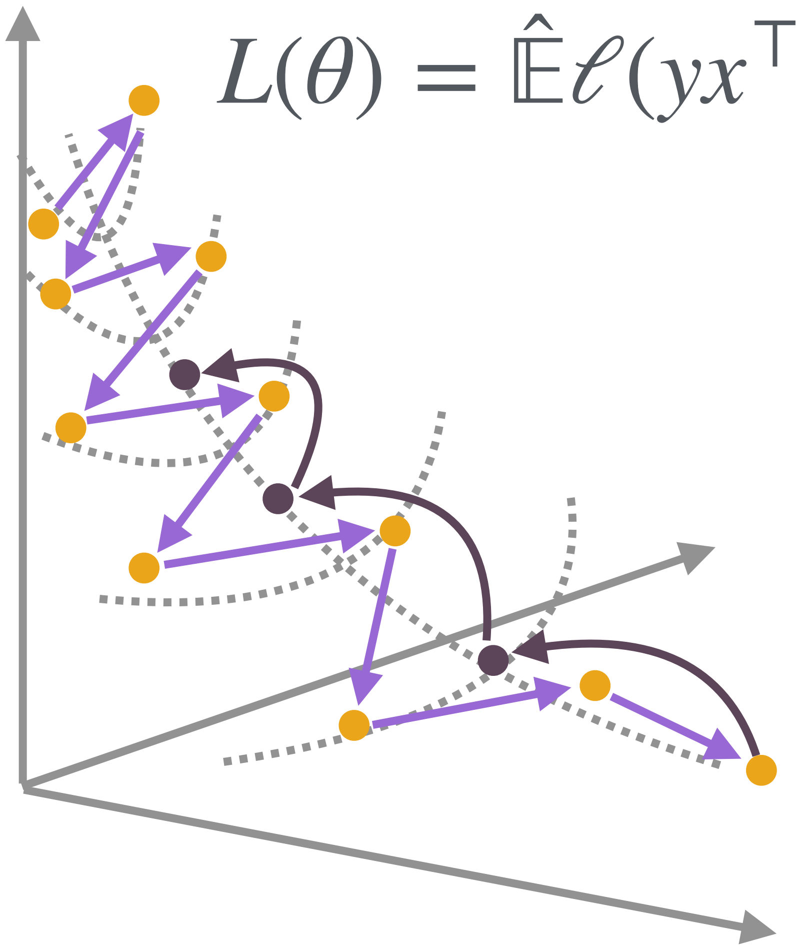
$$\tilde{L}(\theta_{\tau+t}) - \min \tilde{L} \lesssim \exp(-t\eta/\kappa)$$

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

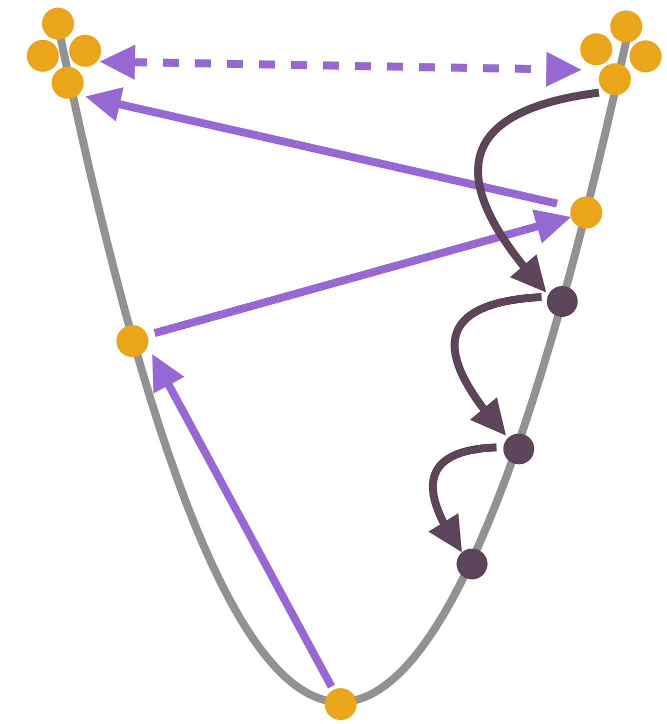
Wu, Marion, Bartlett. "Large stepsizes accelerate gradient descent for regularized logistic regression." NeurIPS 2025

(3/3) Picture: valley + basin

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



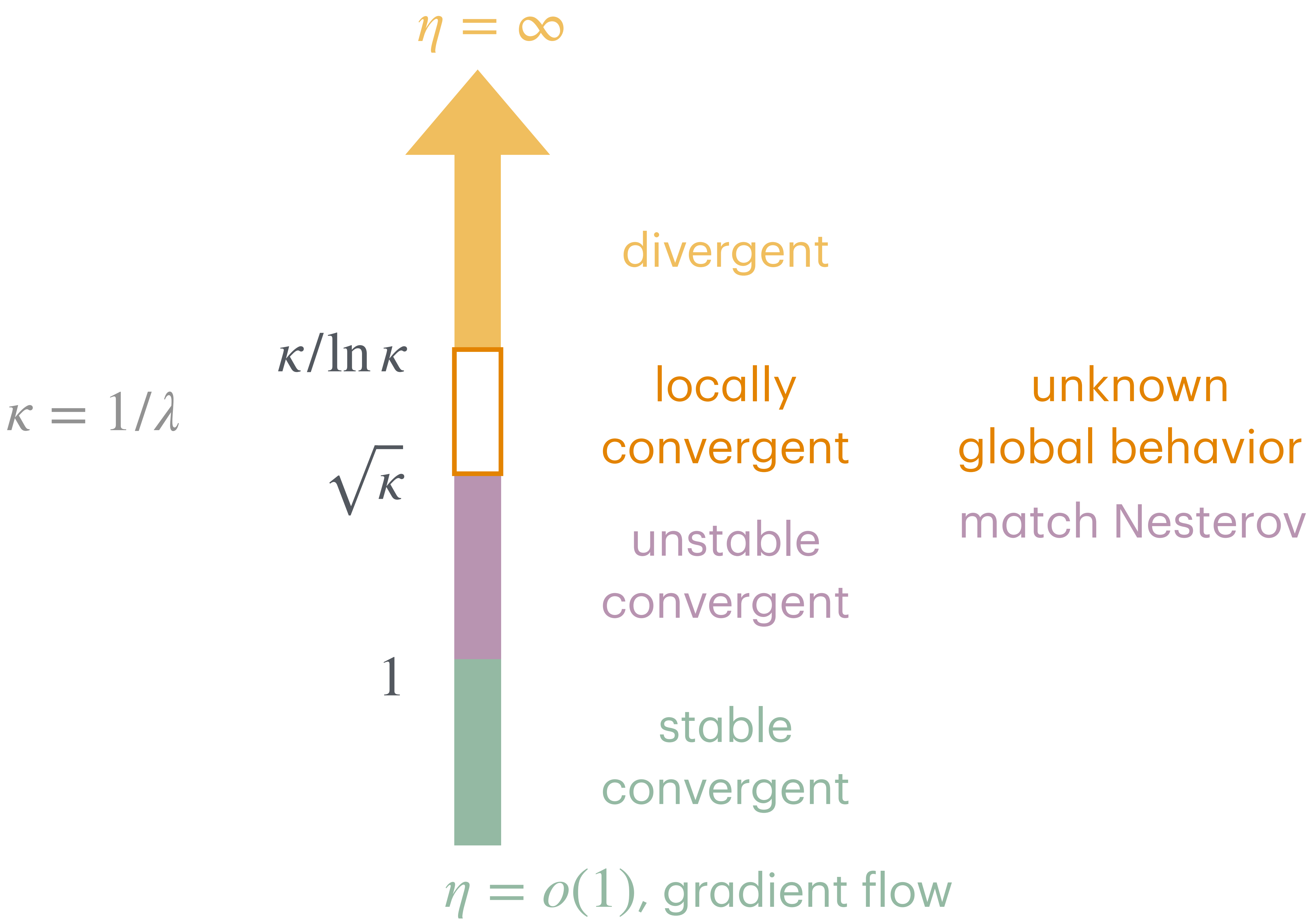
$$R(\theta) = \frac{\lambda}{2}\|\theta\|^2$$



Unstable. $\tilde{L} \approx L$, $R \leq \Theta(1)$, “overshoot” $\|\tilde{\theta}\| = O(\ln \kappa)$

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

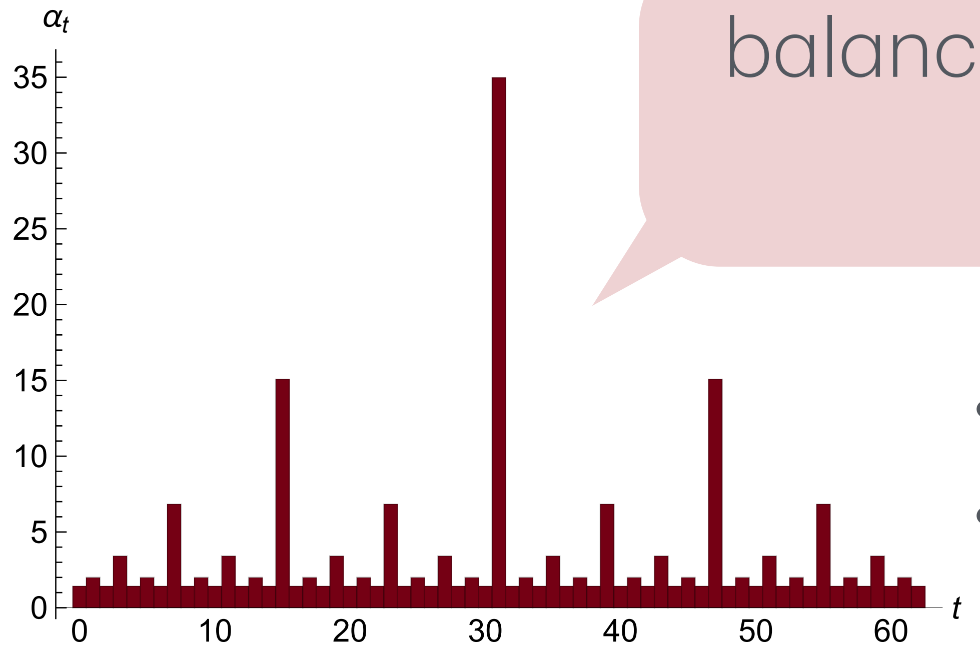
(3/3) Stepsize diagram



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

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



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

- cover more problems, e.g., quadratics
- less practical stepsize scheduler

Altschuler, Parrilo. "Acceleration by stepsize hedging II: silver stepsize schedule for smooth convex optimization." Mathematical Programming 2024

Grimmer, Shu, Wang. "Composing optimized stepsize schedules for gradient descent." Mathematics of Operations Research 2025

Summary

training instability caused by large stepsize

acceleration via large stepsize: three ML examples

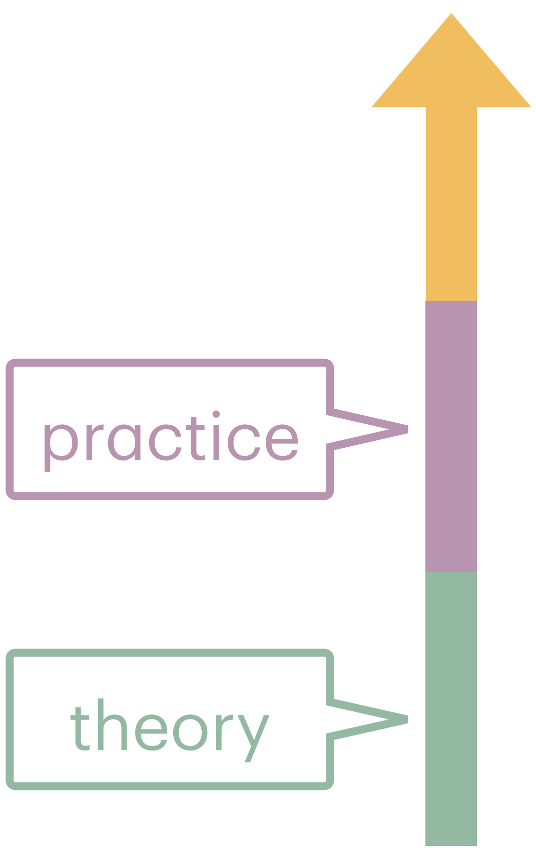
general losses

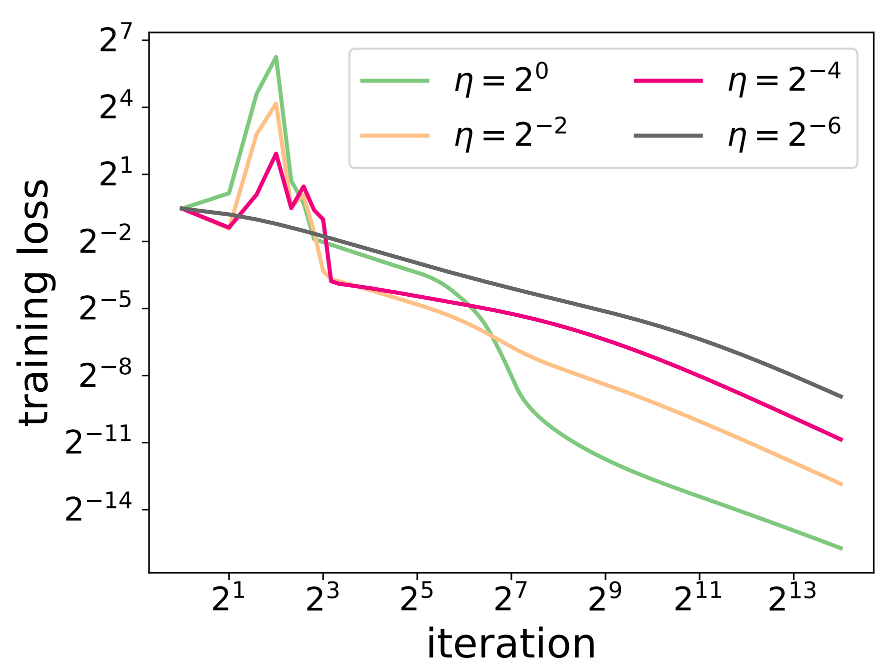
neural networks

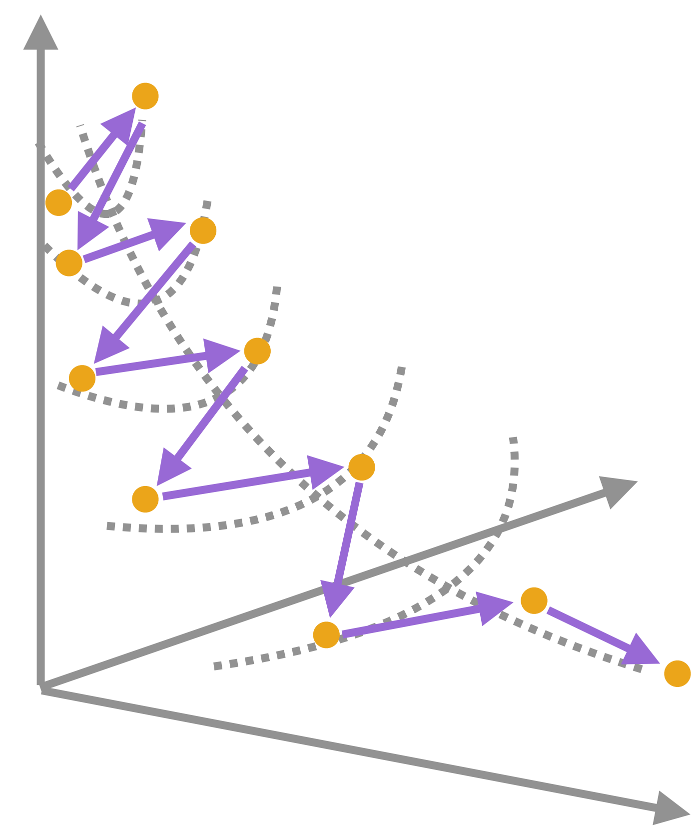
implicit bias, generalization

new mental picture: valley

cross entropy, attention, ...







Open problems (set 1/2)

Call for clear, rigorous understanding on

🤔 what functional property enables large stepsize?

🤔 trackable measures of trajectory: sharpness? local mean?

🤔 early-phase feature learning, especially against NTK?

