SGD with large step sizes learns sparse features (ICML 2023)




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Main theme: *we know that SGD has a strong implicit regularization effect, but what does it imply for the features learned by the model?*

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ELLIS Reading Group on Mathematics of Deep Learning

EPFL

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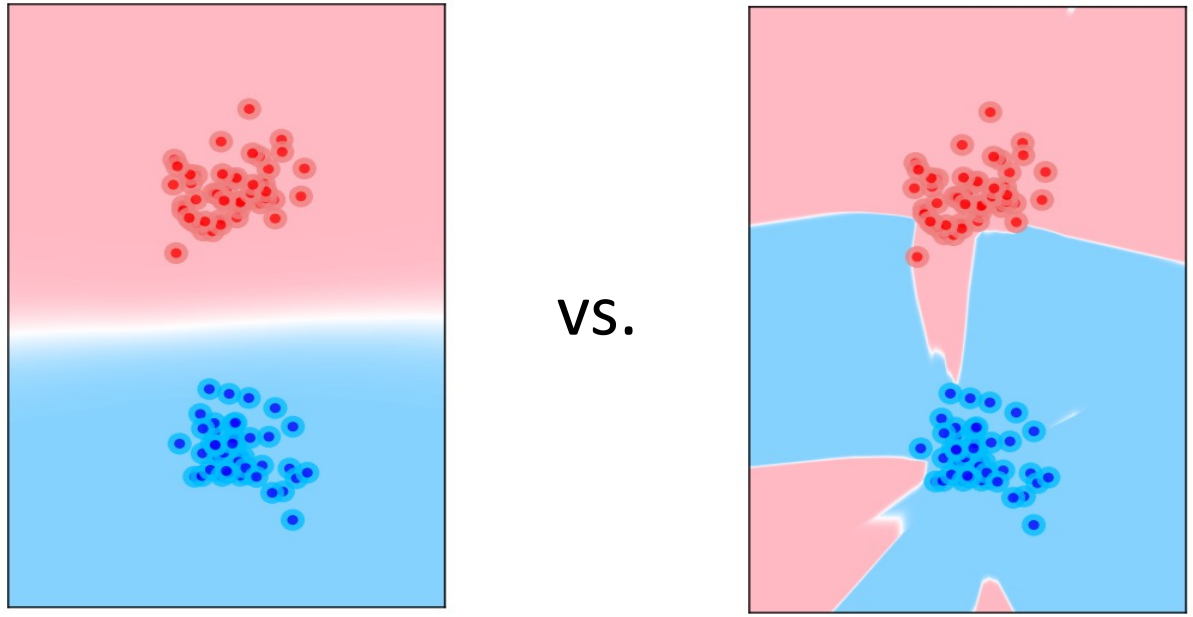
Big picture: understanding the generalization puzzle in *overparametrized* deep learning

- **Underparametrized DL**: training loss / perplexity already correlates very well with generalization! In most cases: we just need to minimize the training loss
- **Overparametrized DL**: different global minima can generalize very differently, so it matters which one we pick (via the opt. algorithm, initialization, regularization, etc)



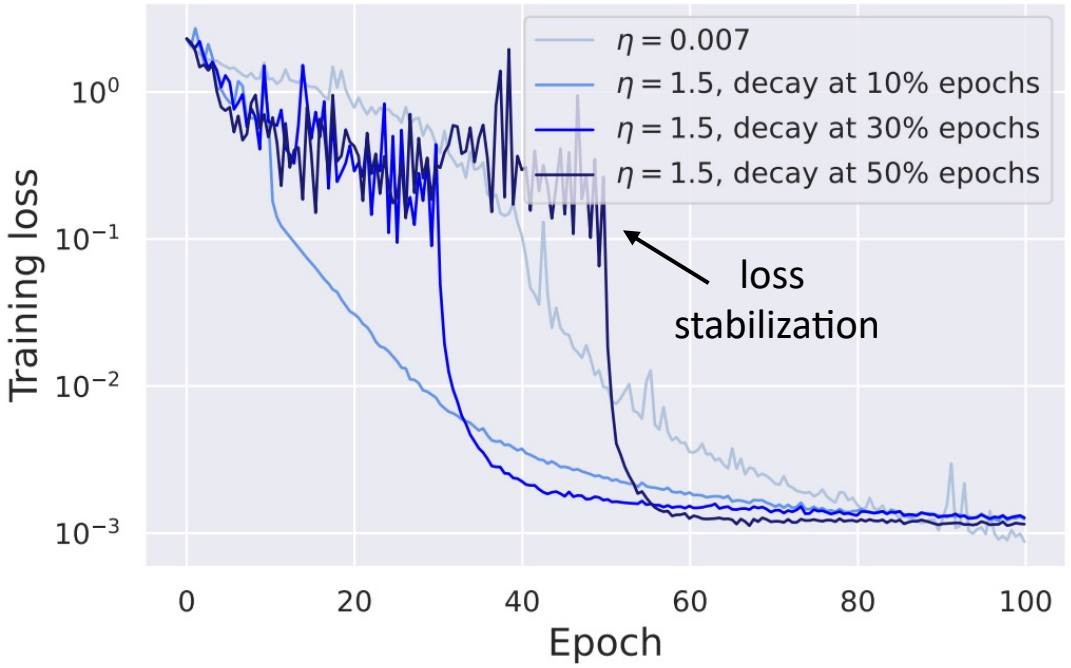
vs.

