Predicting & Optimizing ML Training

Simons “Future of LLMs” Workshop

April 3, 2025

Collaborators

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Graduating now!

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Graduating now (from *undergrad*)!

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Optimizing ML Training with Metagradient Descent

Logan Engstrom*[1], Andrew Ilyas*[2†], Benjamin Chen*[1],
Axel Feldmann[1], William Moses[3], Aleksander Mądry[1]

*Equal contribution [1]MIT, [2]Stanford, [3]UIUC

Motivation

Training requires many design choices. Making the right choice is hard!

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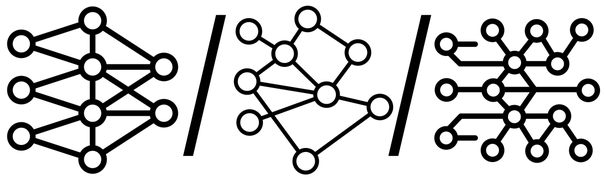
Model architecture



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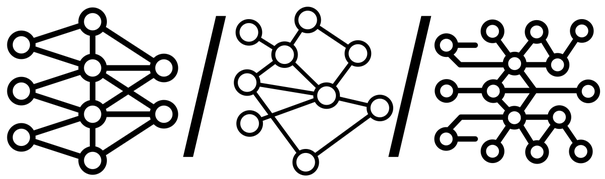
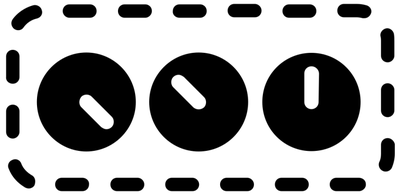


Hyperparameters



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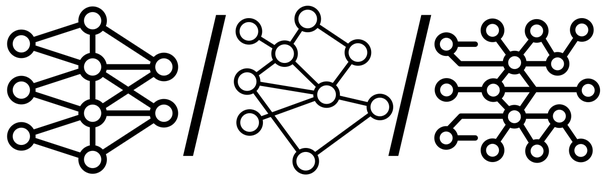

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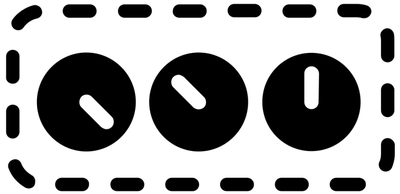
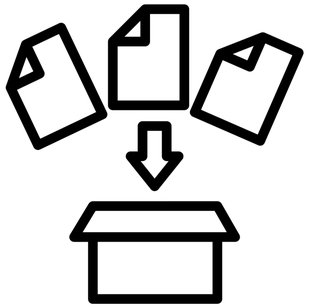


Training dataset



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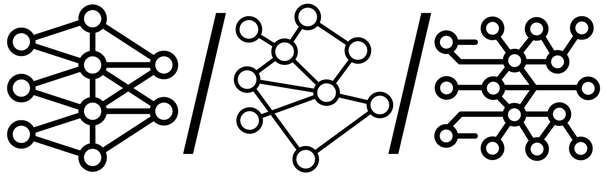

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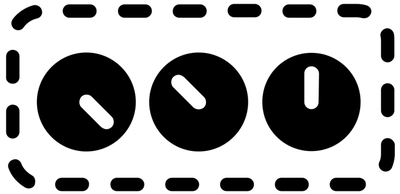

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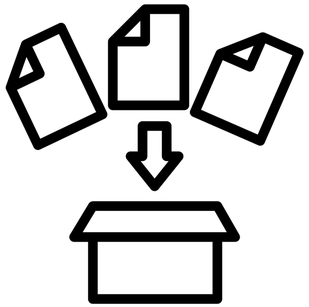

Fundamental Q: Can we predict and optimize the effect of these choices?

E.g.: Architecture search, scaling laws, data curation

The dream

A framework for optimizing and predicting the effect of design choices on model training

Example: Training data

Optimizing: Training data curation

(Sorscher et al. 2022; Gadre et al. 2023; Xie et al. 2024; Xia et al. 2024; Engstrom et al. 2024; many others)

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Scraped internet data

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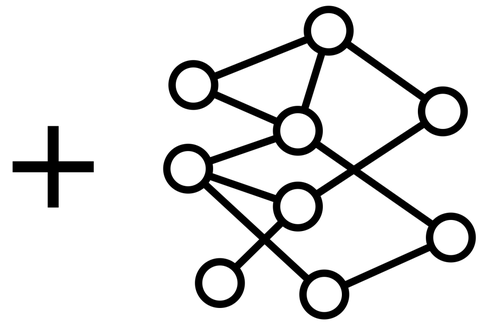

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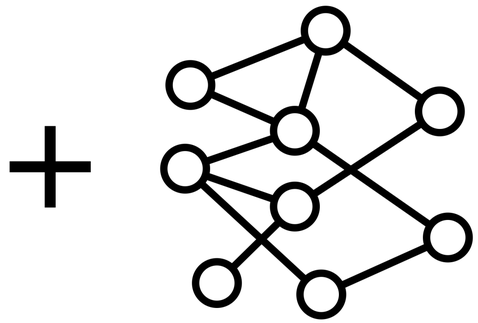