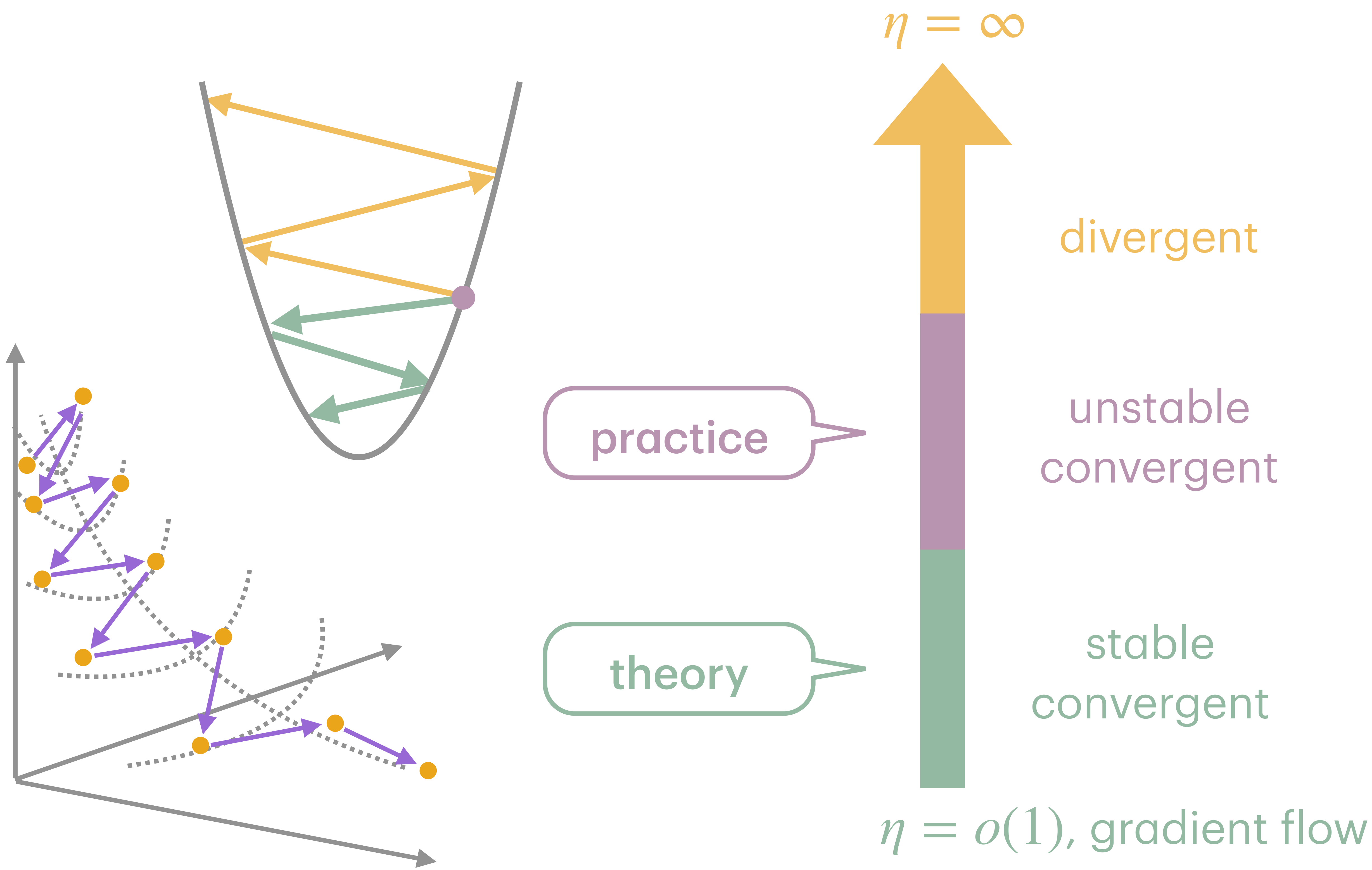
🤔 large stepsize for other optimizers, e.g., SGD, Adam?

Open problems (set 2/2)

Call for useful, heuristic insights on

- 💡 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

NeurIPS Tutorial on "Training Instability"
Part 2: Generalization

Maryam Fazel and Yu-Xiang Wang

Part 1 of the tutorial is about “Rethinking Optimization”

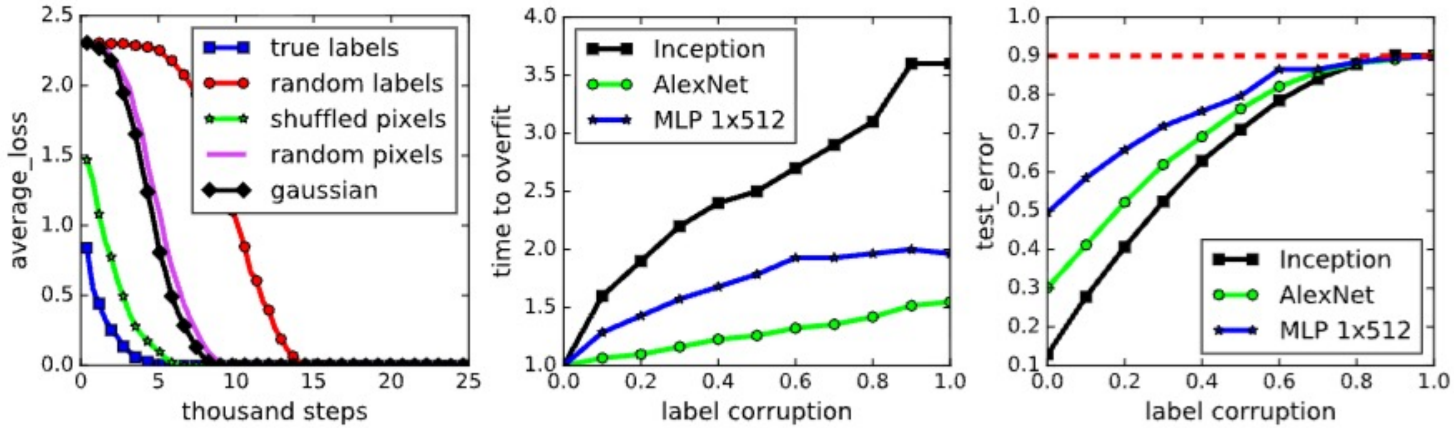
- Go beyond the “stable regime”

- Gradient descent can often converge faster!
  - Linear convergence
  - Nesterov Accelerated Rates
  - (Sometimes) arbitrarily fast (constant iteration complexity)

Part 2 of the tutorial is about “Rethinking Generalization”

Understanding deep learning requires rethinking generalization

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, Oriol Vinyals



(a) learning curves (b) convergence slowdown (c) generalization error growth

- **Deep learning models in practice are NOT capacity limited**
- “generalization” depends on many factors

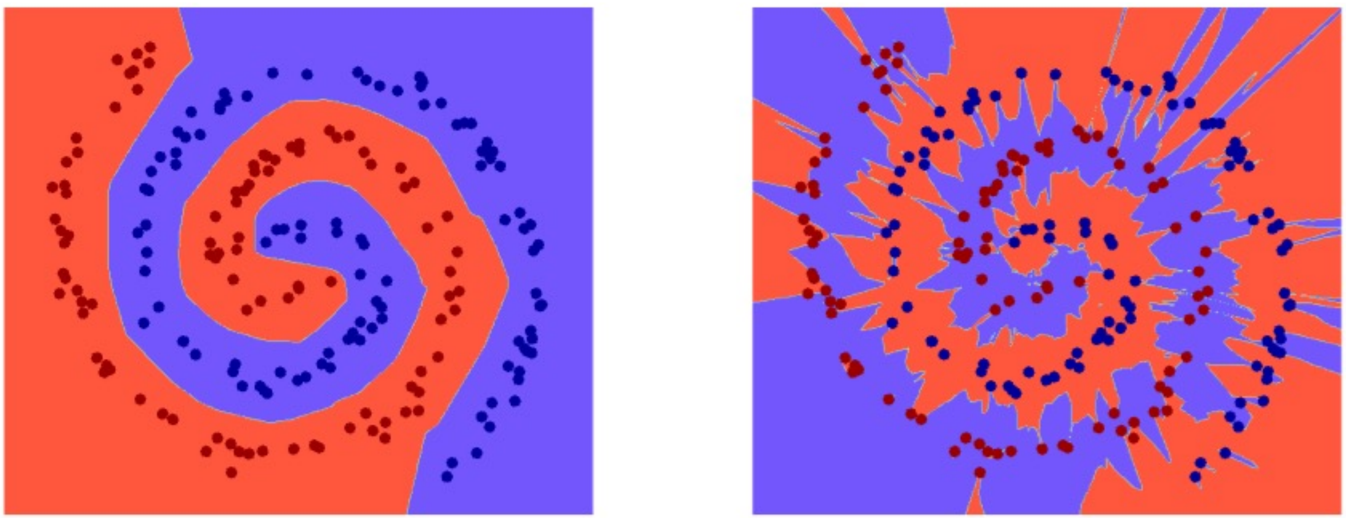
We ask: how does large stepsize affects generalization in overparameterized models?

Let's say the labels are clean… there are many "interpolating" solutions

[Submitted on 7 Jun 2019 (v1), last revised 15 Nov 2020 (this version, v6)]

Understanding Generalization through Visualizations

W. Ronny Huang, Zeyad Emam, Micah Goldblum, Liam Fowl, J. K. Terry, Furong Huang, Tom Goldstein



(a) 100% train, 100% test (b) 100% train, 7% test

Question #1: Does GD with Large Stepsize *find* the generalizing solutions or overfitting solutions?

Things become even more interesting when the labels are noisy.

Benign overfitting (Belkin, Bartlett et al.) : you may have 0 training loss on noisy labels, yet test error / loss → 0

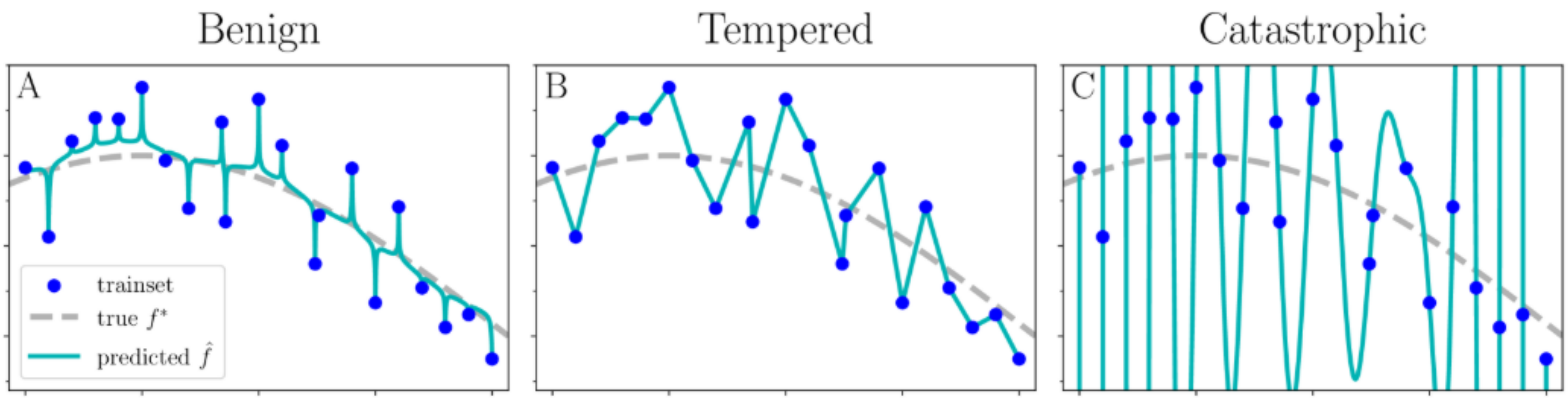


Figure 1: **As $n \to \infty$, interpolating methods can exhibit three types of overfitting. (A)** In *benign overfitting*, the predictor asymptotically approaches the ground-truth, Bayes-optimal function. Nadaraya-Watson kernel smoothing with a singular kernel, shown here, is asymptotically benign. **(B)** In *tempered overfitting*, the regime studied in this work, the predictor approaches a constant test risk greater than the Bayes-optimal risk. Piecewise-linear interpolation is asymptotically tempered. **(C)** In *catastrophic overfitting*, the predictor generalizes arbitrarily poorly. Rank-n polynomial interpolation is asymptotically catastrophic.

Illustration from (Mallinar et al. 2022)

Question #2: What solutions does GD with Large Stepsize find when labels are noisy?

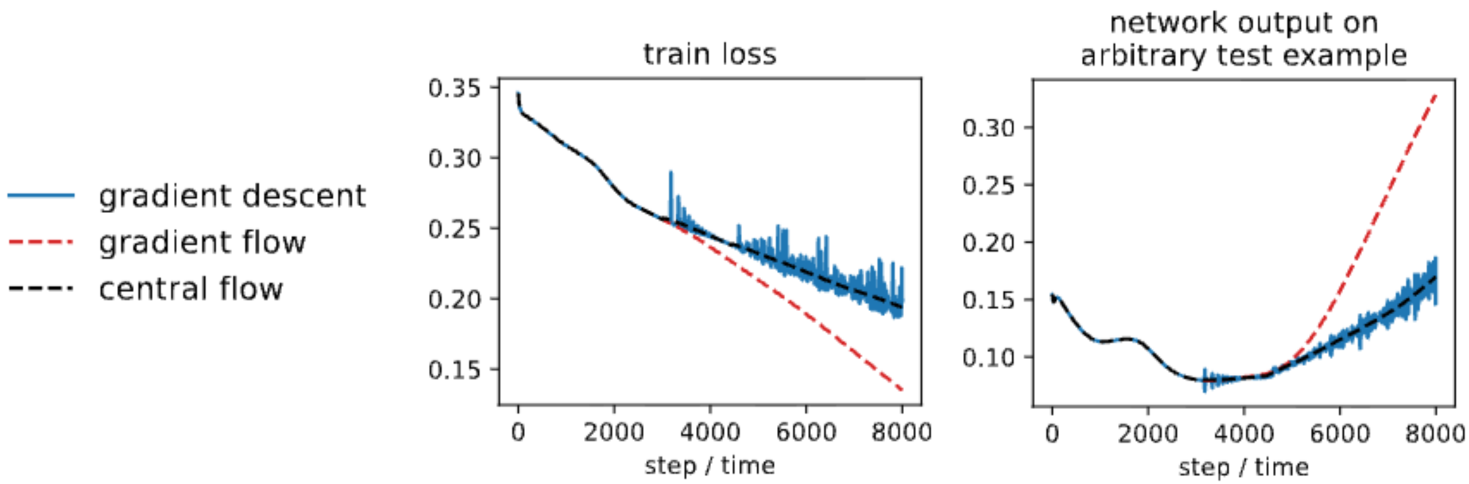
The implicit bias of "Large Stepsize" does not function in isolation.

- Data distribution
  - e.g., Low-dimensional structure, data-augmentation
- Choice of loss functions
  - e.g., Square loss, logistic loss
- Model architecture
  - e.g., with or without "bias", "residual connection", "batch-norm"
- Hyperparameters in training:
  - e.g., weight decay, momentum, adaptive optimizers

Question #3: How does GD with Large Stepsize interact with other "*forces of nature*"?

Gradient descent with *constant stepsize* is qualitatively different from gradient flow.

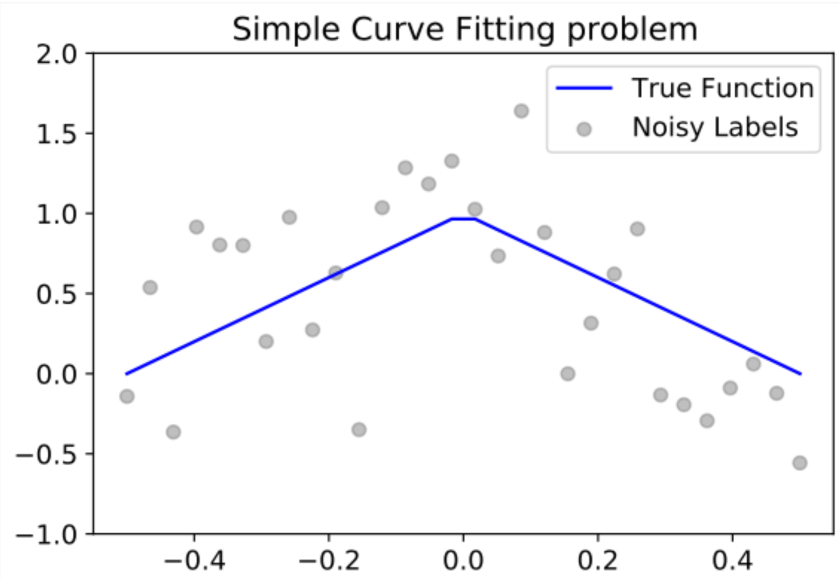
Cohen, Damian, Talwalkar, Kolter, Lee (2025) "Central Flows"



The dynamics is complex and **chaotic**. In: Kong and Tao (2020) "Stochasticity of Deterministic Gradient Descent"

What does the GD solution look like?
Let's start with a simple example.