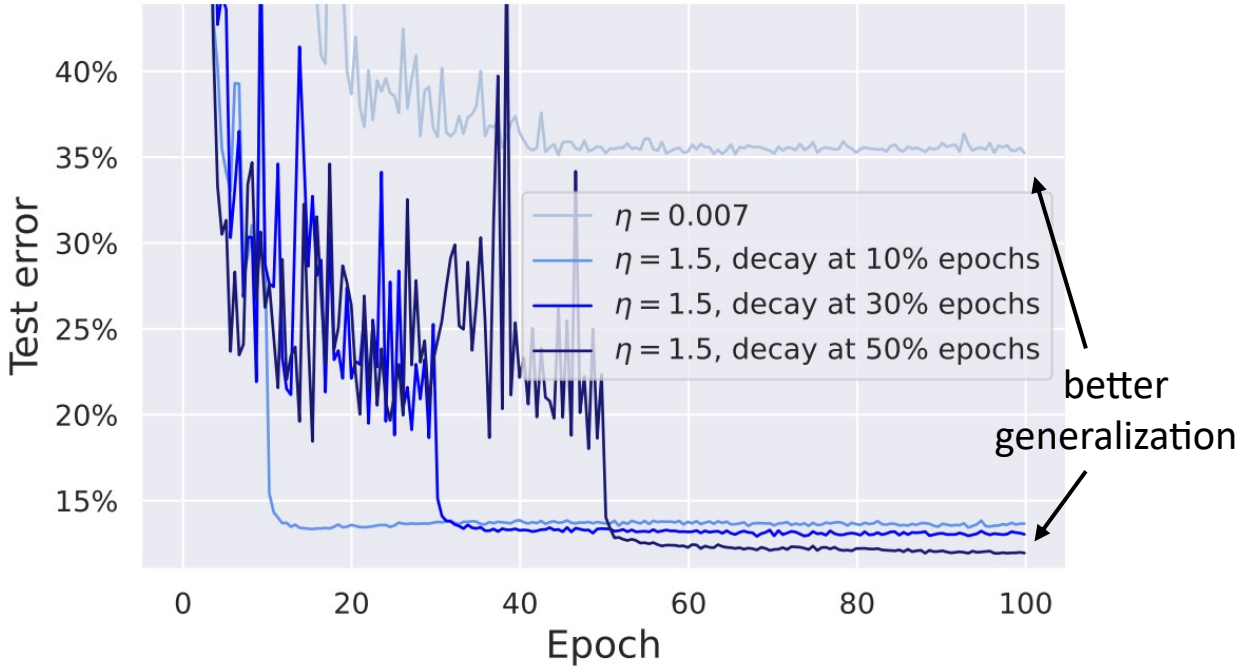
"*Bad Global Minima Exist and SGD Can Reach Them*", NeurIPS'19

Let's start from a known observation

Longer schedules of SGD with large step sizes lead to better generalization

Setting: ResNet-18 on CIFAR-10, standard mini-batch SGD, no data augmentation





This raises multiple questions:

1. Why does the training loss stabilizes?
2. What kind of hidden dynamics is happening in this phase?
3. How is it related to sparsity of the predictor?

A short remark about the paper presented here in June

LOSS LANDSCAPES ARE ALL YOU NEED: NEURAL NETWORK GENERALIZATION CAN BE EXPLAINED WITHOUT THE IMPLICIT BIAS OF GRADIENT DESCENT

Ping-yeh Chiang[1], Renkun Ni[1], David Yu Miller[1,3], Arpit Bansal[1], Jonas Geiping[1], Micah Goldblum[2] & Tom Goldstein[1]

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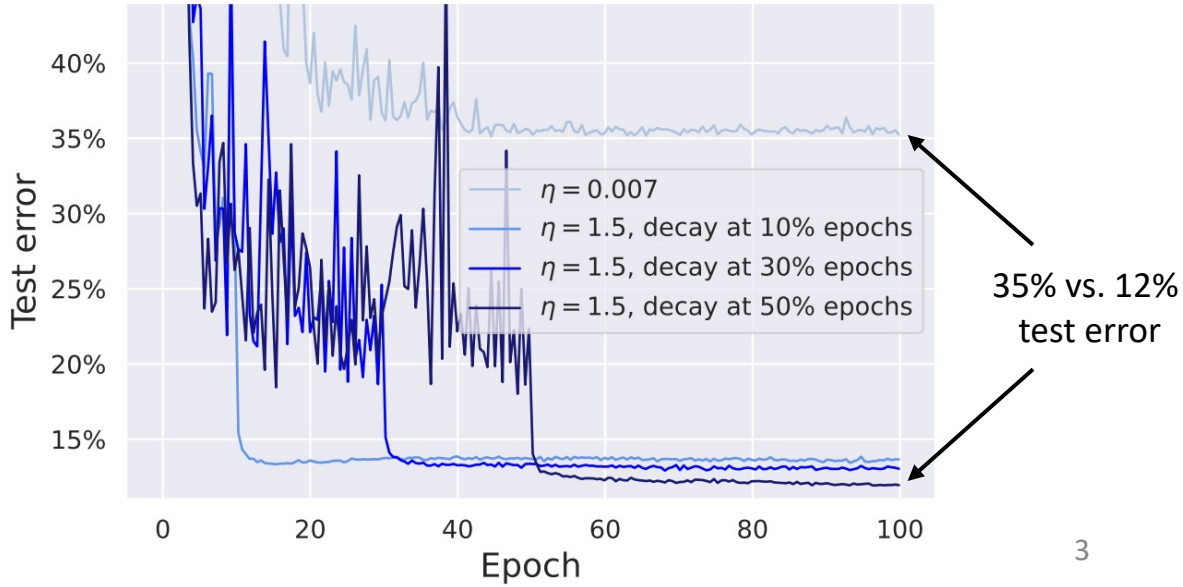
ABSTRACT