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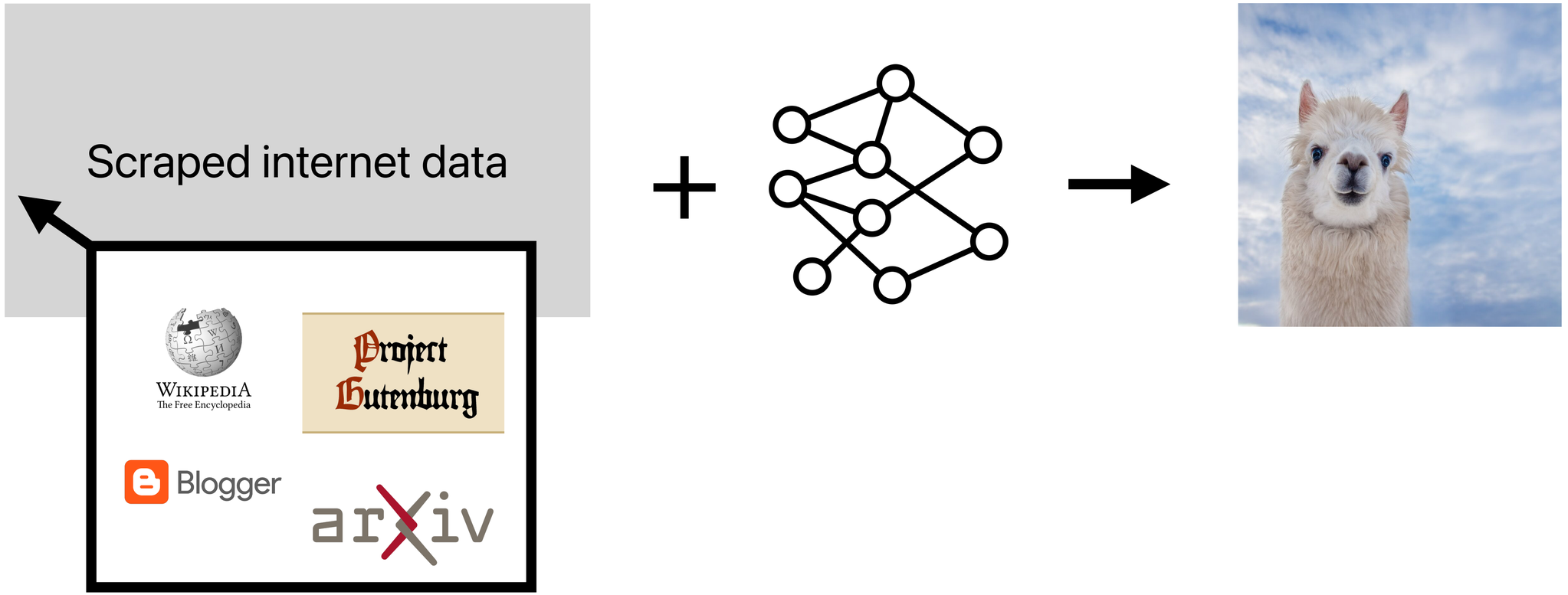

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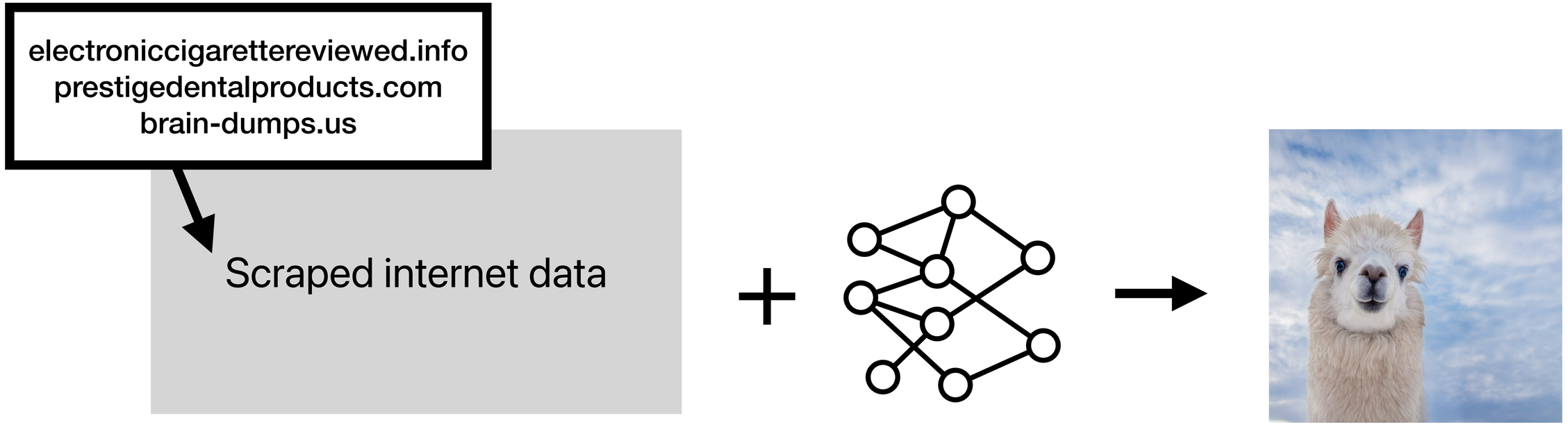

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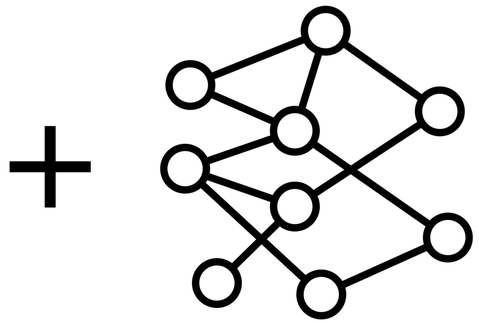

Much of the internet is low-quality: what data should we train on?

Equivalently: can we **optimize** the training data selection for target performance?