Let us train an overparameterized ReLU NN on this "curve fitting" problem



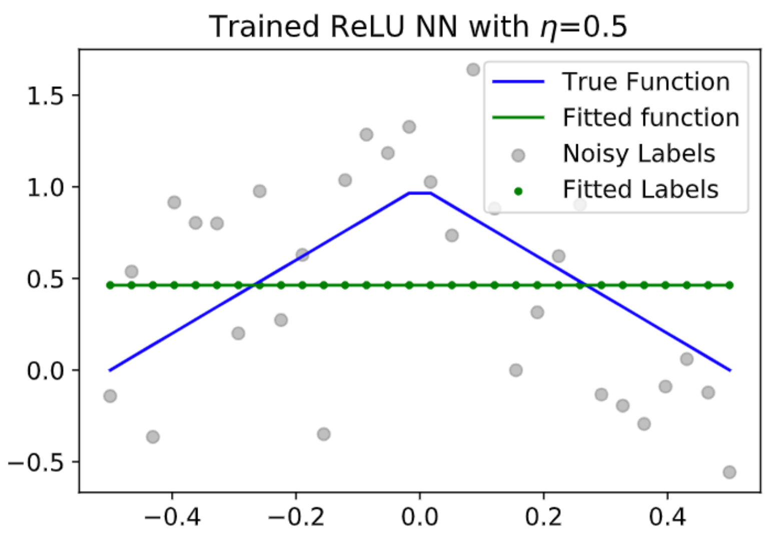
Global optimal solution has 0-loss, i.e., interpolating.

But does GD find these "interpolating" solution?

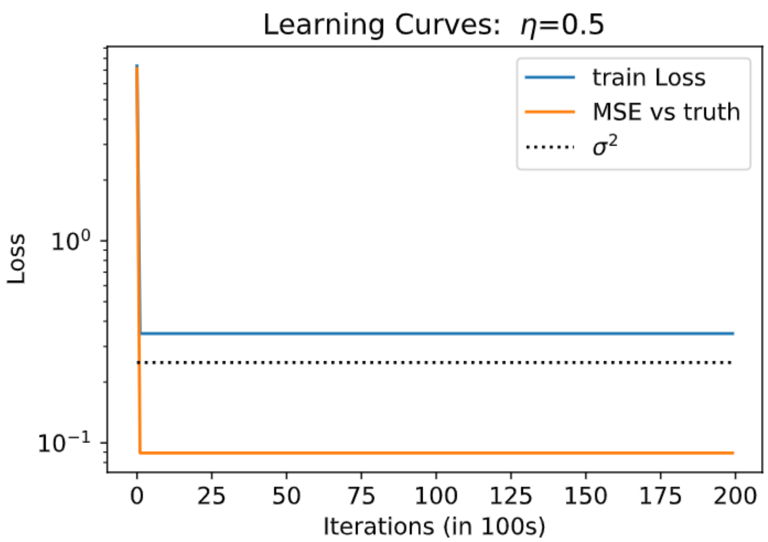
If so, does GD solution satisfies "Benign overfitting"?

30 data points. Noisy labels.
2-Layer ReLU NN with 1000 neurons.
Minimizing square loss.
No regularization.

Stepsize = 0.5

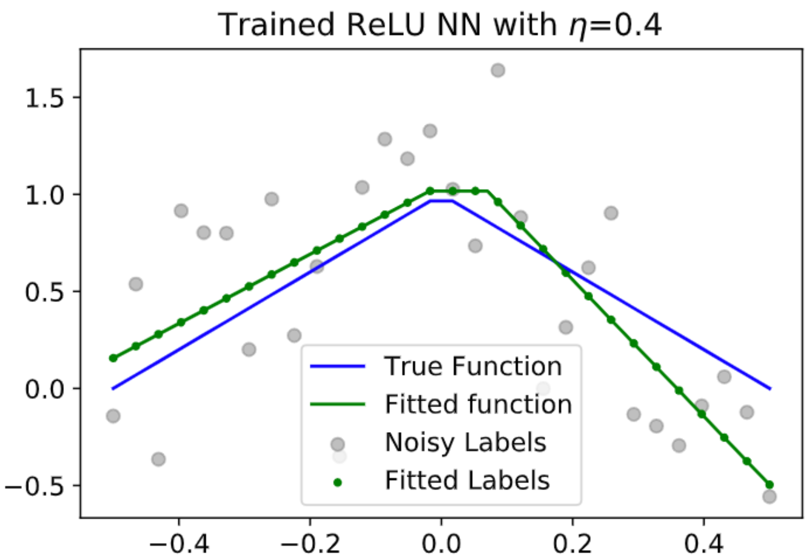


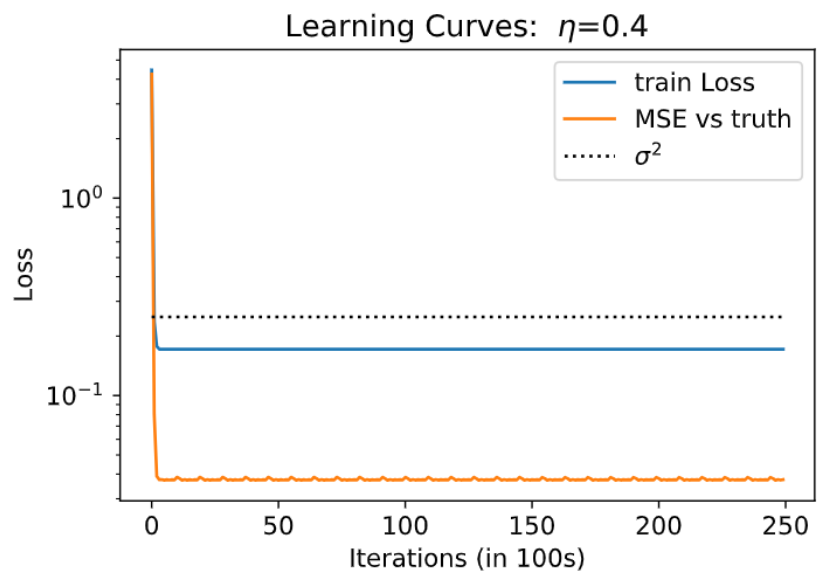
Trained ReLU NN with η=0.5
True Function
Fitted function
Noisy Labels
Fitted Labels
1.5
1.0
0.5
0.0
−0.5
−0.4
−0.2
0.0
0.2
0.4



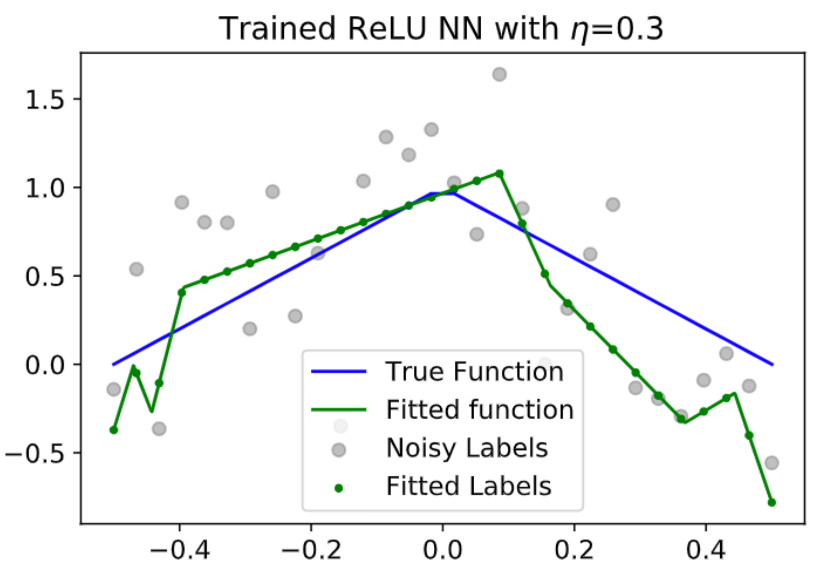
Learning Curves: η=0.5
train Loss
MSE vs truth
σ^2
Loss
10^0
10^{-1}
0
25
50
75
100
125
150
175
200
Iterations (in 100s)

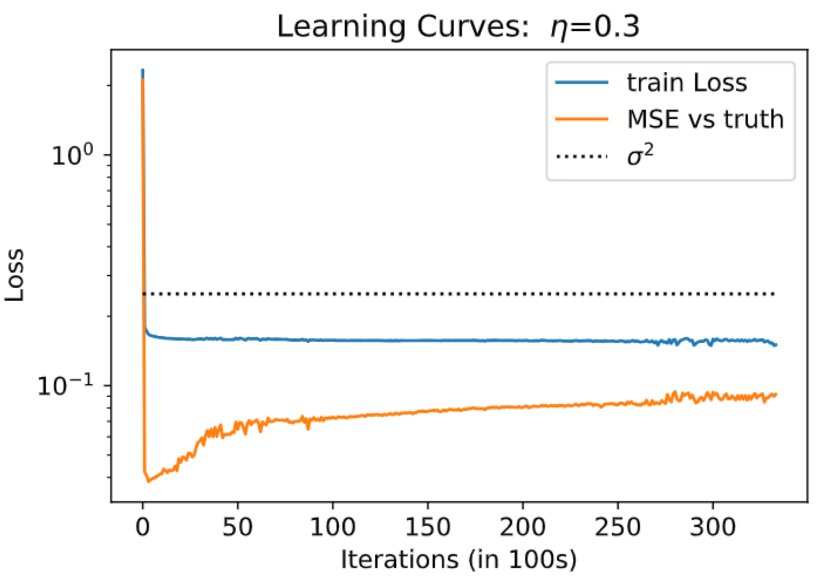
Stepsize = 0.4


Trained ReLU NN with η=0.4
True Function
Fitted function
Noisy Labels
Fitted Labels
1.5
1.0
0.5
0.0
−0.5
−0.4
−0.2
0.0
0.2
0.4

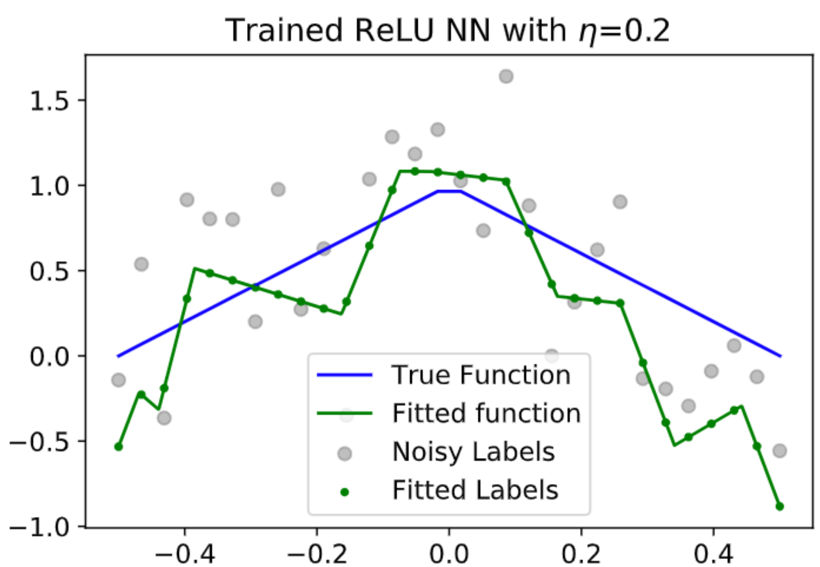

Learning Curves: η=0.4
train Loss
MSE vs truth
σ^2
Loss
10^0
10^{-1}
0
50
100
150
200
250
Iterations (in 100s)

Stepsize = 0.3

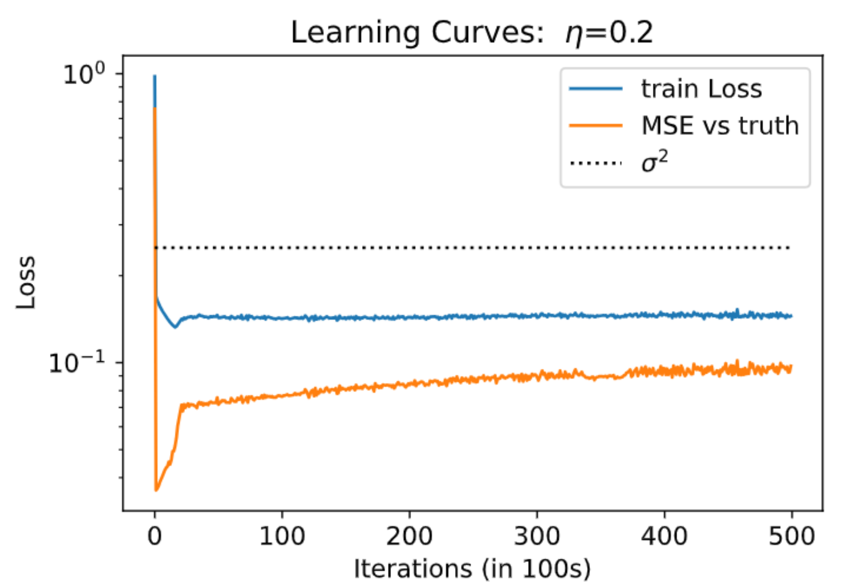

Trained ReLU NN with η=0.3
1.5
1.0
0.5
0.0
−0.5
−0.4
−0.2
0.0
0.2
0.4
True Function
Fitted function
Noisy Labels
Fitted Labels


Learning Curves: η=0.3
train Loss
MSE vs truth
σ^2
Loss
10^0
10^{-1}
0
50
100
150
200
250
300
Iterations (in 100s)

Stepsize = 0.2

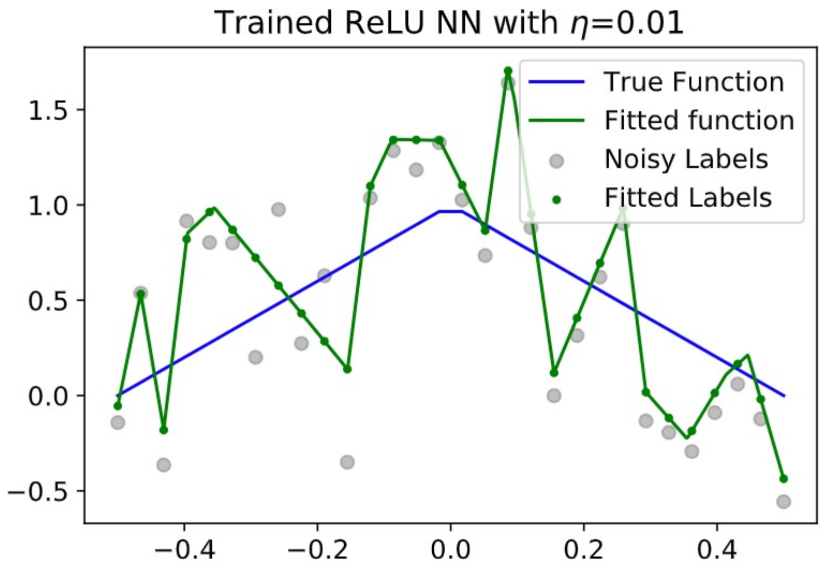


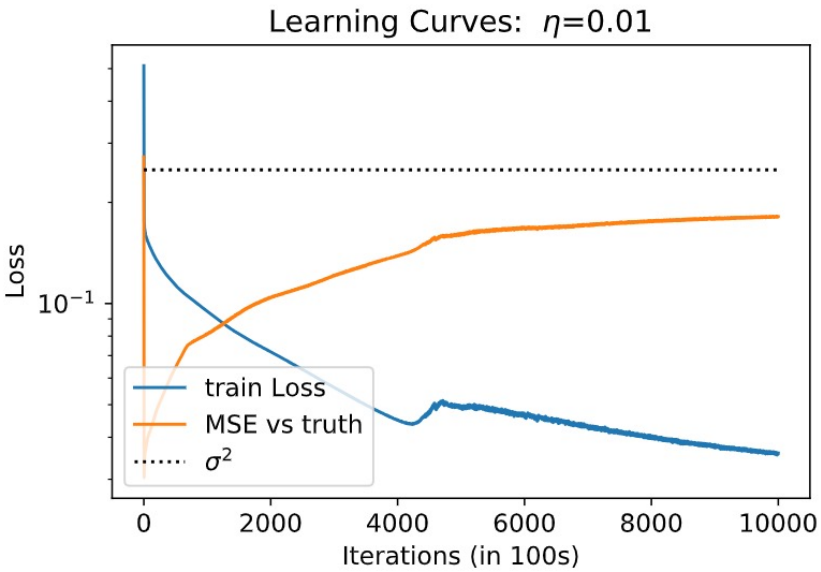
Trained ReLU NN with η=0.2
1.5
1.0
0.5
0.0
−0.5
−1.0
−0.4
−0.2
0.0
0.2
0.4
True Function
Fitted function
Noisy Labels
Fitted Labels