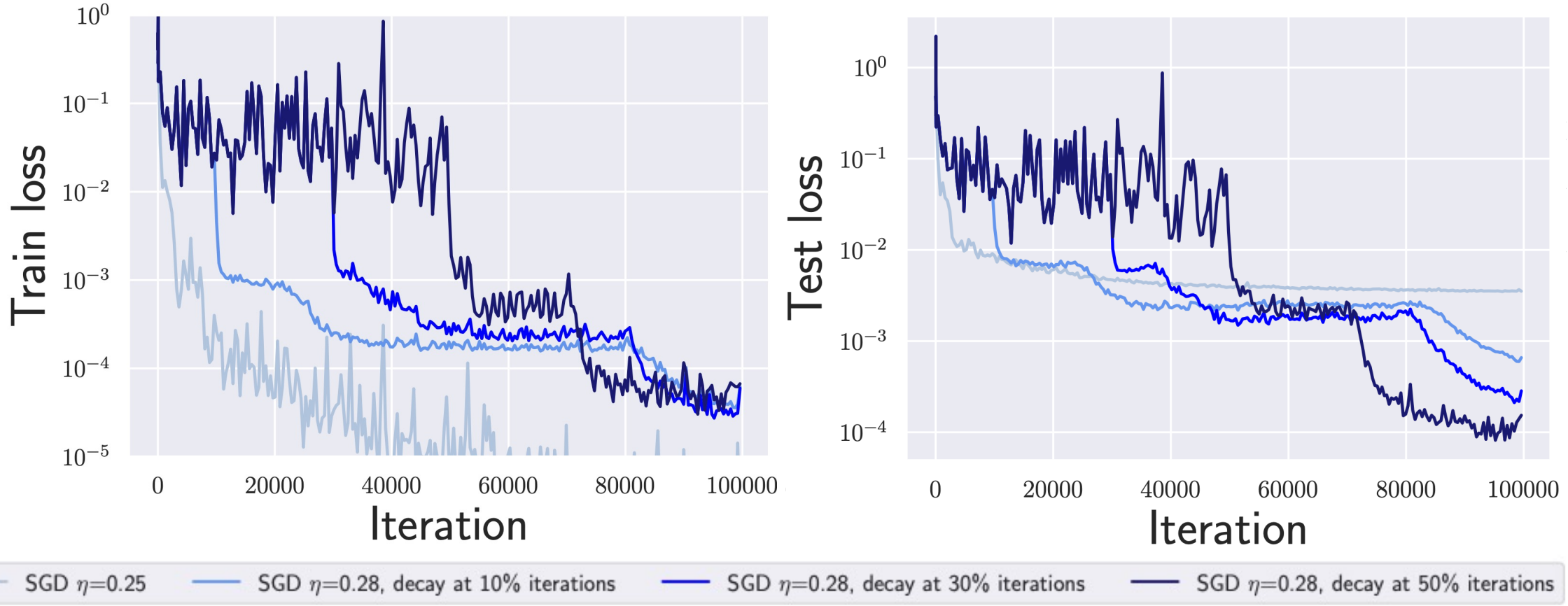
It is commonly believed that the implicit regularization of optimizers is needed for neural networks to generalize in the overparameterized regime. In this paper, we observe experimentally that this implicit regularization behavior is *generic*, i.e. it does not depend strongly on the choice of optimizer. We demonstrate this by training neural networks using several gradient-free optimizers, which do not benefit from properties that are often attributed to gradient-based optimizers. This includes a guess-and-check optimizer that generates uniformly random parameter vectors until finding one that happens to achieve perfect train accuracy, and a zeroth-order Pattern Search optimizer that uses no gradient computations. In the low sample and few-shot regimes, where zeroth order optimizers are most computationally tractable, we find that these non-gradient optimizers achieve test accuracy comparable to SGD. The code to reproduce results can be found at https://github.com/Ping-C/optimizer.

- Quote*: "we observe experimentally that this implicit regularization behavior [of optimizers] is generic, i.e.* ***it does not depend strongly on the choice of optimizer****"*
- Depends on what is "*strongly*"! There is still a consistent difference between SGD with small vs. large step sizes and we want to study that