Predicting: Training data attribution

(Koh & Liang 2017; Feldman 2019; I et al. 2022; Bae et al. 2023, Park et al. 2024; many others)

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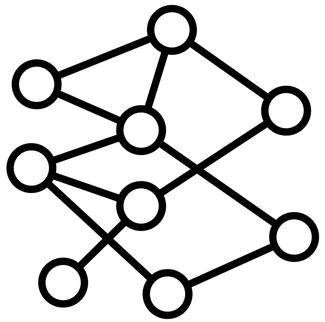

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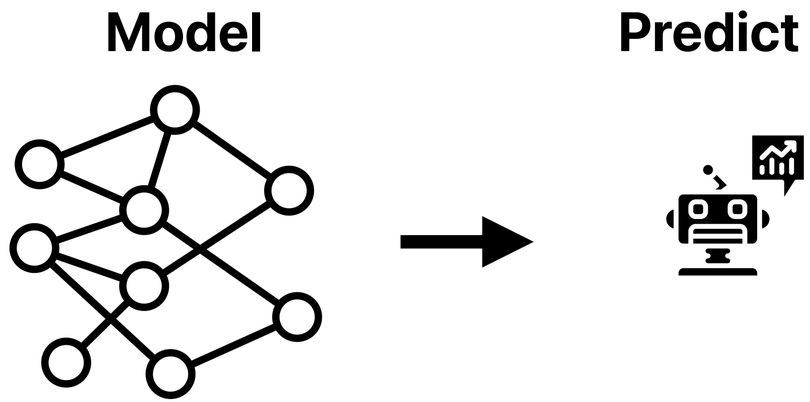

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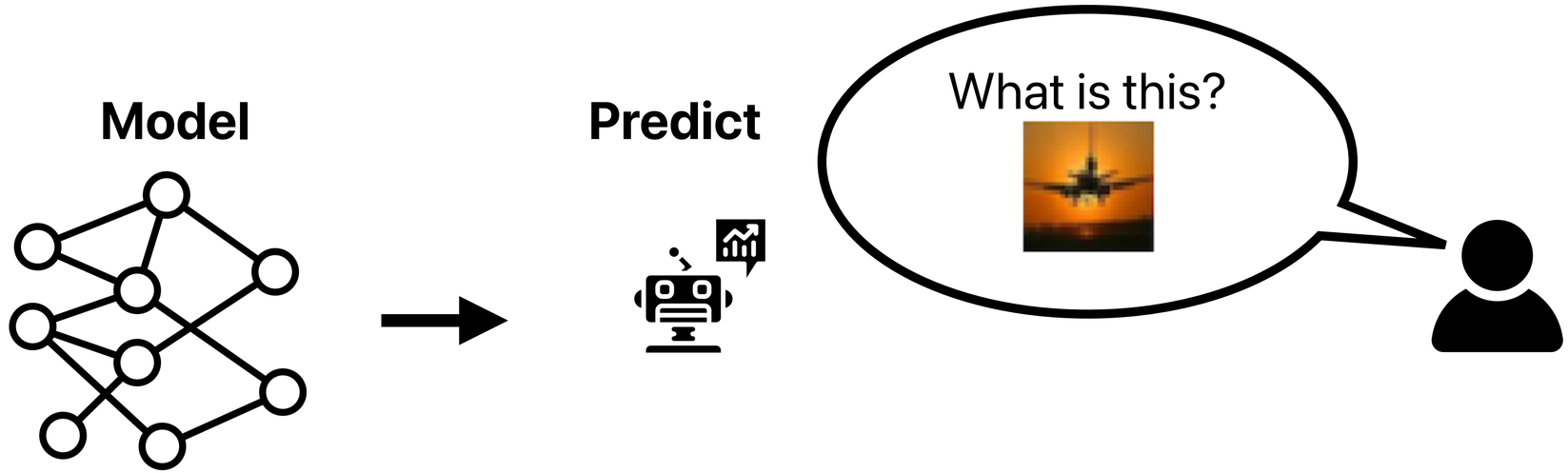

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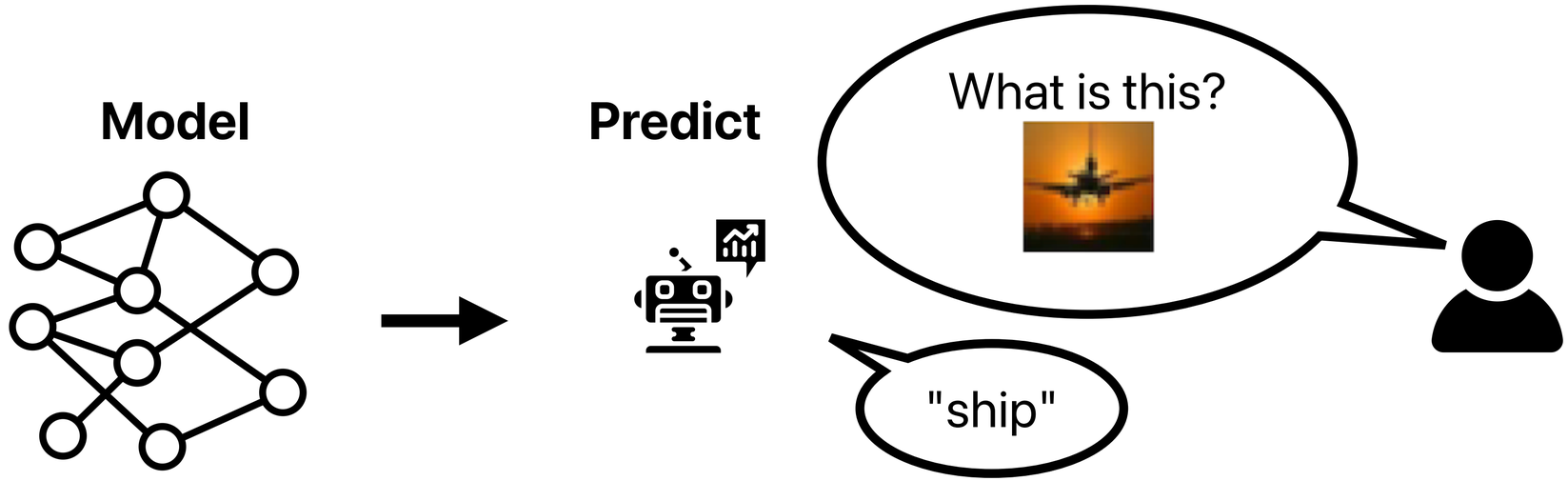