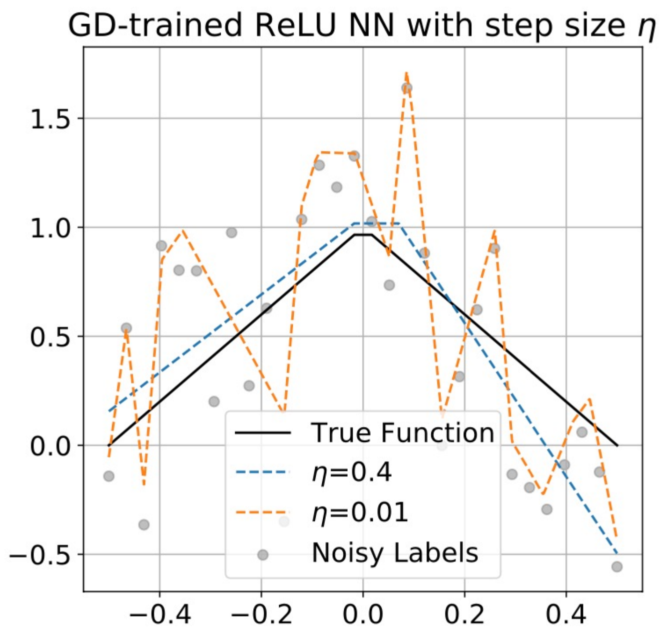
Learning Curves: η=0.2
Loss
10^0
10^−1
0
100
200
300
400
500
Iterations (in 100s)
train Loss
MSE vs truth
σ^2

Stepsize = 0.01





Observation: By tuning the stepsize, we are effectively tuning the number of “linear pieces”. GD with larger stepsize learns **simpler functions**.

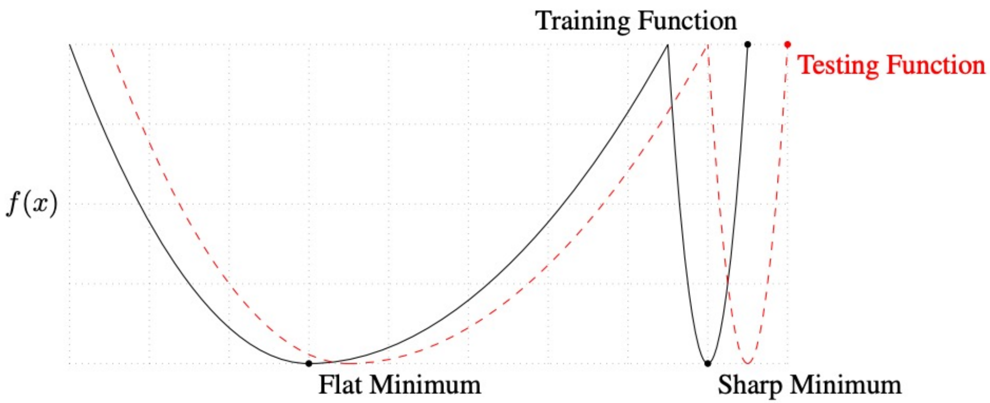


But how did “sparsity” emerge?

Is this a general phenomenon?
Did we get lucky?

Can we prove anything about this phenomenon rigorously?

Large stepsize is intimately connected **flat minima**, and *low-curvature* regions



Minima stability theory:
(Wu et al. 2018, Mulayoff et al. 2021)

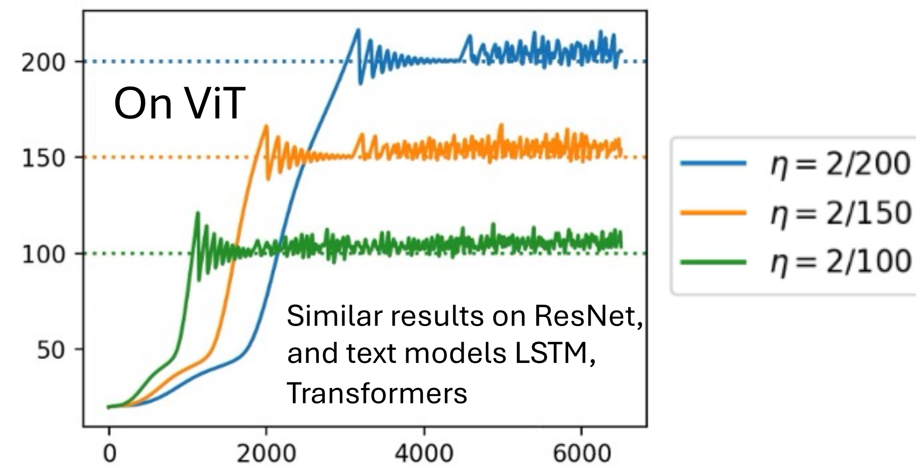
GD tend to diverge at sharp minima. The set of points GD can stabilize around:

$$\{f_\theta | \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \le 2/\eta, \nabla \mathcal{L}(\theta) = 0\}$$

Edge-of-Stability phenomenon
(Cohen et al, 2021; 2025)

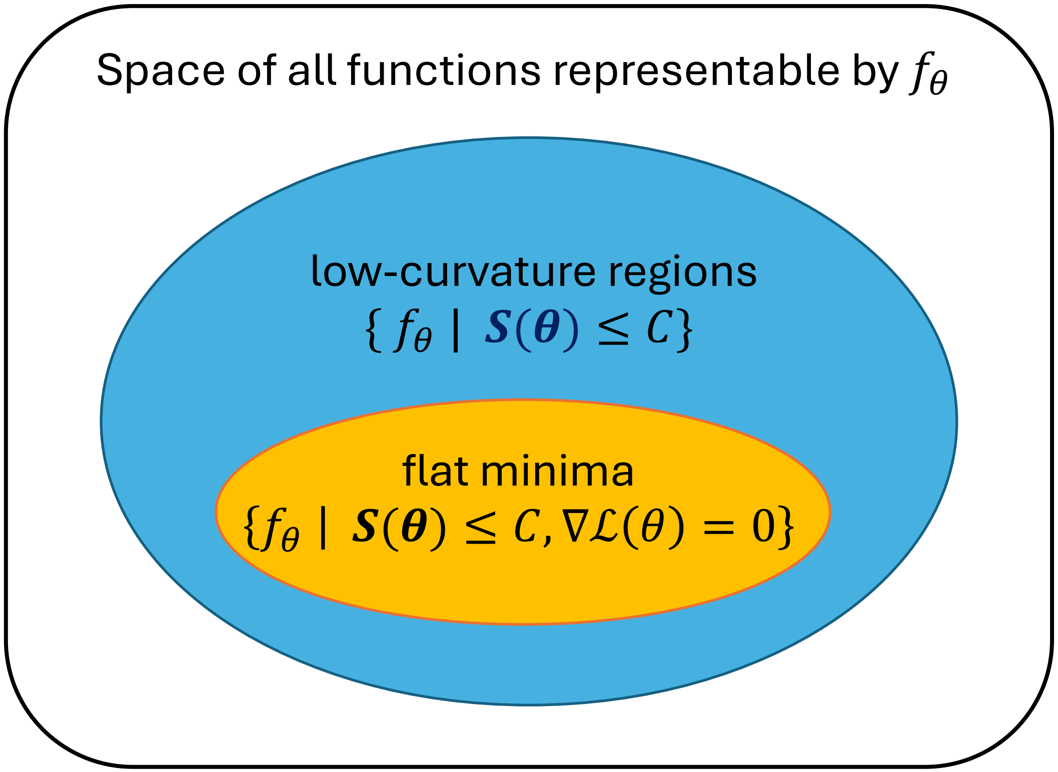
Entire GD trajectory stays inside the following set

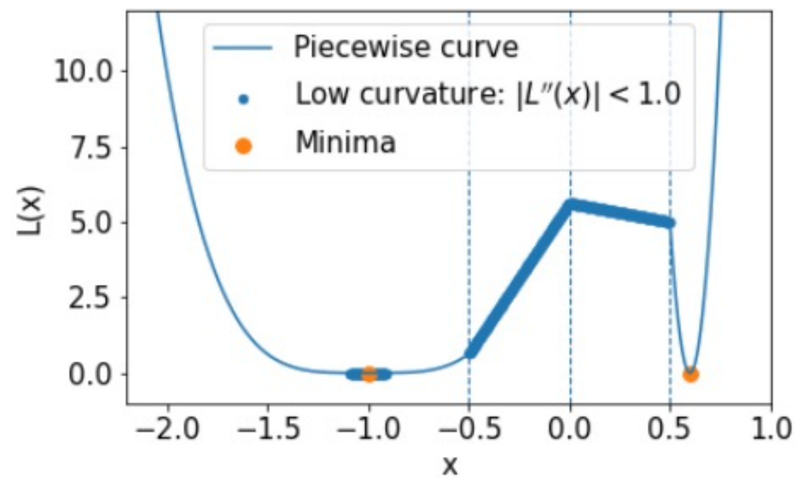
$$\{f_\theta | \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \lesssim 2/\eta\}$$



(illustration from "Central Flow" Cohen et al, 2025)

Flat minima and flat points (low-curvature regions)





$\boldsymbol{S}(\boldsymbol{\theta}) := \lambda_{\max}(\nabla^2\mathcal{L}(\theta))$ for Gradient Descent $\quad C = 2/\eta$

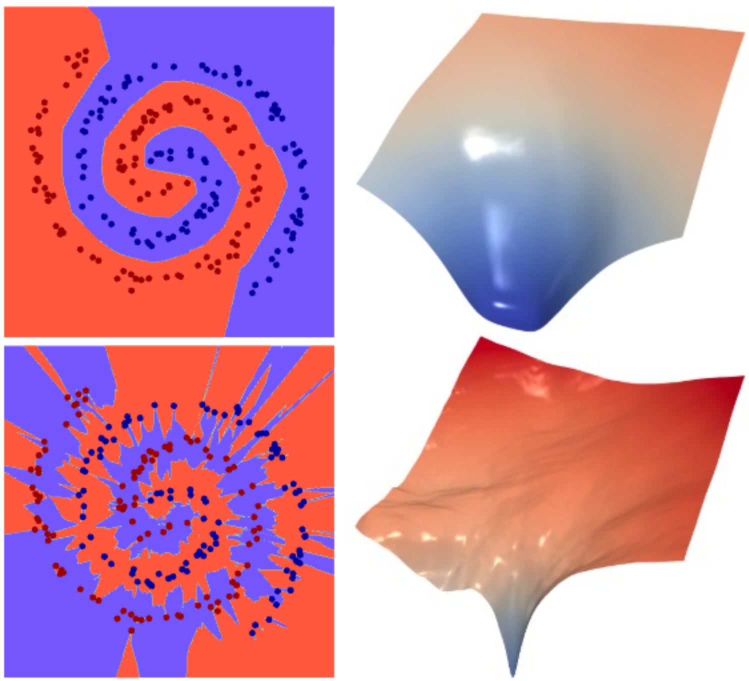
$\boldsymbol{S}(\boldsymbol{\theta}) := \mathrm{trace}(\nabla^2\mathcal{L}(\theta))$ for Stochastic gradient descent $\quad C = O(1/\eta)$

with stepsize = η

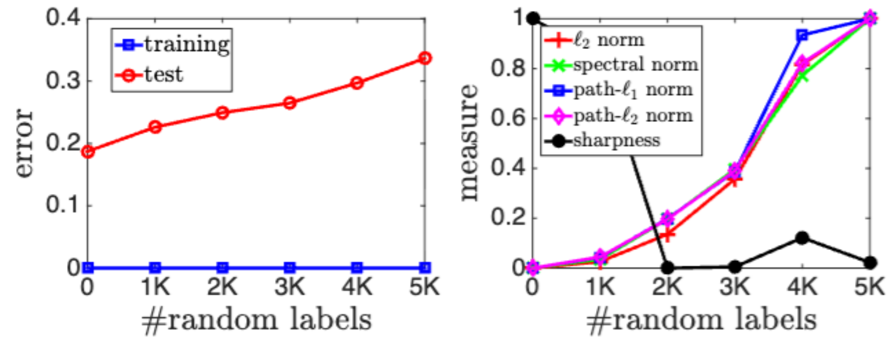
Do flat minima generalize better?

Deep learning folklore that **flat minima generalize better**.

(Hochreiter and Schmidhuber, 1997)



(Huang et al. 2018)



Very flat minima could also overfit.

"Exploring generalization in Deep Learning"
Neyshabur et al. 2017

Sharp Minima Can Generalize For Deep Nets

Laurent Dinh, Razvan Pascanu, Samy Bengio, Yoshua Bengio

How do we make sense of these conflicting observations?

Remainder of this tutorial

1. Flat minima **exactly recover** weights in Matrix Sensing and 2-layer Neural Nets (Maryam)

2. Does **flatness imply generalization** in 2-layer ReLU Neural Networks? (Yu-Xiang)

3. Discussion and Open problems. (Both)

Flat Minima and Generalization: Case studies in Low-rank Recovery and a 2-Layer Network

Outline of this part:

- Overparameterization, generalization & flatness
- Flatness via trace of Hessian
- Prove “flat minima generalize” in 2-layer test cases, including:
  - matrix sensing
  - a 2-layer neural net

Over-parameterization and some consequences

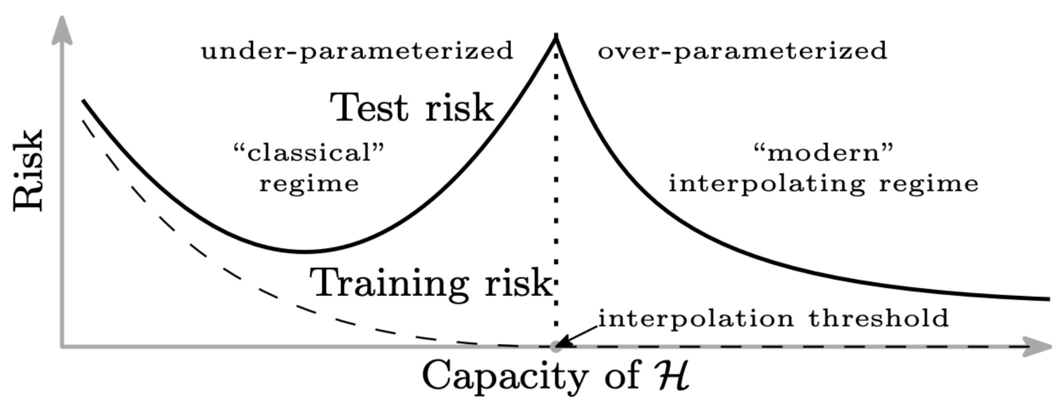
Recall: deep learning seeks **overparameterized** models

$$\min_{\theta \in \mathbb{R}^d} \mathcal{L}(\theta) := \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i))$$

where

$$\underbrace{\#\text{parameters}}_{d} \qquad \gg \qquad \underbrace{\#\text{samples}}_{n}$$

Evidence of **double descent phenomena** (or benign overfitting) in practice and in simple theory models



(Belkin, Hsu, Ma, Mandal '18)

Overparameterization $\implies$ **many** zero-loss solutions

Question: Why do some zero-loss (interpolating) solutions generalize, and others do not?