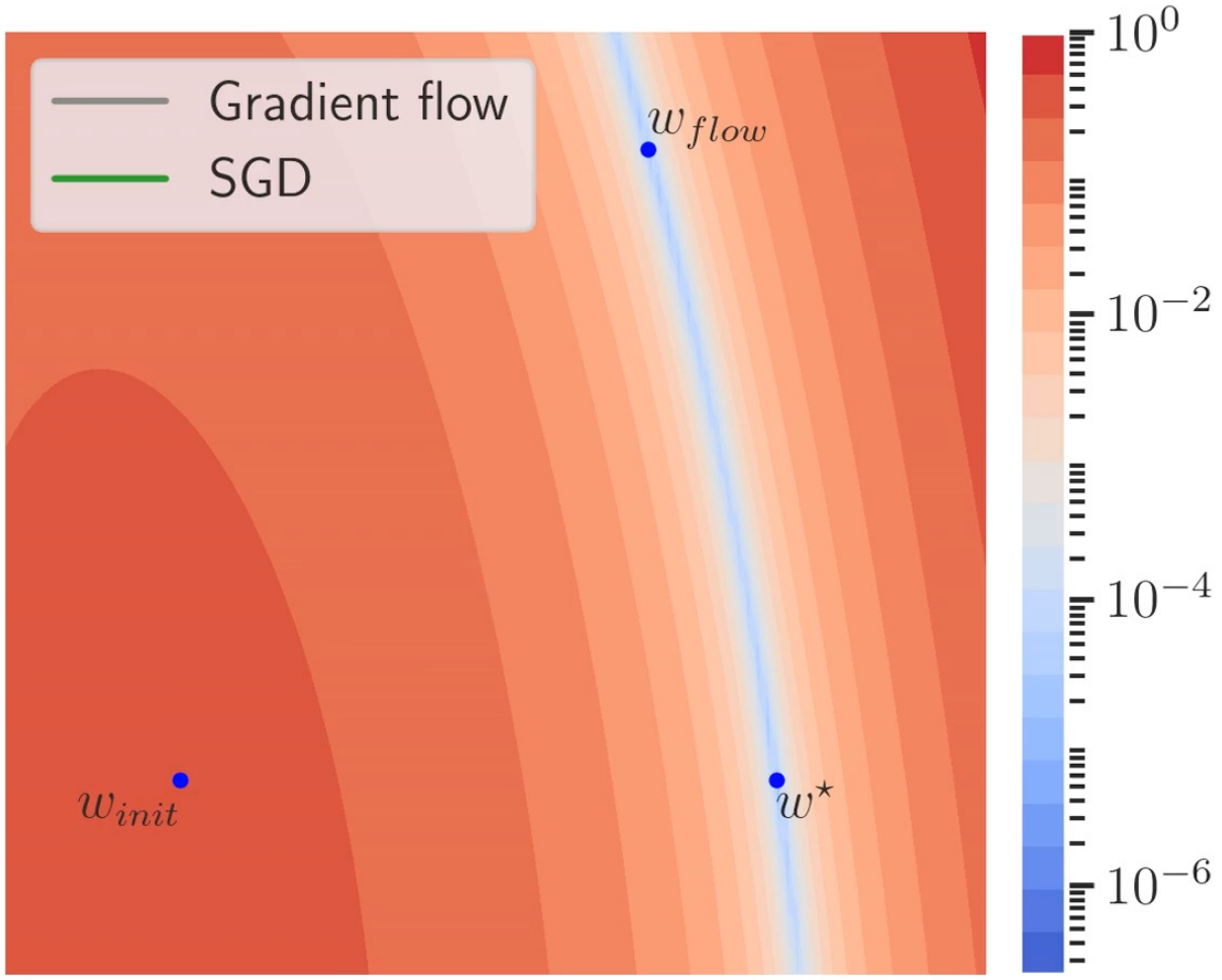
Is this a phenomenon inherent to deep networks? No!

The same observations can be seen even on the **simplest diagonal linear networks** $h(x) = \langle x, u \odot v \rangle$ for a sparse regression problem



⇒ we can try to understand the phenomenon **theoretically** by leveraging prior works on this toy model

How can the training loss stabilize around some level set?



Setting: a 2-D slice of the 60-D training loss surface of a diagonal linear network

General picture:

- Initially, the training loss decreases
- Then, due to the noise, SGD cannot enter the narrow valley and keeps oscillating (⇒ *no convergence but also no divergence*)
- We formalize it in the paper with a proposition that describes how this can occur **provably** for a 1D diagonal linear net
- In addition, it's apparent that SGD slowly moves to a certain direction. **Can we better understand that?**

Modelling SGD with a Stochastic Differential Equation (Part I)

- **Observation:** the noise intensity of SGD is proportional to the training loss
  ⇒ when the loss stabilizes, we can assume **constant noise intensity**
- Thus, we can model the **large step size SGD phase** with the following **constant-noise SDE**:

Constant-noise SDE: $$\mathrm{d}\theta_t = -\nabla_\theta \mathcal{L}(\theta_t)\mathrm{d}t + \sqrt{\eta\delta}\,\underbrace{\phi_{\theta_t}(X)^\top}\,\mathrm{d}B_t$$

- step size: η
- constant noise intensity due to loss stabilization: δ
- the Jacobian of the network: $\underbrace{\phi_{\theta_t}(X)^\top}$, $[\nabla_\theta h_\theta(x_i)^\top]_{i=1}^n \in \mathbb{R}^{n\times p}$
- $\mathrm{d}B_t$: Brownian motion in $\mathbb{R}^n$, i.e., Gaussian noise

- We check empirically that this **SDE fully agrees with SGD** in terms of the generalization improvements and other key metrics (*we'll see these experiments later*)
- This SDE can be seen as the effective **slow dynamics** (due to the gradient + the noise term) that drives the θ_t while they bounce rapidly due to the noise (**fast dynamics**)

Modelling SGD with a Stochastic Differential Equation (Part II)

Constant-noise SDE: $\mathrm{d}\theta_t = -\nabla_\theta \mathcal{L}(\theta_t)\mathrm{d}t + \sqrt{\eta\delta}\,\phi_{\theta_t}(X)^\top \mathrm{d}B_t$

- **Prior works**: for diagonal linear networks, Pillaud-Vivien et al. (COLT 2022) proved the **sparsity of the solution** using a similar SDE derived for **label noise SGD**
- **Our work**: we conjecture that for arbitrary deep networks, a **similar sparsifying effect** is taking place for **standard SGD with large step sizes** (no label noise needed)
  - **Observation**: for the Brownian motion $\mathrm{d}B_t \in \mathbb{R}^n$: $\phi_{\theta_t}(x_i)^\top dB_t = ||\phi_{\theta_t}(x_i)||_2 dW_t$ where $dW_t \in \mathbb{R}$ is a 1D Brownian motion (*basic property of the Gaussian distribution*)
  - Thus, the SDE resembles the **geometric Brownian motion** (Oksendal, 2013):