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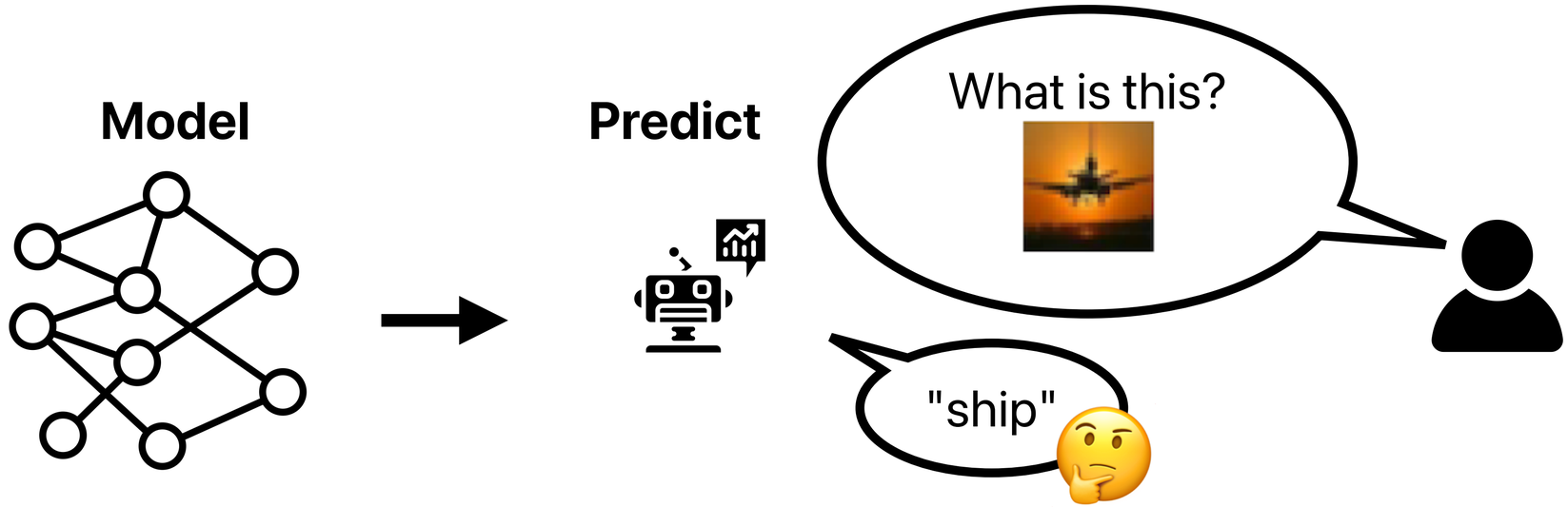

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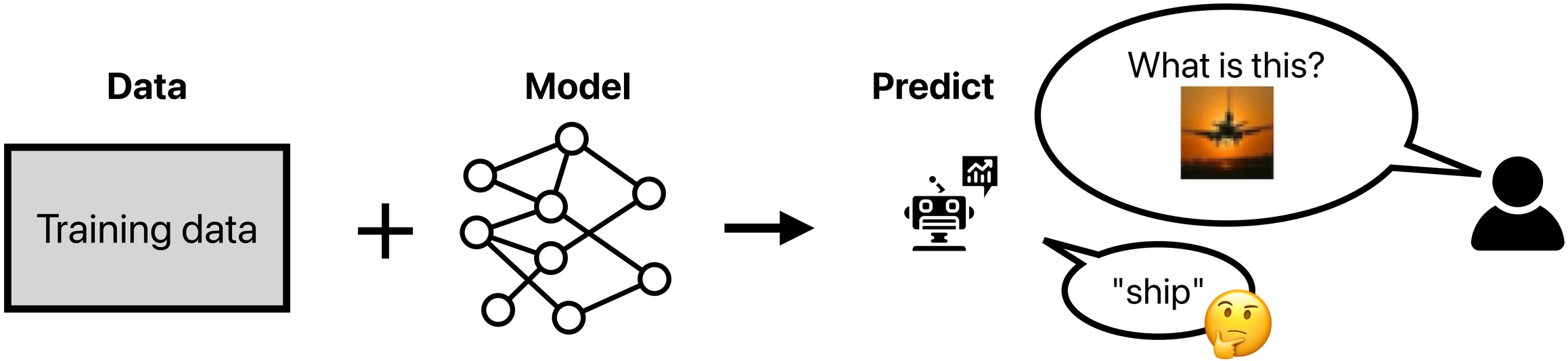