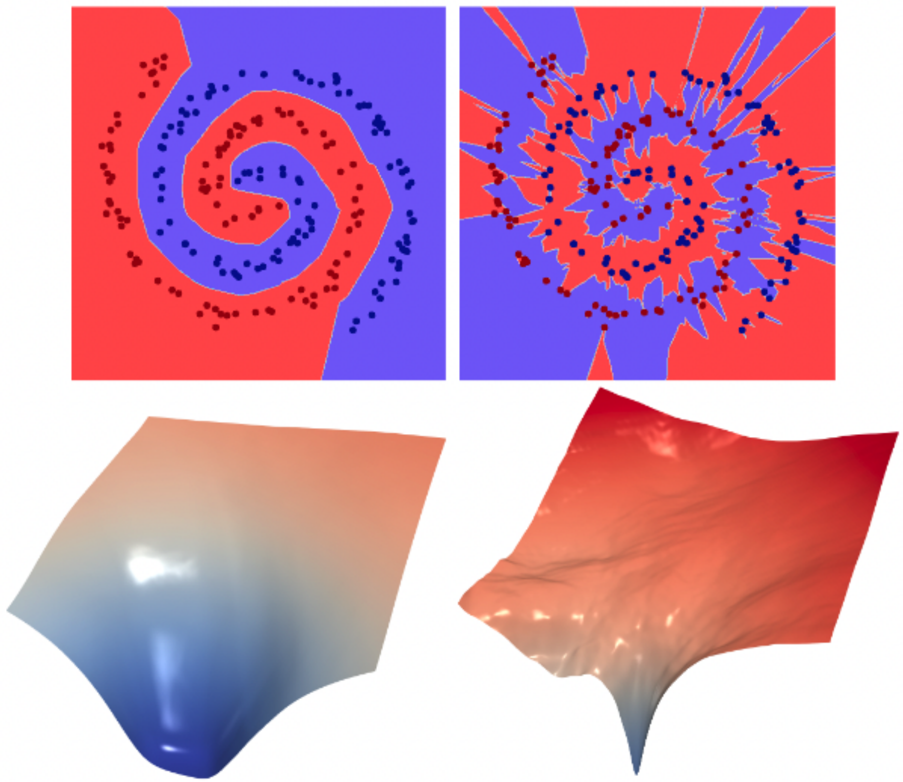
Value of training loss is **not enough**; other properties that predict good generalization?

1. explicit or implicit regularization (training algorithm)
2. **flatness** (loss function + architecture, ℓ and f_θ) $\rightarrow$ **this part**
   algorithm-agnostic, focus on loss landscape $\mathcal{L}(\theta)$

Empirical evidence favoring flatness

(Huang, Emam, Goldblum, Fowl, Terry, Huang, Goldstein '2020)

As seen earlier: Binary classification, with swiss-roll data:



- Classification boundaries (top), training loss landscapes (bottom), 6-layer network: left generalizes well (& more robust), right has perfect train accuracy but *bad generalization*

Can we prove flat minimizers generalize?

For many **over-parametrized low-rank matrix** recovery problems: Yes!

- matrix recovery/sensing
- matrix completion (approximate recovery)
- phase retrieval
- bilinear matrix sensing
- robust PCA
- one-hidden-layer NN with quadratic activation

Flat minima **exactly** recover the ground-truth generative model under standard statistical assumptions, i.e., they generalize (in a strong sense)

Ref: L. Ding, D. Drusvyatskiy, M. Fazel, Z. Harchaoui, *IMA Journal on Information and Inference*, 2024.

“Matrix sensing” problem

Problem: recover matrix $M_\sharp \in \mathbb{R}^{d \times d}$ from $b_i = \langle A_i, M_\sharp \rangle = \mathrm{Tr}$, where

$$\mathcal{A}(X) = (\langle A_1, X \rangle, \langle A_2, X \rangle, \ldots, \langle A_m, X \rangle)$$

and $r_\sharp := \mathrm{rank}(M_\sharp) \ll d$.

Classical approach: (Fazel et al. 01, '02, Recht-Fazel-Parrilo '10)

$$\min_{X \in \mathbb{R}^{d \times d}} \underbrace{\|X\|_*}_{\text{complexity}} \qquad \text{subject to} \qquad \mathcal{A}(X) = b$$

- Explicit nuclear norm regularization: well-understood by now
- Possible to pick **low-complexity solutions** without this regularizer and just via 'flatness'?

Case study in nonconvex matrix sensing

Problem: recover matrix $M_\sharp \in \mathbb{R}^{d\times d}$ from $b = \mathcal{A}(M_\sharp)$, where

$$\mathcal{A}(X) = (\langle A_1, X\rangle, \langle A_2, X\rangle, \ldots, \langle A_m, X\rangle)$$

and $r_\sharp := \mathrm{rank}(M_\sharp) \ll d$.

Rewrite as **over-parametrized low-rank matrix recovery**:
Let $X = LR^T$,

$$\min_{L,R\in\mathbb{R}^{d\times k}} \mathcal{L}(L,R) = \|\mathcal{A}(LR^\top) - b\|_2^2$$

where $b = \mathcal{A}(M_\sharp)$ and

$$k \gg \mathrm{rank}(M_\sharp) := r_\sharp$$

'Learning' interpretation: A two-layer linear network

- (L, R) are the model parameters (layer weights)
- A_i, b_i are the data
- $M_\sharp$ captures the generative model (teacher network)

▶ a prototype for nonconvex learning (Gunasekar et al, '17, Du et al. '18, Li et al. '18, Tian and Du '18)

Flatness measure

(Zero-loss) solution set: $\mathcal{S} = \{(L, R) : \mathcal{A}(LR^\top) = b\}$

Second-order expansion around $(L, R) \in \mathcal{S}$:

$$\mathcal{L}(L+U, R+V) \quad \approx \quad \tfrac{1}{2} D^2\mathcal{L}(L,R)[U,V]$$

Flatness measure: $\operatorname{tr}(D^2\mathcal{L}(L,R))$

An **average measure of curvature**:

$$\operatorname{tr}(D^2\mathcal{L}(L,R)) = \; c \cdot \mathop{\mathbb{E}}_{U,V\sim\mathcal{N}(0,I)} \mathcal{L}(L+U, R+V)$$

Flat (flattest) solutions are the argmin of:

$$\boxed{\min_{L,R\in\mathbb{R}^{d\times k}} \underbrace{\operatorname{tr}(D^2\mathcal{L}(L,R))}_{\text{quadratic}} \qquad \text{subject to} \qquad \underbrace{\mathcal{A}(LR^\top)}_{\text{quadratic}} = b}$$

Warm-up: $\mathcal{A} = \mathcal{I}$

$$\min_{L,R\in\mathbb{R}^{d\times k}} \mathcal{L}(L,R) = \|LR^\top - M_\sharp\|_F^2$$

Second-order expansion around $(L,R)\in\mathcal{S}$:

$$D^2\mathcal{L}(L,R)[U,V] = 4\langle \underbrace{LR^\top - M_\sharp}_{=0}, UV^\top\rangle + 2\|LV^\top + UR\|_F^2$$

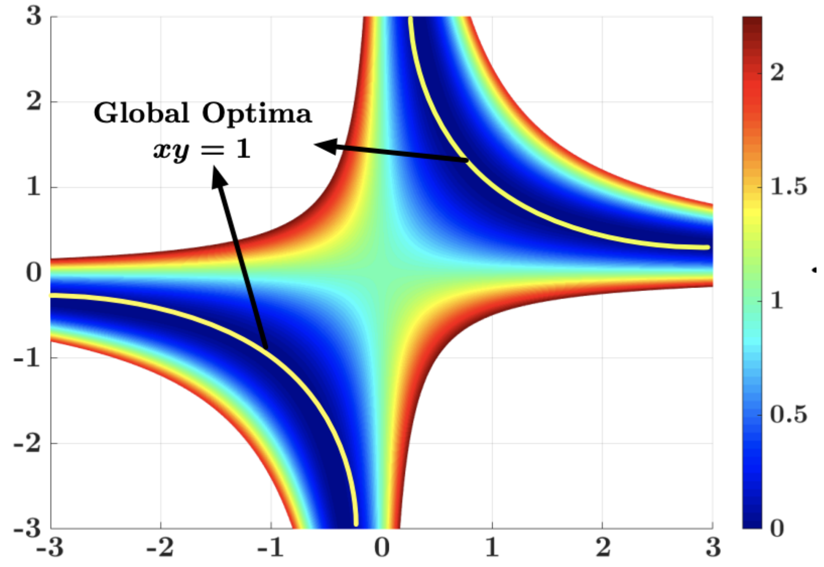


Figure: $l(x,y) = (xy-1)^2$. (1,1), (-1,-1) are flat solutions.

(we prove when $\mathcal{A} = \mathcal{I}$, flat is equivalent to "norm minimal" and "balanced")

Back to $\mathcal{A} \neq \mathcal{I}$

Goal: (Exact recovery)

Show that under standard statistical assumptions (on measurement map $\mathcal{A}$, i.e., randomness of data A_i) flat solutions $(L, R) \in \mathcal{S}$ satisfy $LR^\top = M_\sharp$.

Strategy: Show that $M_\sharp$ is the **unique solution** of the following convex relaxation of flatness maximization:

$$\min_{X \in \mathbb{R}^{d \times d}} \quad \|D_1 X D_2\|_* \qquad \text{subject to} \qquad \mathcal{A}(X) = b$$

where D_1 and D_2 are data-dependent weights, hence both objective and constraints are **data-dependent**.

Matrix sensing

Random data/measurements:

$$\mathcal{A}(X) = (\mathrm{tr}(A_1 X), \mathrm{tr}(A_2 X), \ldots, \mathrm{tr}(A_m X))$$

- Gaussian ensemble: A_i are i.i.d standard Gaussian (also holds for many more cases via matrix Restricted Isometry Property) (Recht-Fazel-Parrilo '10)

Theorem (Matrix sensing)

When $m \gtrsim r_\sharp d$, with probability at least $1 - e^{-\Omega(m)}$, any flat solution (L_f, R_f) satisfies

$$L_f R_f^\top = M_\sharp.$$

Moreover, for any $\delta > 0$ w.h.p. we have

$$\|L_f\|_F^2 + \|R_f\|_F^2 \le (1+\delta)\|M_\sharp\|_* \qquad \text{[Norm-minimal]}$$

$$\|L_f^\top L_f - R_f^\top R_f\|_* \le \delta\|M_\sharp\|_* \qquad \text{[Balanced]}$$

- matches sample complexity for nuclear norm minimization (though not the same solution)
- result extends to **noisy labels** (recovery up to noise level)

Case study: Single hidden-layer NN (quadratic activation)

Problem: (Li-Ma-Zhang '18, Soltanolkotabi et al. '18)

Given data $x \in \mathbb{R}^d$, output $y(x)$ is given by the "teacher" network

$$y(U_\sharp, x) = v^\top q(U_\sharp^\top x)$$

- $U_\sharp$ is $d \times r_\sharp$; $v \in \mathbb{R}^{r_\sharp}$ has r_1 positive and r_2 negative entries
- $q(s) = s^2$ applied coordinate-wise

Prediction $\hat{y}$ of the "student" NN on x can be expressed as

$$\hat{y}(U, x) = u^\top q(U^\top x)$$

with a fixed u, so problem simplifies to seeking U.

Overparameterized problem:

$$\min_{U \in \mathbb{R}^{d \times k}} \mathcal{L}(U) := \frac{1}{n} \sum_{i=1}^{n} (\hat{y}(U, x_i) - y_i)^2$$

Flatness: $U_f \in \mathcal{S}$ is **flat** if it solves the problem

$$\min_{U \in \mathcal{S}} \operatorname{tr}(D^2 \mathcal{L}(U)).$$

Exact recovery

Lemma (Reduction to matrix sensing): We can reformulate the loss as

$$\mathcal{L}([U_1, U_2]) = \frac{1}{n}\|\mathcal{A}(U_1U_1^\top - U_2U_2^\top - M_\sharp)\|_2^2,$$

where $A_i = x_i x_i^\top$ and $M_\sharp = U_\sharp \mathrm{diag}(v) U_\sharp^\top$.

Theorem (Exact recovery)

When $m \gtrsim r_\sharp d$, with probability at least $1 - e^{-\Omega(d)}$, any flat solution U_f recovers the teacher model $U_\sharp$.

Summary & take-away

- For a family of overparameterized nonconvex problems, flat minima do generalize!
- Relation to other properties: norm minimality ("weight decay"), balancedness
- Ideas from *compressed sensing, low-rank recovery* are useful
- Some implications:
  - regularization: (approximate) Hessian trace can serve as a good regularizer
  - algorithmic: a theoretical basis for methods that bias iterates towards flat solutions

Remainder of this tutorial

1. Flat minima **exactly recover** weights in Matrix Sensing and 2-layer Neural Nets (Maryam)

2. Does **flatness imply generalization** in 2-layer ReLU Neural Networks? (Yu-Xiang)

3. Discussion and Open problems. (Yu-Xiang and Maryam)

So far, we considered “exact recovery” and “stable recovery” by flat minima.

- Can we weaken the data assumptions?
  - No assumption on the labeling function

- What can we say about other points GD discovers?
  - No interpolation. Not even local minima, e.g., early stopping.

- Can we obtain results for more realistic neural networks?
  - ReLU activation? Training all weights.

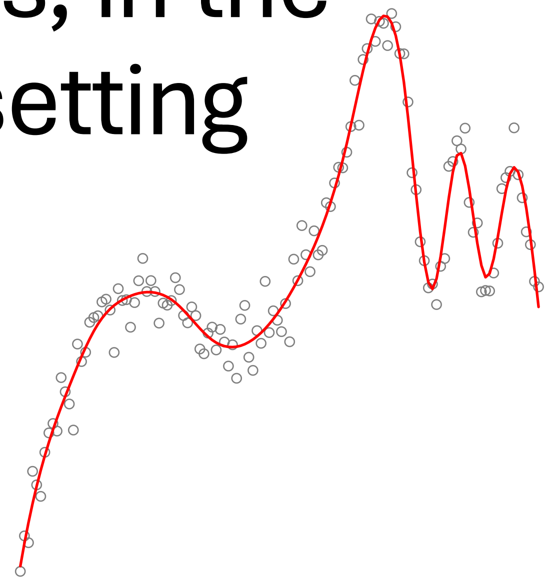
Problem setup: statistical theory of ML

- Data $(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$
- A family of models $\mathcal{F}$ parameter space Θ
- Each element $f_\theta : \mathcal{X} \to \mathcal{Y}$
- Loss function $\ell : (\mathcal{X} \times \mathcal{Y}) \times \mathcal{F} \to \mathbb{R}$
- Training: try to minimize the loss on training data

How do we measure generalization?

- Loss function ℓ
- Train loss (empirical risk): $\frac{1}{\mathrm{n}}\sum_i \ell(train\_data_i, f)$
- Test loss (aka risk): $\mathbb{E}_{data\sim P}[\ell(data, f)]$
- **Generalization Gap = |Training Loss - Test Loss|**
  - Useful when we do not make strong assumptions about the data.