    $d\theta_t = \mu\theta_t dt + \delta\theta_t dW_t \;\rightarrow$ closed-form solution $\;\theta_t = \theta_0 \exp((\mu - \delta^2/2)t + \delta W_t)$

  - Thus, we expect the SDE to induce a similar **shrinkage effect** for each multiplicative factor to dW_t, i.e., $||\phi_{\theta_t}(x_i)||_2$ with strength proportional to the loss stabilization level δ

Notions of sparsity for arbitrary architectures

Constant-noise SDE: $\mathrm{d}\theta_t = -\nabla_\theta \mathcal{L}(\theta_t)\mathrm{d}t + \sqrt{\eta\delta}\,\phi_{\theta_t}(X)^\top \mathrm{d}B_t$

We empirically track **two quantities** related to the Jacobian $\phi_\theta(X) \in \mathbb{R}^{n\times p}$:

1. **Rank of the Jacobian** that reflects
   - how many columns collapsed completely to zero (e.g., if ReLU = 0 for all x_i)
   - how many columns are linearly dependent on others (e.g., if two ReLUs implement the same function, up to a constant rescaling)

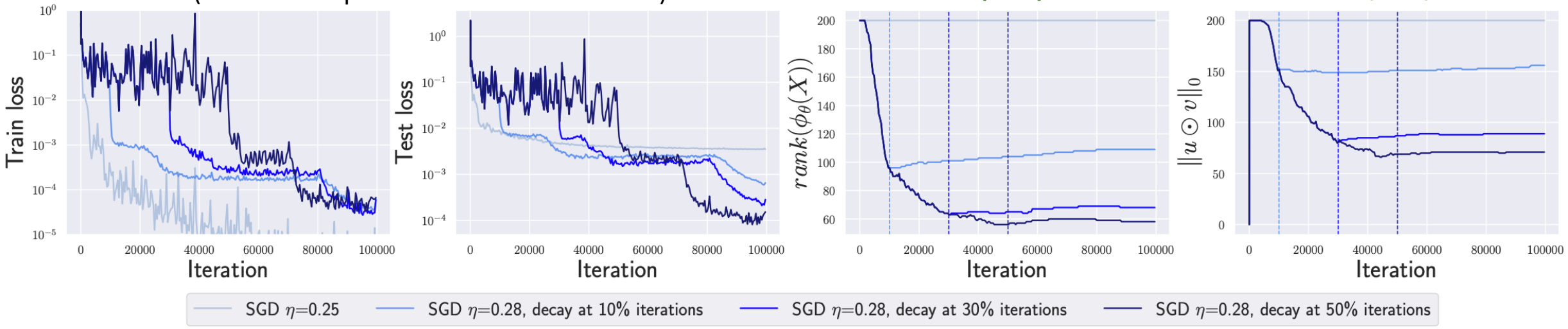
2. **"Feature sparsity coefficient"**: the average number of distinct (we count highly-correlated neurons as one), non-zero activations
   - formally: $\frac{1}{n}\sum_{i=1}^{n}\frac{1}{m}\sum_{j=1}^{m}\mathbf{1}_{g(x_i)_j>0}$ where $g(x_i) \in \mathbb{R}^m$ is the feature vector at some layer where we merge beforehand *highly correlated neurons*
   - this serves as a cheap proxy of the rank that **scales to deep networks**

Sparse feature learning for diagonal linear networks

(the first two plots are the same as before)

(new)

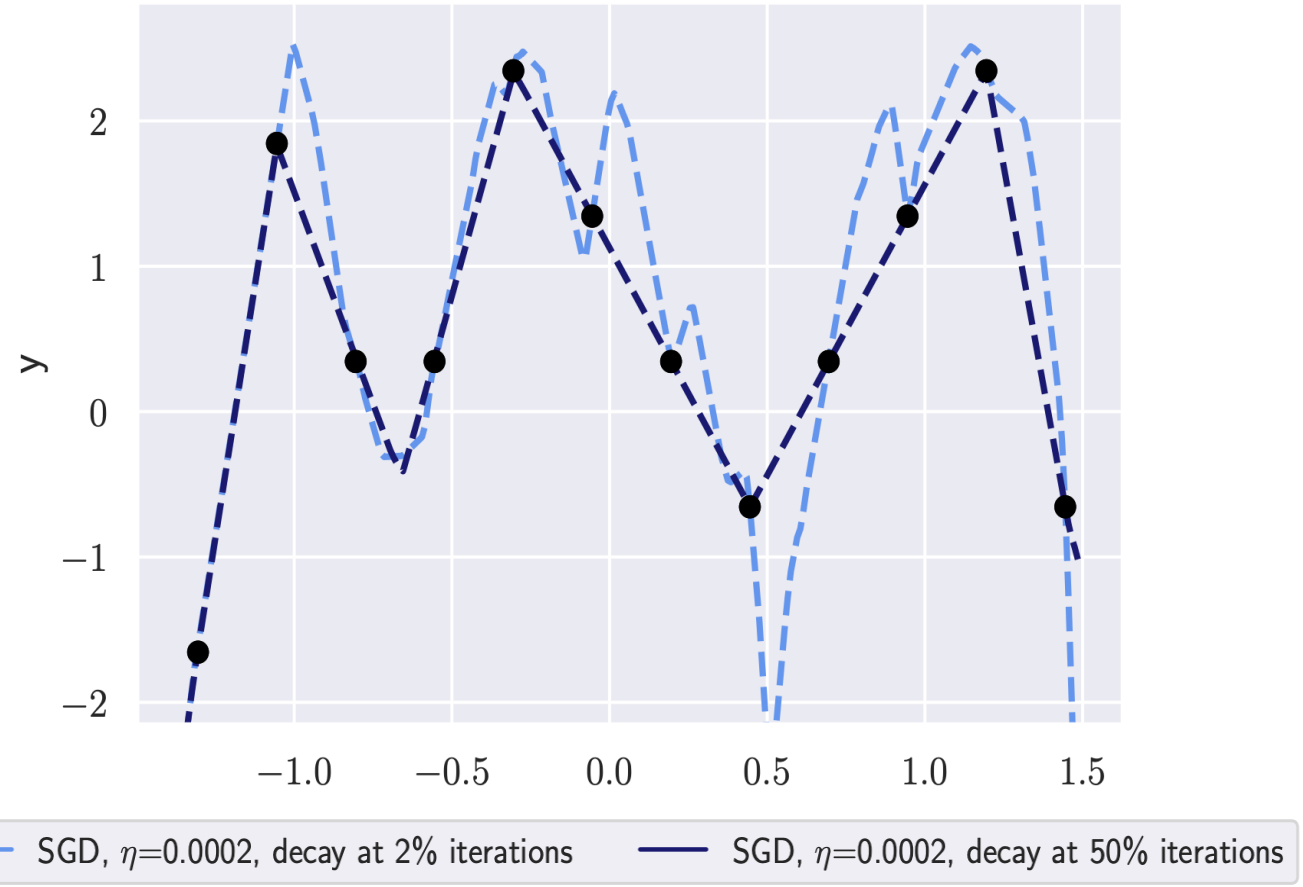
(new)