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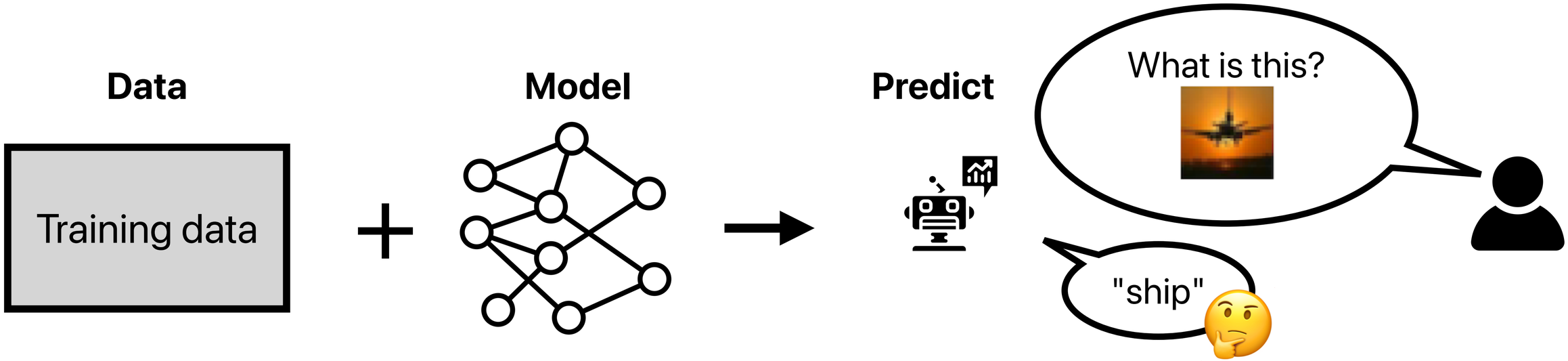

"What examples in the training data caused this behavior?"

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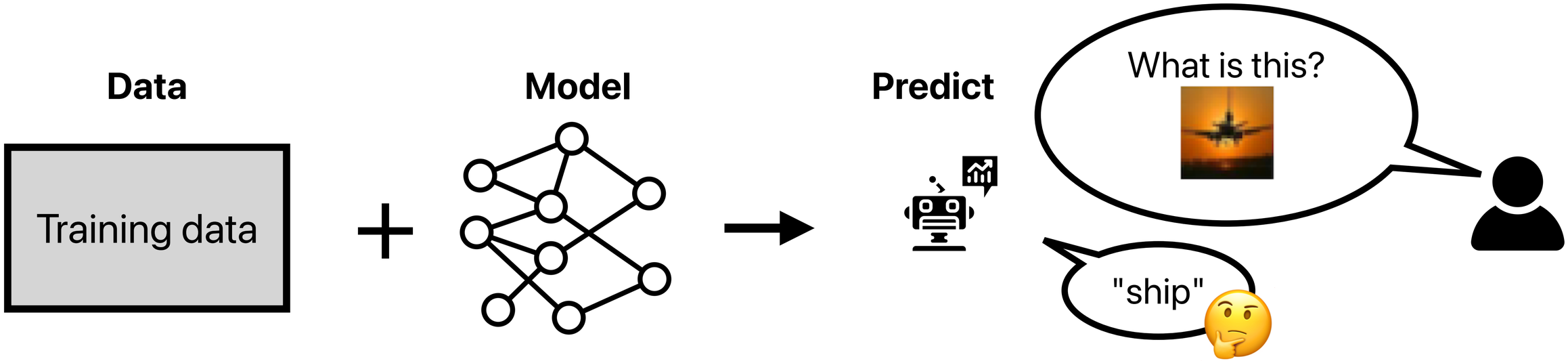

"What examples in the training data caused this behavior?"

Equivalently: Can we **predict** change in this behavior as a function of training data?

Full problem statement

Problem: Metaparameter selection

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Idea: write **model output** as a direct function of **training setup** (“metaparameter”)

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Metaparameter

$$\mathbf{z} \in \mathbf{Z} \subset \mathbb{R}^d$$

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The aspect(s) of the training setup that we want to study

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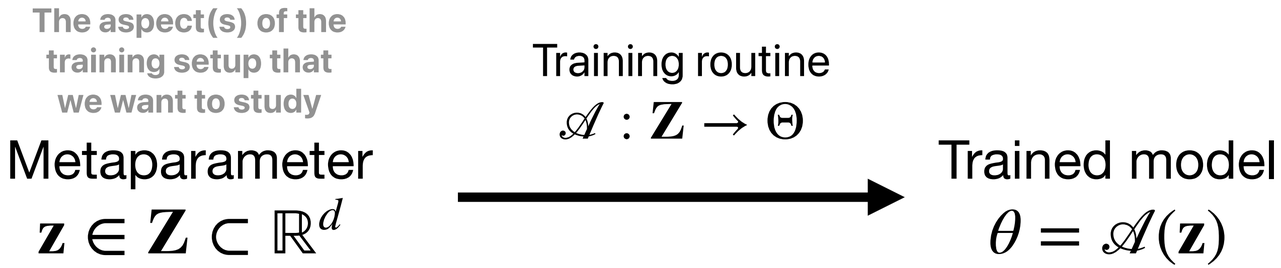