In the case of the square loss, in the non-parametric regression setting



- If $\boldsymbol{y_i = f_0(x_i) + N(0, \sigma^2)}$

- Then:

$$\mathrm{MSE}(f) \coloneqq \mathbb{E}\left[\left(f(x) - f_0(x)\right)^2\right]$$

$$= \underbrace{\mathbb{E}[(f(x) - y)^2] - \overbrace{\mathbb{E}[(f_0(x) - y)^2]}^{\sigma^2}}_{\text{“Excess Risk”, aka “Regret”}}$$

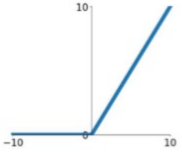
$$\leq TrainLoss(f) \; - \sigma^2 + Gen.Gap(f)$$

We consider two-Layer ***overparameterized*** *ReLU*-Neural Networks

$$\mathcal{F} = \left\{ f : \mathbb{R} \to \mathbb{R} \;\middle|\; f(x) = \sum_{i=1}^{k} w_i^{(2)} \phi\left(w_i^{(1)} x + b_i^{(1)}\right) + b^{(2)} \right\}$$

- ReLU activation

ReLU
$\max(0, x)$



- Square loss

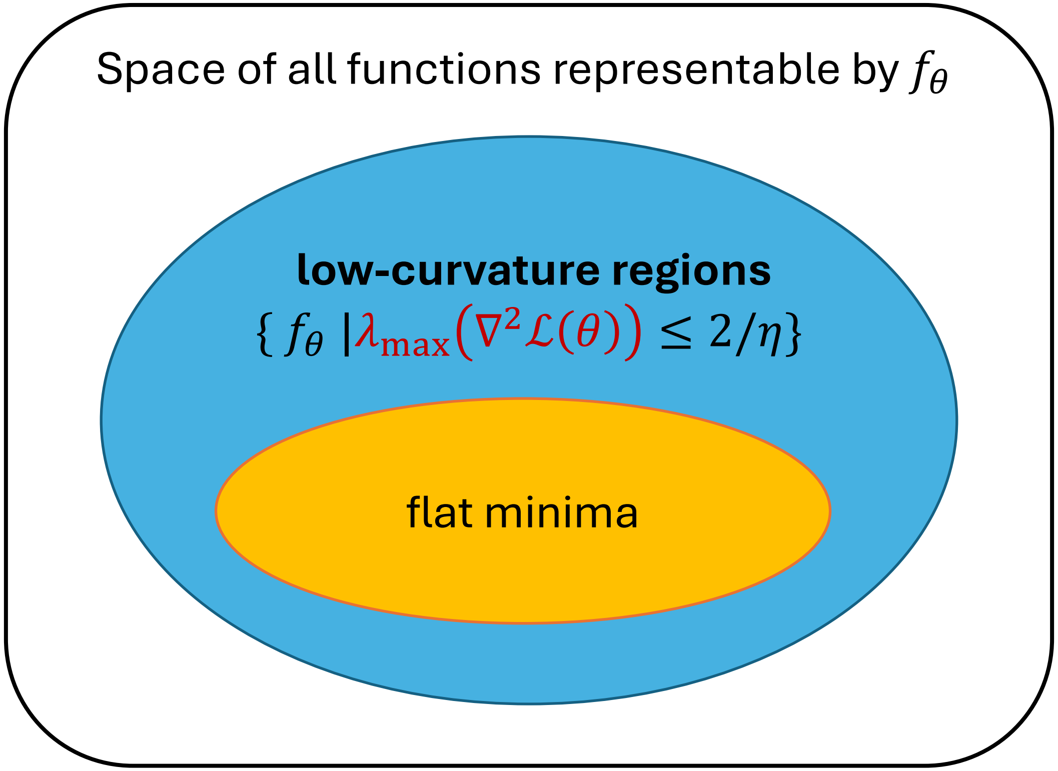
$$\mathcal{L}(\theta) = \frac{1}{2n} \sum_{i=1}^{n} (f_\theta(x_i) - y_i)^2$$

- Let's train with gradient descent with no regularization.

$$\theta_{t+1} = \theta_t - \eta \nabla \mathcal{L}(\theta_t), \; t \geq 0,$$

Stepsize (aka learning rate) parameter

Recall that GD finds points in low-curvature region: $\{f_\theta | \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \leq 2/\eta\}$

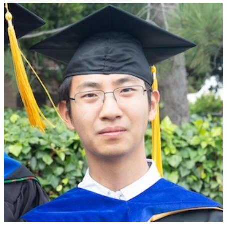


We will study the generalization of the whole class via **Uniform Convergence.**

Note: The set is data-dependent, since $\mathcal{L}$ depends on training data.

Our plan is to focus on the following work.

- Univariate-input + Square loss
  - Qiao, Zhang, Singh, Soudry, Wang. (2024) **Stable Minima Cannot Overfit in Univariate ReLU Networks: Generalization by Large Step Sizes**: https://arxiv.org/abs/2406.06838

- (If time permit) more general cases
  - Logistic loss: (Qiao et al. 2025)
  - High-dimension: (Liang et al. 2025a)
  - Adaptation and data-geometry: (Liang et al. 2025b)

What does class look like? **A Weighted TV1** class.

$$\left\{f_\theta \middle| \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \leq 2/\eta\right\}$$

$$\subseteq$$

$$\left\{f \,\middle|\, \int |f''(x)| g(x) dx \leq C\right\} =: \mathrm{TV}_g^{(1)}(C)$$

where $C = 2/\eta + \tilde{O}(1)$

Mulayoff, Rotem, Tomer Michaeli, and Daniel Soudry. "The implicit bias of minima stability: A view from function space." *NeurIPS'2021*

Qiao et al. (2024) Stable Minima Cannot Overfit in Univariate ReLU Networks: Generalization by Large Step Sizes. NeurIPS'2024

Flatness of Loss (in parameter space) implies a TV-type constraint (in function space)

Theorem (Qiao, Zhang, Singh, Soudry and W., 2024): Let f be any function represented by a ReLU activated two-layer NN f_θ. Let $\mathcal{L}(\theta)$ be the square (training) loss.

$$\int_{-x_{\max}}^{x_{\max}} |f''(x)| g(x) dx \leq \frac{\lambda_{\max}(\nabla^2_\theta \mathcal{L}(\theta))}{2} - \frac{1}{2} + x_{\max}\sqrt{2\mathcal{L}(\theta)},$$

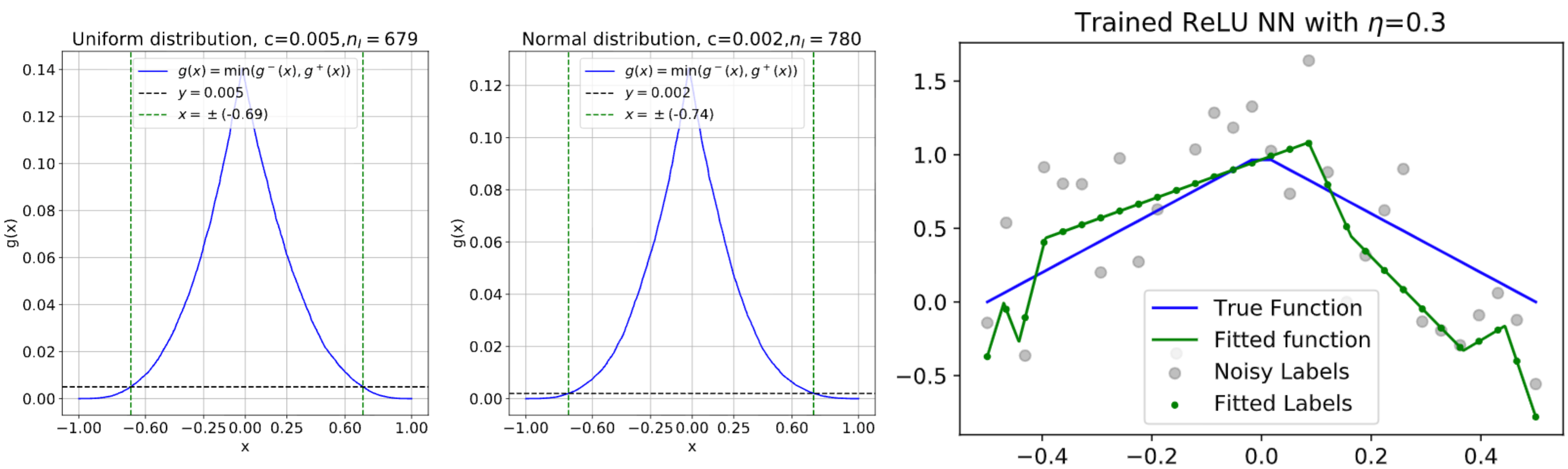
Assume data is coming from $\boldsymbol{y_i = f_0(x_i) + noise}$, then w.h.p.

$$\int_{-x_{\max}}^{x_{\max}} |f''(x)| g(x) dx \leq \frac{\lambda_{\max}(\nabla^2_\theta \mathcal{L}(\theta))}{2} - \frac{1}{2} + \widetilde{O}\left(\sigma x_{\max} \cdot \min\left\{1, \sqrt{\frac{k}{n}}\right\}\right) + x_{\max}\sqrt{\mathrm{MSE}(f)}.$$

- Tune learning rate => select smoothness of f
- Smoothness of f => Generalization bounds

The weighting function g(x) depends only on the distribution of x.

$$\int_{-x_{\max}}^{x_{\max}} |f''(x)| \boxed{g(x)} dx \leq \frac{\lambda_{\max}(\nabla_\theta^2 \mathcal{L}(\theta))}{2} - \frac{1}{2} + x_{\max}\sqrt{2\mathcal{L}(\theta)},$$



The implicit regularization is **stronger in the interior** of the data distribution…
Nearly no regularization towards the boundaries.

Interpolating solutions must have high curvature (must be sharp)

- Theorem from the previous slide

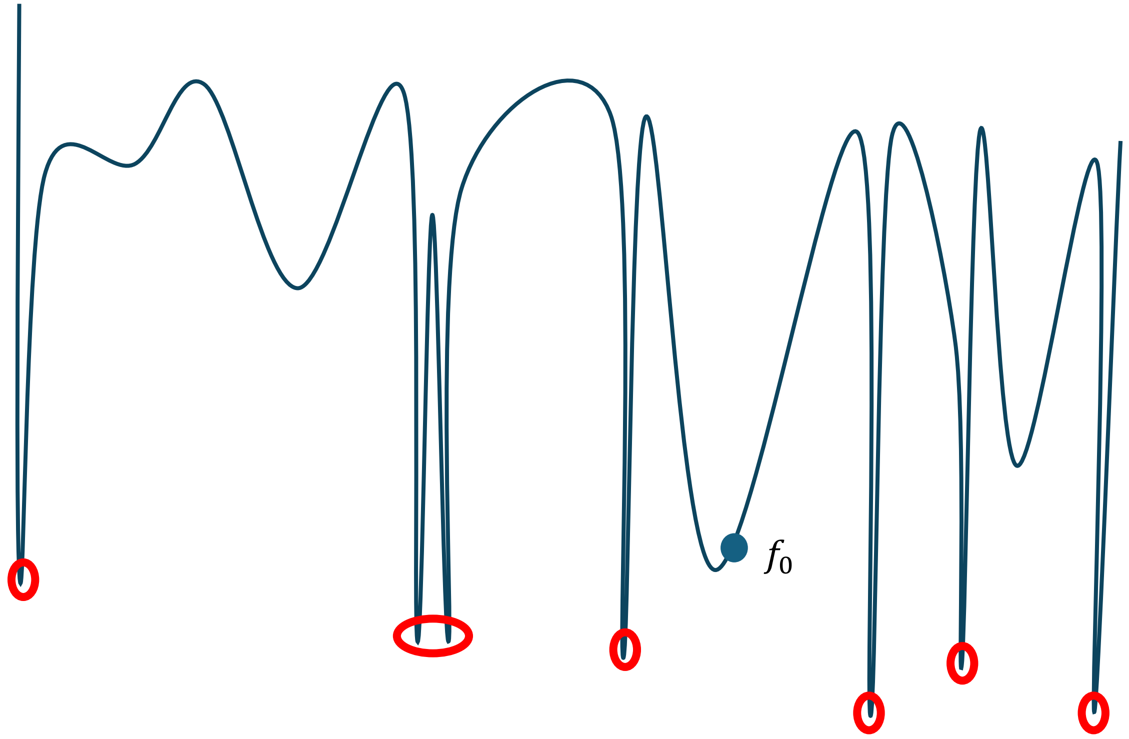
$$\int_{-x_{\max}}^{x_{\max}} |f''(x)| g(x) dx \leq \frac{\lambda_{\max}(\nabla_\theta^2 \mathcal{L}(\theta))}{2} - \frac{1}{2} + x_{\max}\sqrt{2\mathcal{L}(\theta)},$$

- We prove that for any interpolating solution (noise level):

$$\int_{-x_{\max}}^{x_{\max}} |f''(x)| g(x) dx = \Omega\left(\sigma n \left[n - 24 \log\left(\frac{1}{\delta}\right)\right]\right),$$

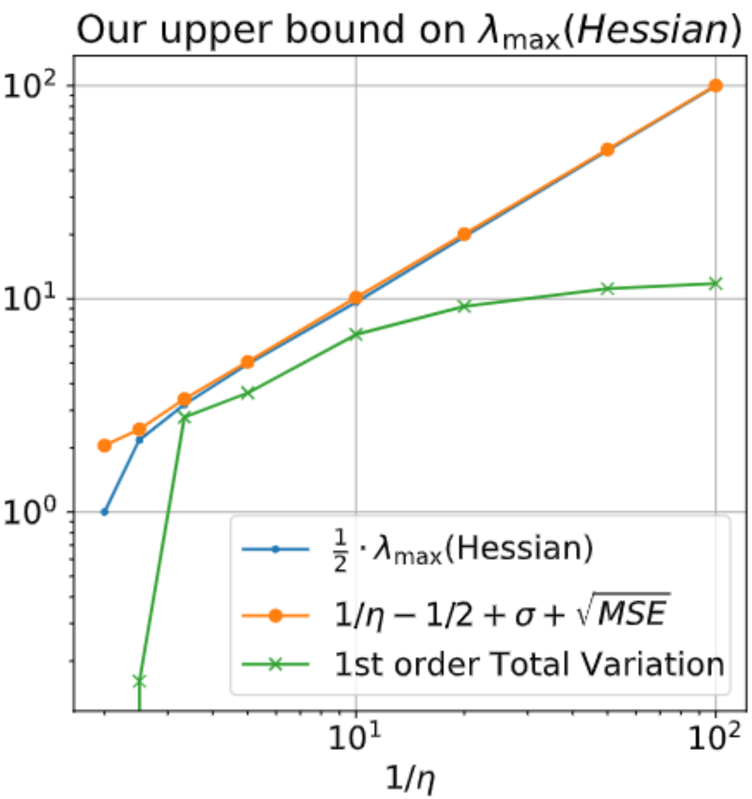
- Implies that stepsize η needs to be extremely small $O\left(\frac{1}{n^2 \sigma}\right)$ for GD to stably converge to interpolating solutions.

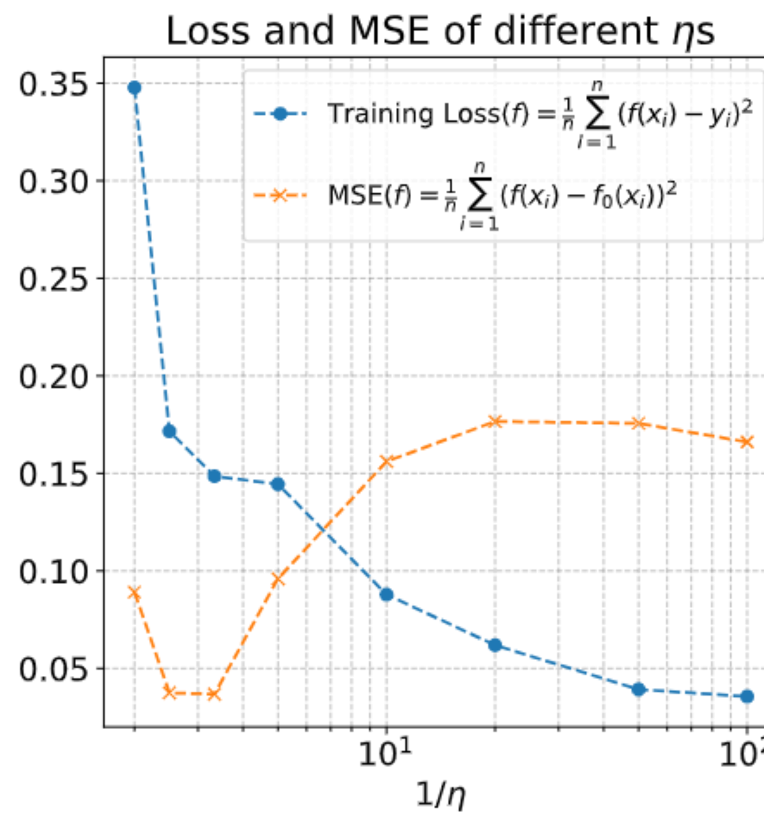
It tells us something new about the energy landscape of overparameterized NN training on noisy problems



Training with GD automatically avoids these sharp and overfitting solutions

Edge-of-Stability appears to hold.
2/η very precisely predicts the sharpness, and gives a classical U-shape risk curve.