- The last two plots clearly show that **sparsity is progressively achieved** in the large step size phase
- **Note**: for this task, sparsity is desirable because the ground truth vector w^* was selected to be sparse
- If there is no alignment between the ground truth and implicit bias, we don't expect to see improvements in generalization!

Sparse feature learning for a simple one-layer ReLU network

Illustration: a classical textbook picture about overfitting

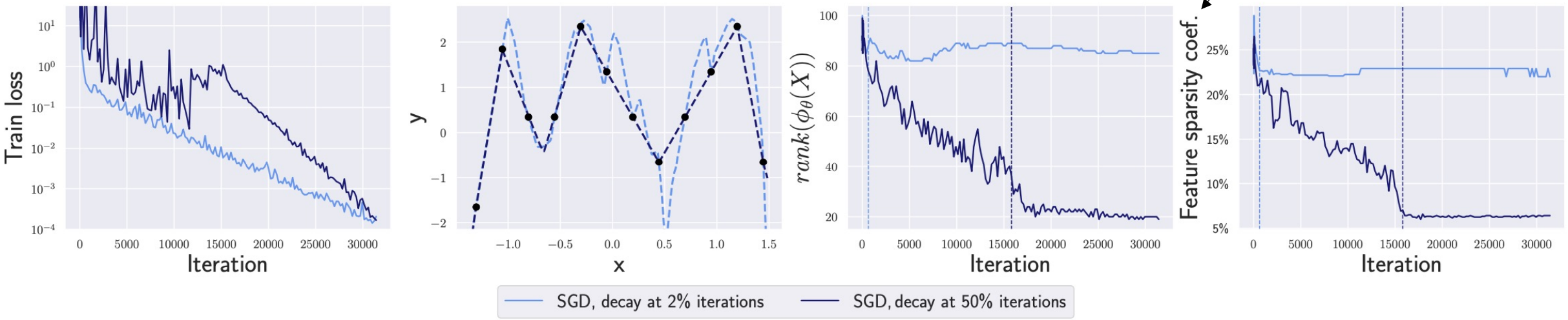


Here, however, the nice interpolation between the points
is **due to the implicit regularization effect** of large step sizes

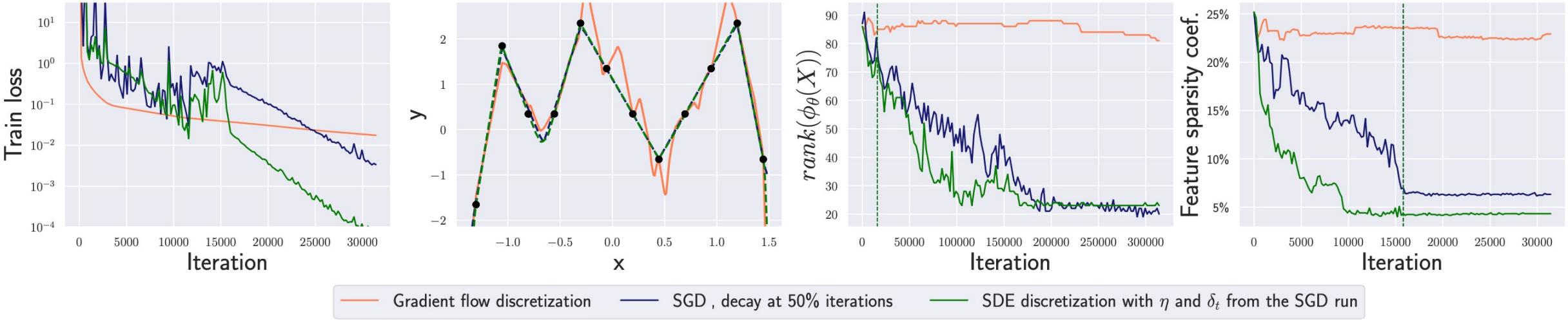
A simple one-layer ReLU network: sparsity metrics

$\frac{1}{n}\sum_{i=1}^{n}\frac{1}{m}\sum_{j=1}^{m}\mathbf{1}_{g(x_i)_j>0}$ for deduplicated features $g(x_i)$