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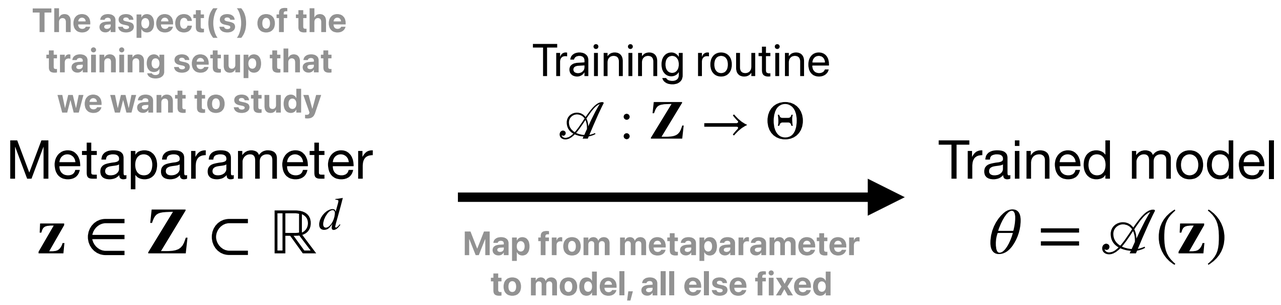

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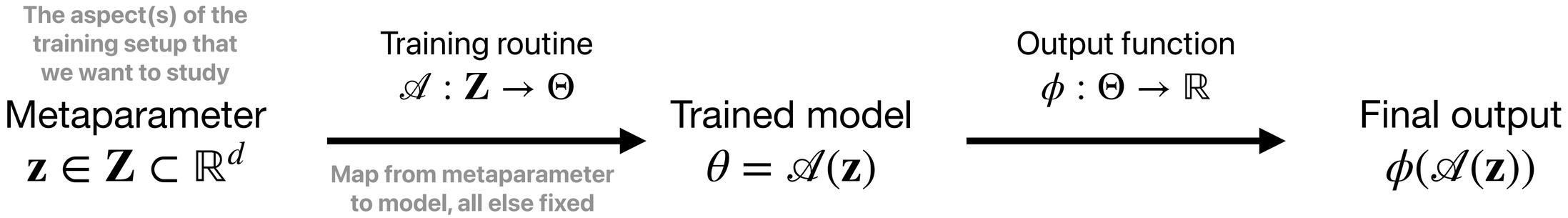

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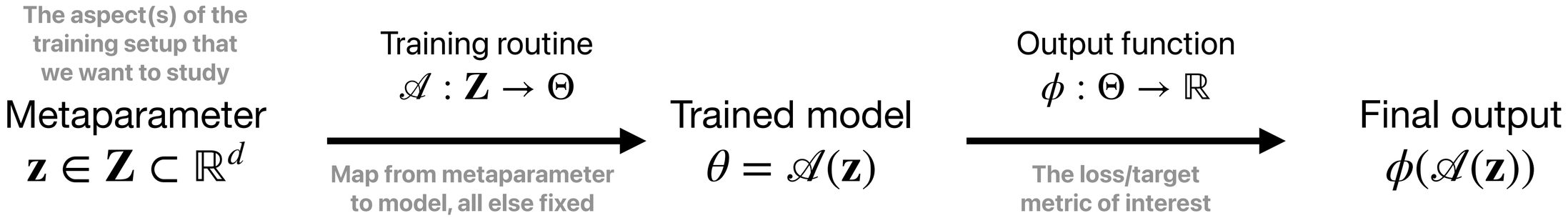

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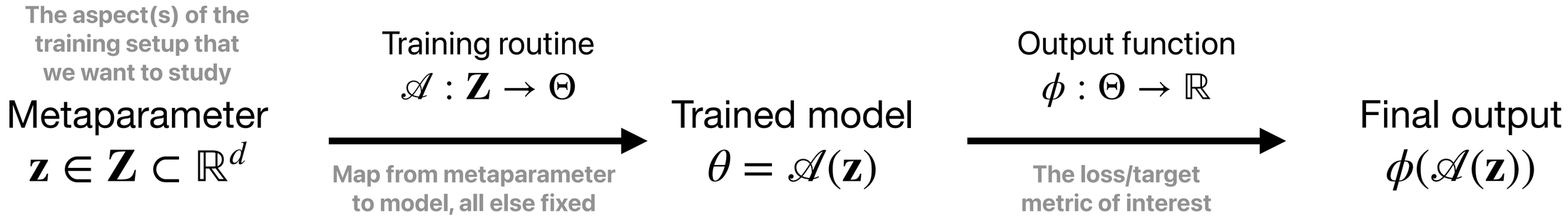

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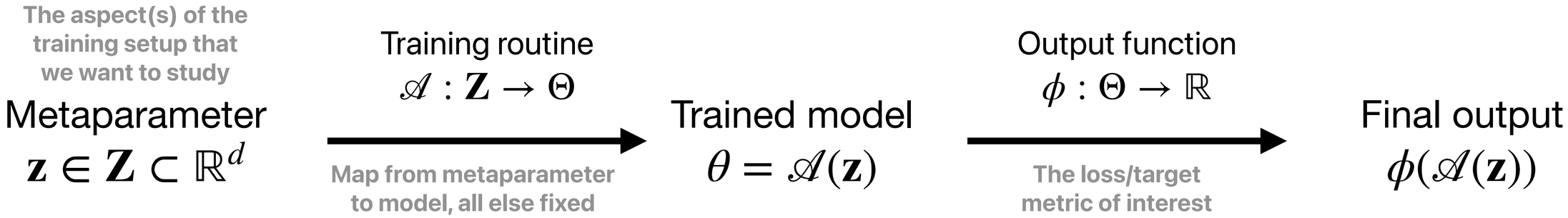