Generalization bounds that stem from these function space characterization

Theorem (informal): We proved that in the **strict interior of the data support:**

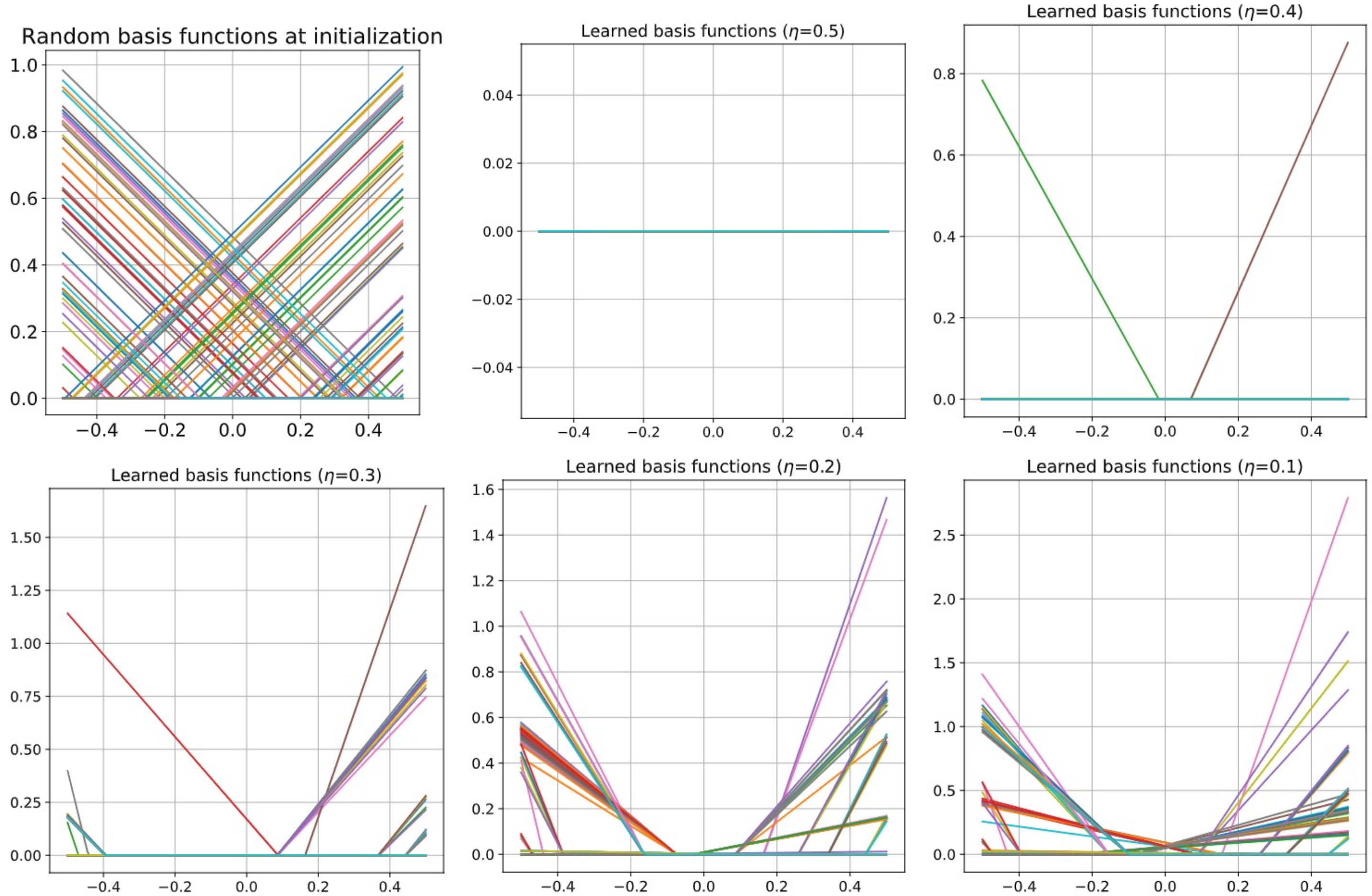
1. Agnostic case: generalization gap = O(n^{-2/5})
2. In the non-parametric regression setting, if training loss smaller than σ^2 then w.h.p., get an MSE

$$\mathrm{MSE}_{\mathcal{I}}(f) = \frac{1}{n_{\mathcal{I}}} \sum_{x_i \in \mathcal{I}} (f(x_i) - f_0(x_i))^2 \leq \widetilde{O}\left(\left(\frac{\sigma^2}{n_{\mathcal{I}}}\right)^{\frac{4}{5}} \left(\frac{x_{\max}}{\eta} + \sigma x_{\max}^2\right)^{\frac{2}{5}}\right)$$

* near minimax optimal (for estimating TV1-functions).

	NN with optimally tuned stepsize	Kernel ridge regression (any RKHS)
MSE	$O(n^{-4/5})$	$\Omega(n^{-3/4})$

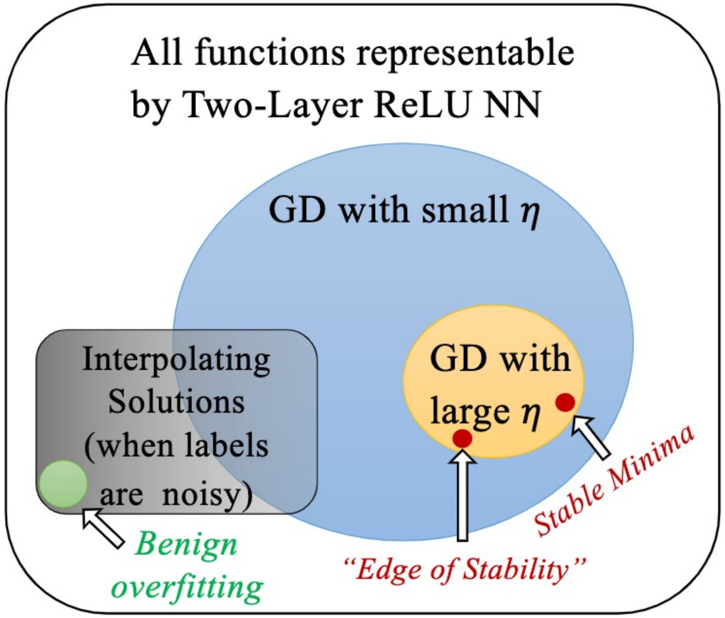
Large-stepsize generalizes better due to extensive "Feature learning": only a few neurons are active!



Checkpoint:

Qiao et al. (2024) **Stable Minima Cannot Overfit in Univariate ReLU Networks: Generalization by Large Step Sizes:**
https://arxiv.org/abs/2406.06838

- In simple "curve fitting" problem, two-layer ReLU NN does not overfit if trained with GD (regardless how overparameterized it is)
- Tuning learning rate choice is connected to an L1-type smoothness that we can quantify.
- Provably stronger than NTK. New insight into representation learning.



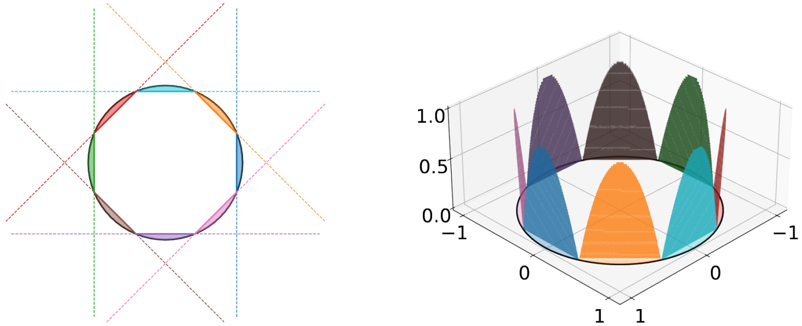
Extension of the theory

Qiao and W. (2025) **Does Flatness imply Generalization for Logistic Loss in Univariate Two-Layer ReLU Network?:** https://arxiv.org/abs/2512.01473

$\{ f_\theta \mid \lambda_{\max}\left(\nabla^2 \mathcal{L}(\theta)\right) \le 2/\eta \}$ insufficient for generalization.

$\{ f_\theta \mid \lambda_{\max}\left(\nabla^2 \mathcal{L}(\theta)\right) \le \frac{2}{\eta},\ \boldsymbol{\|\theta\| = o(n)} \}$ works.

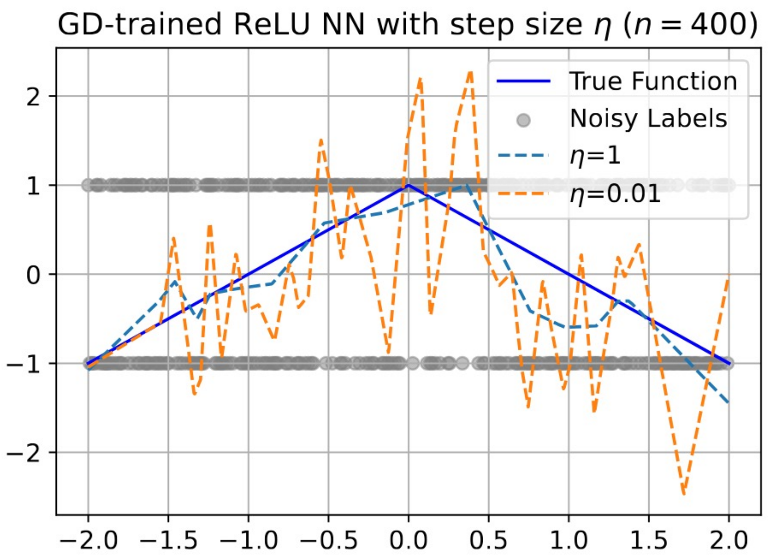
Liang, Qiao, W. and Parhi (2025) **Stable Minima of ReLU Neural Networks Suffer from the Curse of Dimensionality: The Neural Shattering Phenomenon**:
https://arxiv.org/abs/2506.20779
(NeurIPS 2025 Spotlight)



Liang, Cloninger, Parhi and W. (2025) **Generalization Below the Edge of Stability: The Role of Data Geometry**: https://arxiv.org/abs/2506.20779

Does Flatness imply Generalization for **Logistic Loss** in Univariate Two-Layer ReLU Network?

- Empirically, kinda yes.
- Data: y ~ Bernoulli(Sigmoid(f_0(x))



But we can no longer talk about the set of all flat solutions.

$$\left\{ f_\theta \middle| \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \leq 2/\eta \right\}$$

$$\subseteq$$

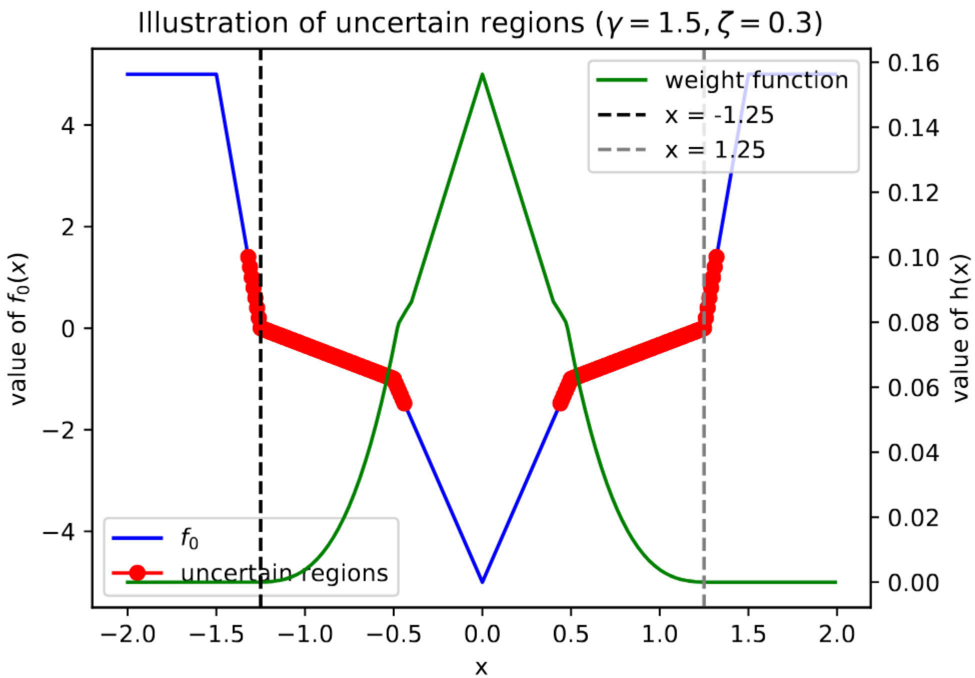
$$\left\{ f \middle| \int |f''(x)| g(x) dx \leq \frac{2}{\eta} \right\}$$

But the weighting function g now depends on f!

Qiao and W. (2025) "Does Flatness imply Generalization for Logistic Loss in Univariate Two-Layer ReLU Network?" New manuscript.

The weighting function now depends on the uncertainty region of the current NN configuration.

$$\left\{ f \,\middle|\, \int |f''(x)| g(x) dx \leq \frac{2}{\eta} \right\}$$



What's worse, we can construct a solution that is

1. interpolating

2. arbitrarily flat loss

"flat" when simple and generalizing

But also "flat" if you are **confidently interpolating** training data.

$\{ f_\theta \mid \lambda_{\max}(\nabla^2 \mathcal{L}(\theta)) \leq 2/\eta \}$ **insufficient** for generalization.

Why does it still generalize in the non-parametric classification setting?

- Assumption: y ~ Bernoulli(Sigmoid(f_0(x))
  - f_0 is bounded.

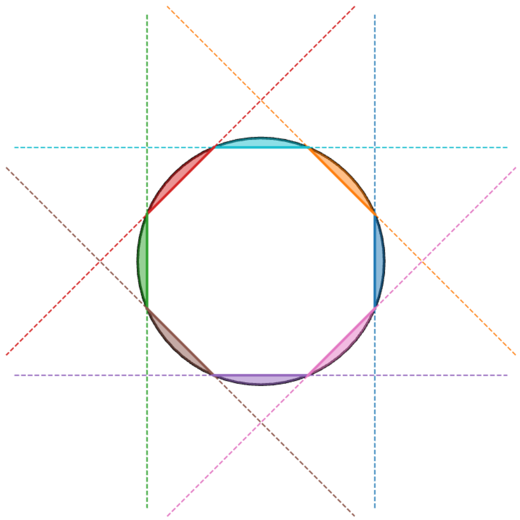
(Informal) Claim: within the convex hull of the uncertain region of f_0, near ***optimal excess risk*** for an "optimized" $f \in \{ f_\theta \mid \lambda_{\max}\left(\nabla^2 \mathcal{L}(\theta)\right) \leq \frac{2}{\eta},\ \|\boldsymbol{\theta}\| = \boldsymbol{o}(\boldsymbol{n})\}$

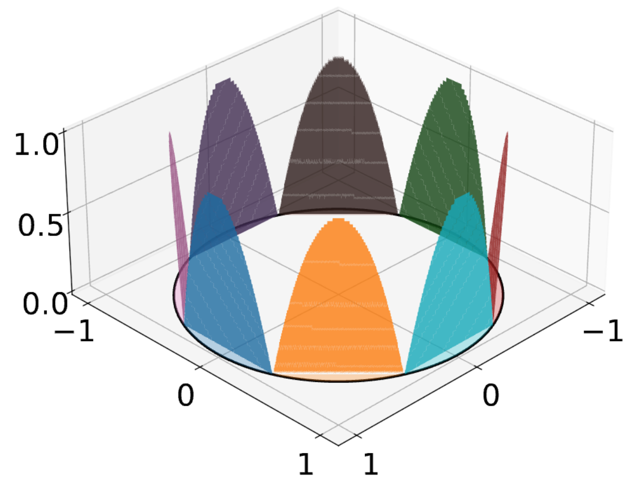
Weak-generalization by weight decay → Strong **(near-optimal) generalization** by large-stepsize

Qiao and W. (2025) **Does Flatness imply Generalization for Logistic Loss in Univariate Two-Layer ReLU Network?**

How about the multivariate case? It works, but suffers from the curse of dimensionality.