Sparse feature learning



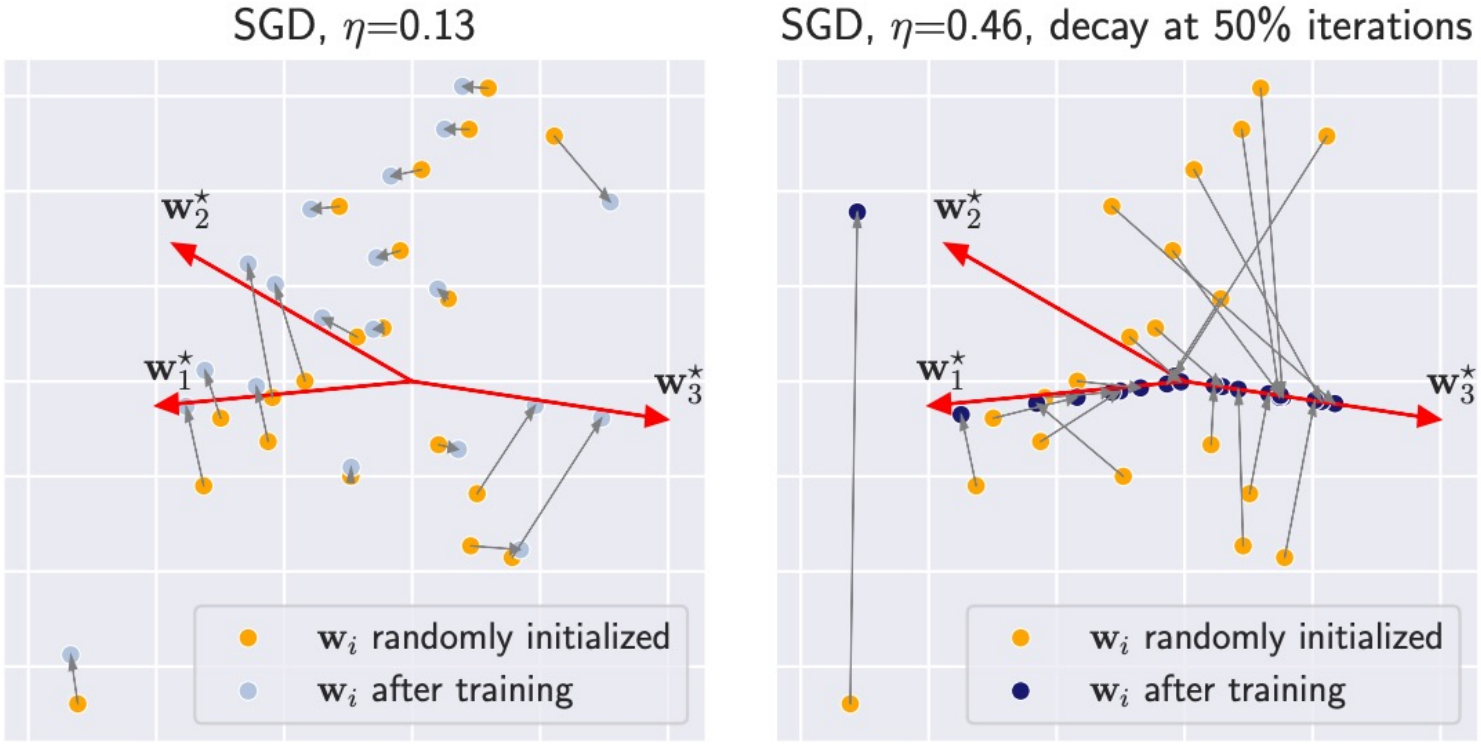
Validity of the SDE modeling



Dynamics of individual neurons in 2D

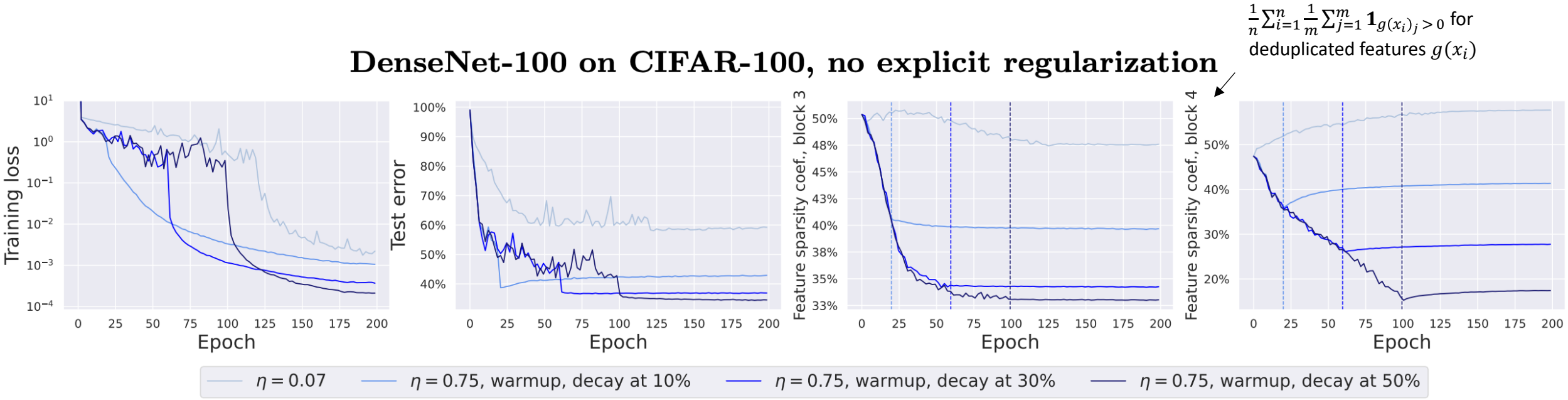
- How do the weight vectors corresponding to neurons move depending on the step size?

Setting: input dimension $d = 2$, teacher with 3 neurons $w_1^\star, w_2^\star, w_3^\star$, student with 20 neurons



- With small step sizes, the neurons barely move! i.e., **the network fits the data with effectively fixed random features** → not desirable
- **Sparse feature learning occurs only for large step sizes**

Sparse feature learning for deep networks (part I)

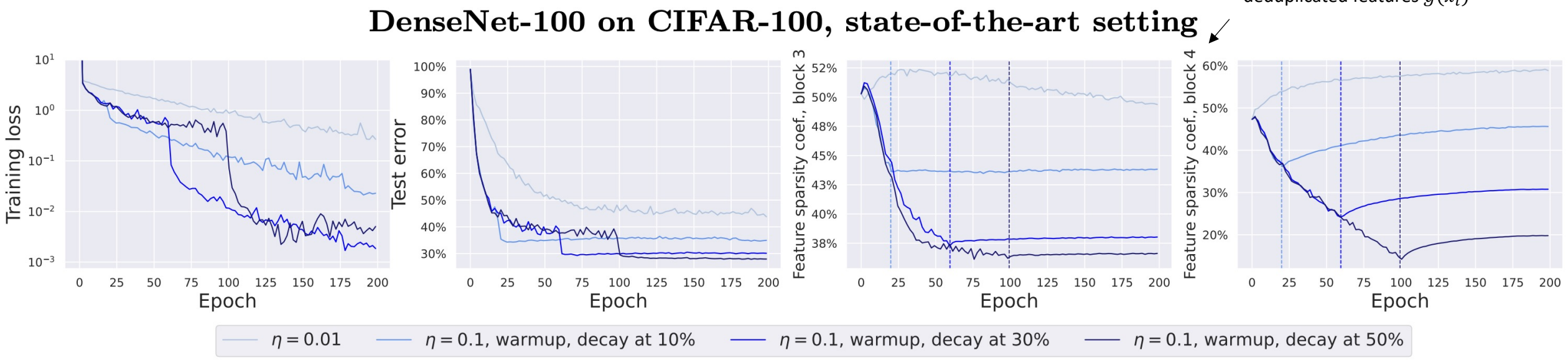


Main observations:

- Plot 1: the **training loss** stabilizes
- Plot 2: the **test error** noticeably depends on the length of the schedule
- Plots 3 & 4: the **feature sparsity coefficient** *at top layers* (blocks 3 and 4 out of 4 blocks in total) is minimized during the large step size phase

Sparse feature learning for deep networks (part 2)

$\frac{1}{n}\sum_{i=1}^{n}\frac{1}{m}\sum_{j=1}^{m}\mathbf{1}_{g(x_i)_j>0}$ for deduplicated features $g(x_i)$



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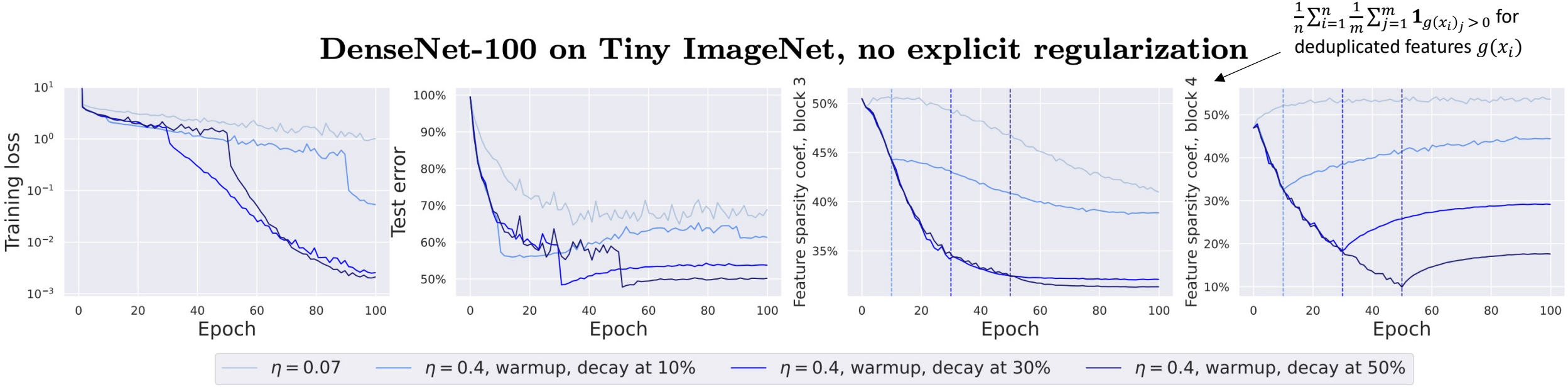
Sparse feature learning for deep networks (part 3)



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Conclusions and takeaways

- **Our picture**: SGD noise drives the iterates to a sparse solution which we observe on many models (from **diagonal linear networks** to **DenseNets on Tiny ImageNet**)
- Sparse features are likely to be often (but surely not always) beneficial for generalization on natural data
- We can learn them via the SGD dynamics **if we don't converge too early**
- The same training dynamics is likely to be achieved via different means but **with SGD we get this effect "for free"** unlike, e.g., for gradient/Jacobian regularizers
- May be of interest: recent work "*Stochastic Collapse: How Gradient Noise Attracts SGD Dynamics Towards Simpler Subnetworks*" (June 2023, arXiv) with similar high-level claims but a bit different perspective

Thanks for your attention!