- Lower bound reveals a **Neural Shattering Phenomenon:** *It's very easy for each neuron to single out one data point at boundary.*

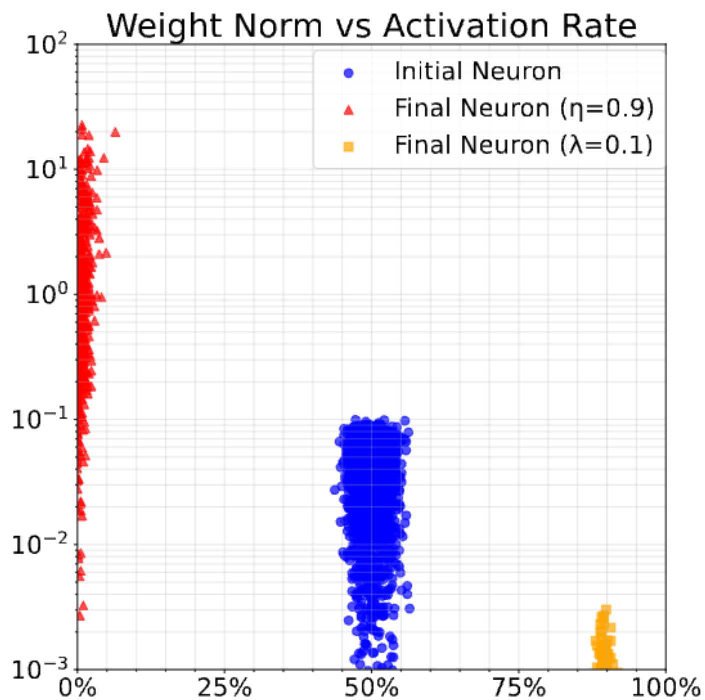




Liang, T., Qiao, D., Wang, Y. X., & Parhi, R. (2025). Stable Minima of ReLU Neural Networks Suffer from the Curse of Dimensionality: The Neural Shattering Phenomenon. *NeurIPS'25*.

Neural Shattering does not happen if there is **weight decay** or if we **remove “bias”** parameter from MLP

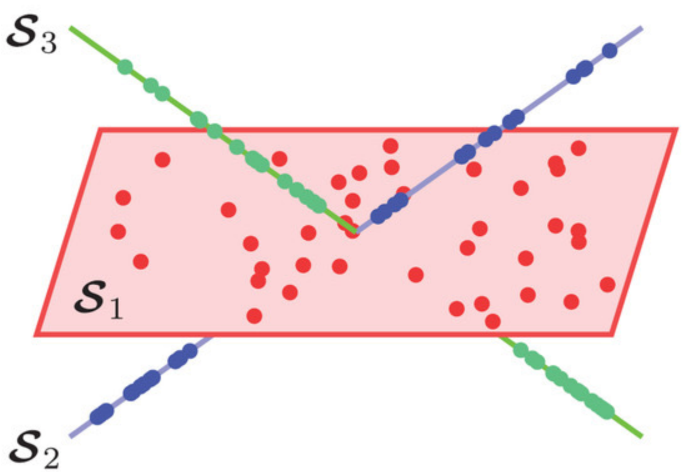
Weights $|w_i^{(1)} w_i^{(2)}|$

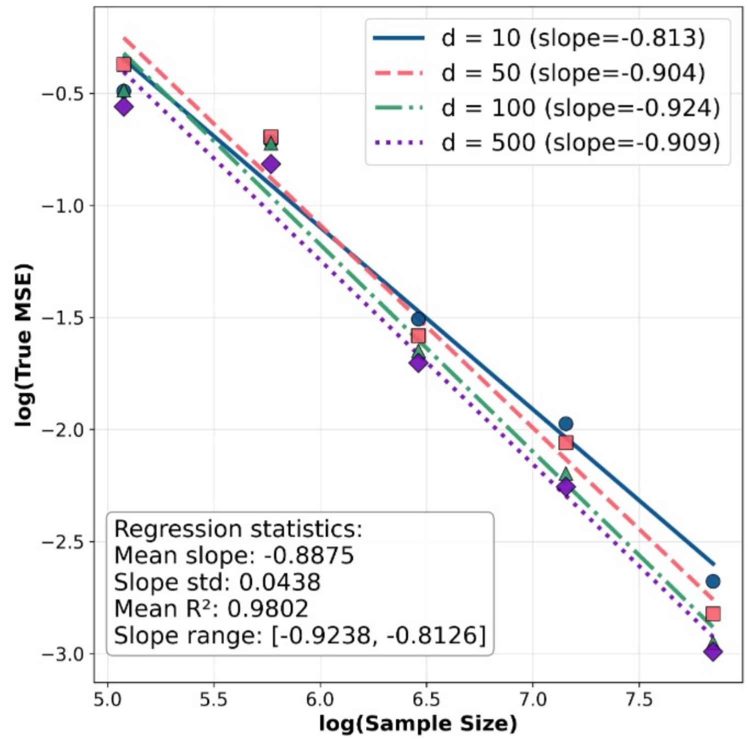


Percentage of training data where a neuron is active

What happens if the input data is secretly low-dimensional (embedded in a high-dim ambient space)

- Assumption: data comes from a union of low-dim subspaces

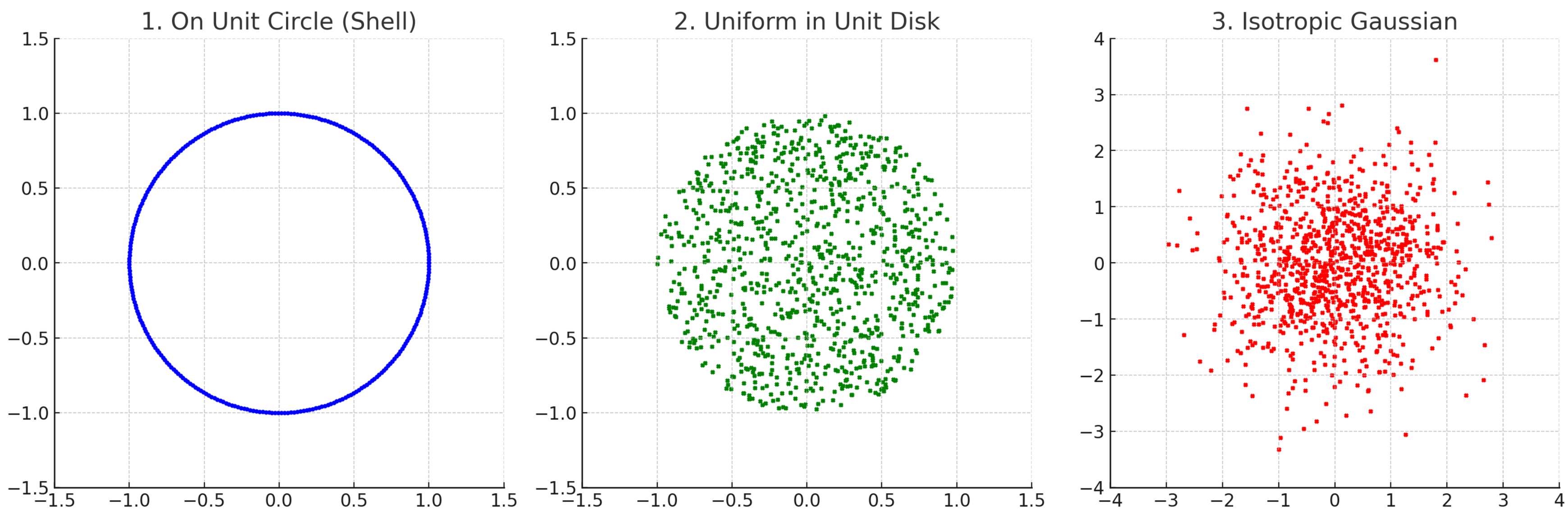




(a) Adaptation to intrinsic dimension

Liang et al (2025) **Generalization Below the Edge of Stability: The Role of Data Geometry.**
https://arxiv.org/abs/2510.18120

The shape of data distribution matters in flatness induced generalization



Cannot generalize at all

Generalize but suffer from Curse-of-Dimensionality

Liang et al (2025) **Generalization Below the Edge of Stability: The Role of Data Geometry.**
https://arxiv.org/abs/2510.18120

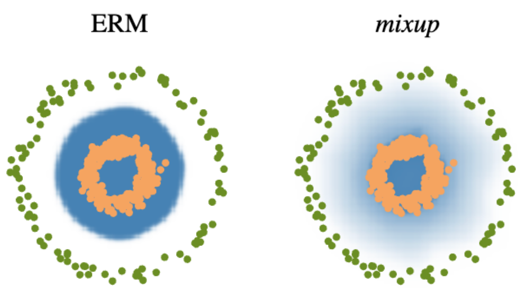
Mixup: a prominent approach for data augmentation.

mixup: BEYOND EMPIRICAL RISK MINIMIZATION

by H Zhang · 2017 · Cited by 13963 — We have proposed **mixup, a data-agnostic and straightforward data augmentation principle**. We have shown that mixup is a form of vicinal risk ...

```
# y1, y2 should be one-hot vectors
for (x1, y1), (x2, y2) in zip(loader1, loader2):
    lam = numpy.random.beta(alpha, alpha)
    x = Variable(lam * x1 + (1. - lam) * x2)
    y = Variable(lam * y1 + (1. - lam) * y2)
    optimizer.zero_grad()
    loss(net(x), y).backward()
    optimizer.step()
```

(a) One epoch of *mixup* training in PyTorch.



(b) Effect of *mixup* ($\alpha = 1$) on a toy problem. Green: Class 0. Orange: Class 1. Blue shading indicates $p(y = 1|x)$.

Figure 1: Illustration of *mixup*, which converges to ERM as $\alpha \to 0$.

Our theory explains “mixup" quite well. But can we do better?

Checkpoint: provable generalization bounds for low-curvature points, but..

- Trickier in high-dimension and beyond square loss.
- Known fixes: Data-augmentation, Weight Decay, Architecture tweaks.
- Many interesting theoretical / empirical directions to explore.

Remainder of this tutorial

1. Flat minima **exactly recover** weights in Matrix Sensing and 2-layer Neural Nets (Maryam)

2. Does **flatness imply generalization** in 2-layer ReLU Neural Networks? (Yu-Xiang)

3. Discussion and Open problems. (Both)

Flat minima / regions in **Multi-layer** Neural networks appears to behave qualitatively different.

- For two-layers networks:
  - Mostly similar to weight decay, give L1-type sparsity (or low nuclear norm)
- For L-layer diagonal linear networks
  - As L → large, weight decay => ||. ||_2/L norm. (sparser!)
  - But flat minima => ||. ||_$\{2-\frac{2}{L}\}$ norm (denser!)

(Lemma 9.2, Ding et al., 2024)

What do we know and what's open?

- L-layer linear (non-diagonal) neural networks
  (Gatmiry et al, NeurIPS'22).
  similar to when L=2, i.e., nuclear-norm.

- What happens with nonlinear activations?

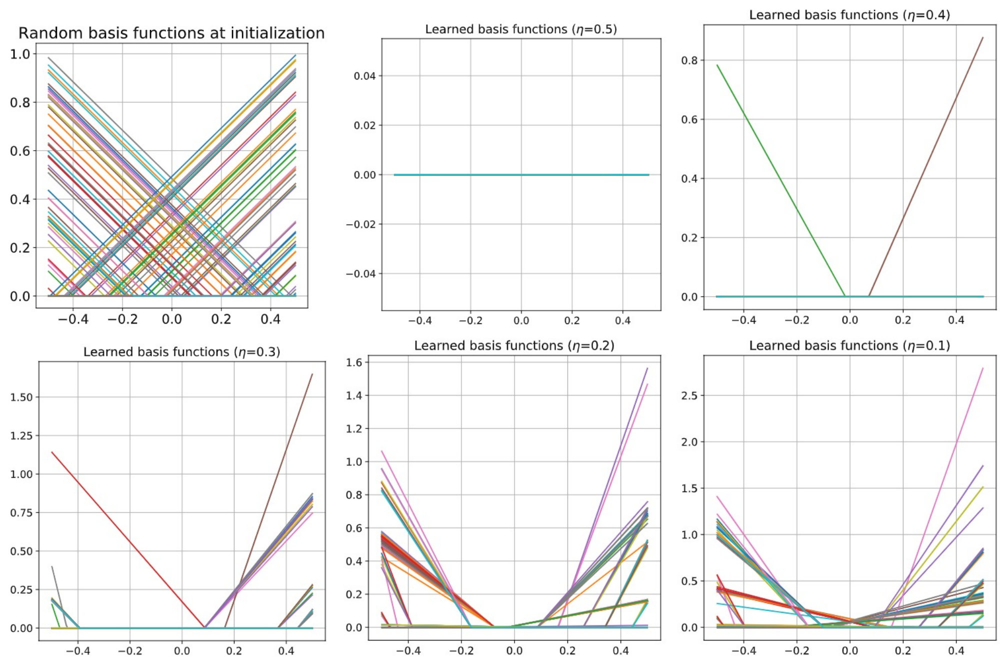
- In between diagonal vs fully-connected weights?
  - Convolutional layers?
  - Block-diagonal weights?

Interaction with architecture choices.

- BERT models have biases
- GPT models do not use biases
- Provably better generalization when there is no bias?

The modality of representation learning is quite interesting

- It's pushing neurons out of data support.
- "Dead" neurons will never recover.
- They may be active on OOD data.
  - Culprits of non-robustness



How can we characterize the dynamics?

Thank you for your attention!

Jingfeng Wu
UC Berkeley

Yu-Xiang Wang
UC San Diego

Maryam Fazel
UW

References and other materials on the website:
https://uuujf.github.io/instability/

Supplementary slides

What about depth?

Overparameterized sparse recovery:

$$\min_{v_1,\ldots,v_k \in \mathbb{R}^d} \quad f(v) := \frac{1}{m}\|A(\underbrace{v_1 \odot \cdots \odot v_k}_{x}) - b\|_2^2,$$

where $b = A(x_\sharp)$ and we seek x that's $r_\sharp$-sparse.

Flat $(v_1, \ldots, v_k)$ are those solving:

$$\min_{v_i \in \mathbb{R}^d, i=1,\ldots,k} \operatorname{tr}(D^2 f(v_1, \ldots, v_k)) \quad \text{s.t.} \quad A(v_1 \odot \cdots \odot v_k) = b.$$

Lemma: For Gaussian A, any flat solution $(v_1, \ldots, v_k)$ yields a minimizer $x = v_1 \odot \cdots \odot v_k$ of the problem:

$$\min_{x \in \mathbb{R}^d} \sum_{i=1}^{d} |D_{ii}||x_i|^{2-\frac{2}{k}} \quad \text{s.t.} \quad Ax = b.$$

Conclusion: Exact recovery for $k = 2$ and poor recovery as $k \to \infty$.

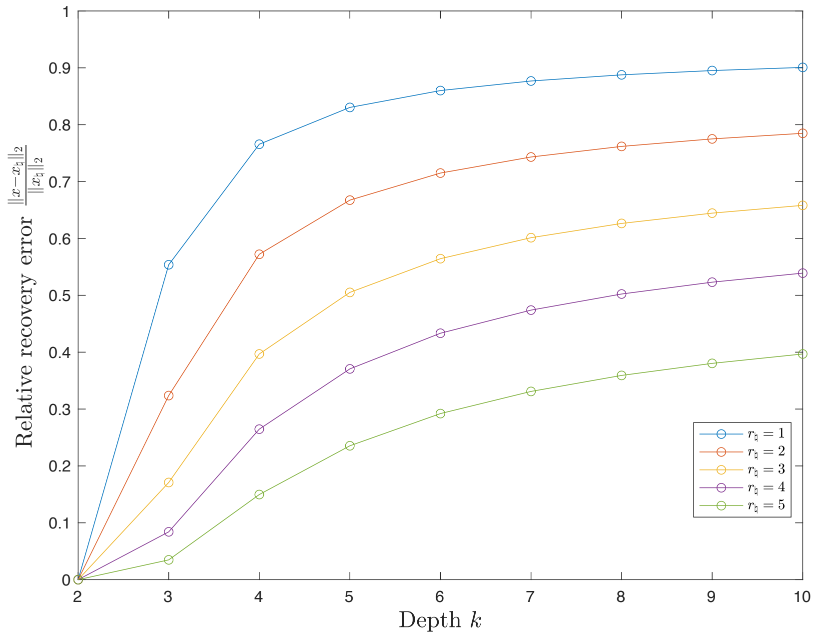


Figure: The effect of depth for different choice of sparsity $r_\sharp$

- (Gatmiry et al. Neurips'23) showed approximate recovery bounds for k-layer but **non-diagnonal** linear network
- Theoretical explanation is still open for $k > 2$ for networks with nonlinear activation