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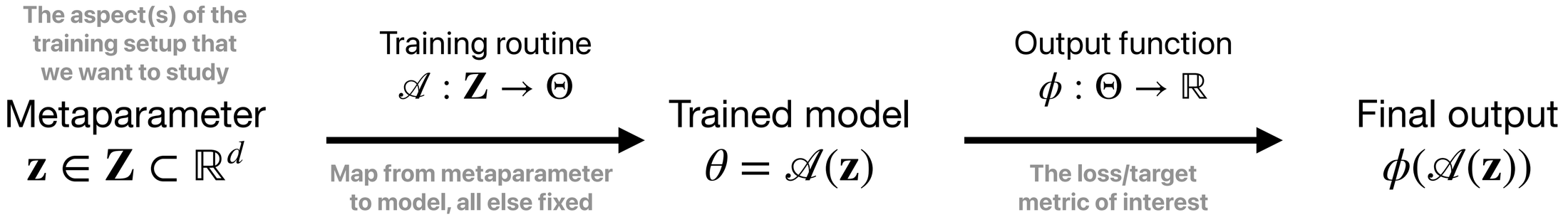

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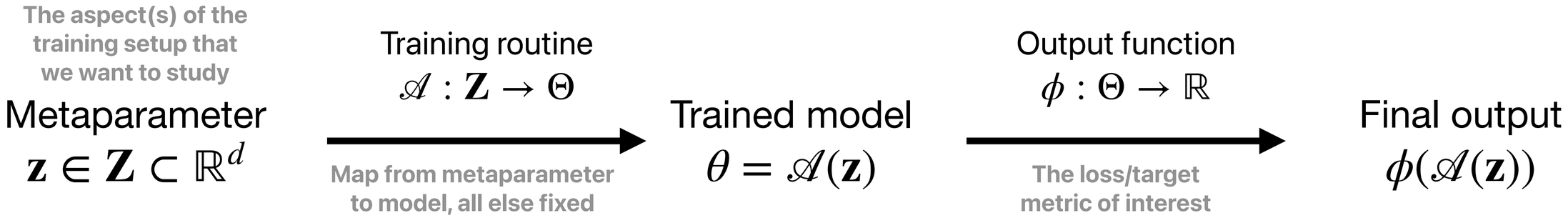

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Captures data curation & attribution but also <u>many</u> established ML challenges

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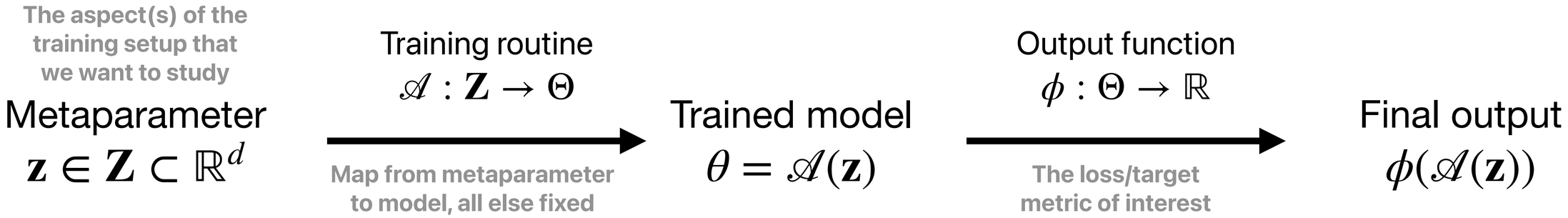

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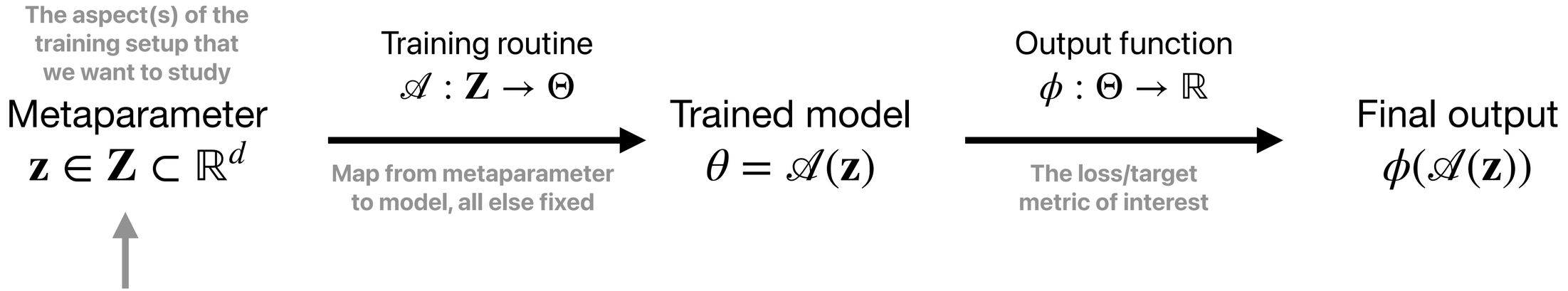

This will be our data selection:

d = number of training examples

$\mathbf{z}_i = 0$ means don’t train on i

$\mathbf{z}_i > 0$ means train on i with importance weight $\mathbf{z}_i$

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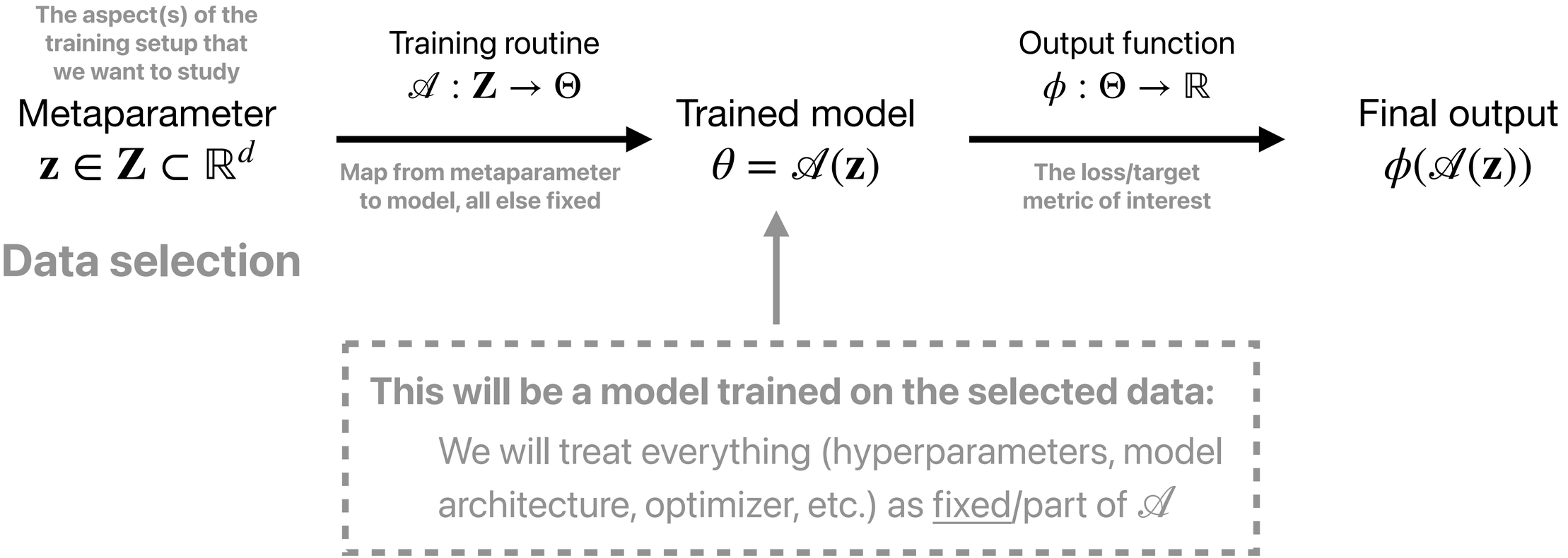

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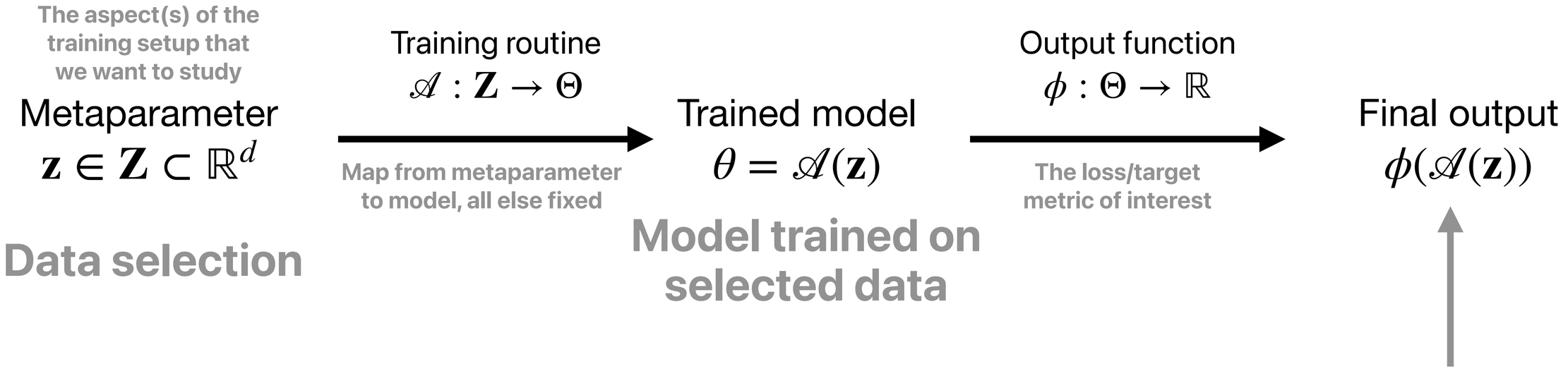

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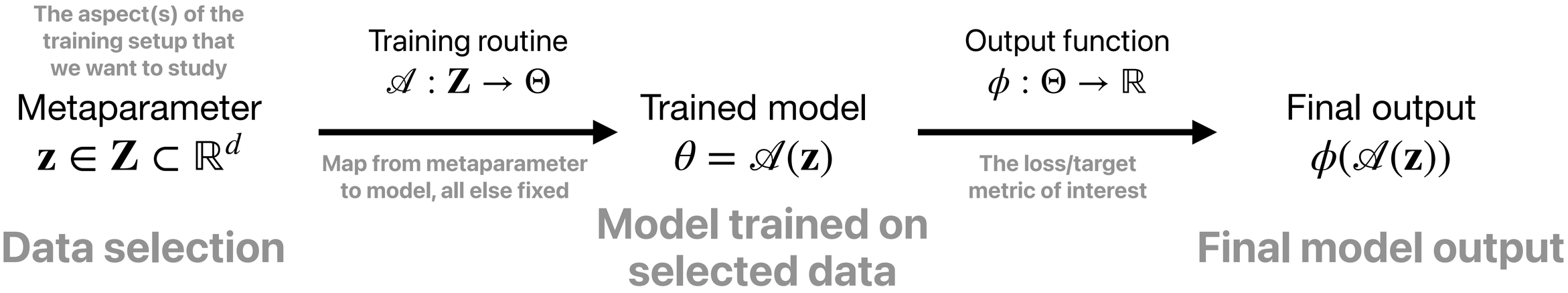

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Find the selection $\mathbf{z}$ that minimizes the resulting model’s test loss

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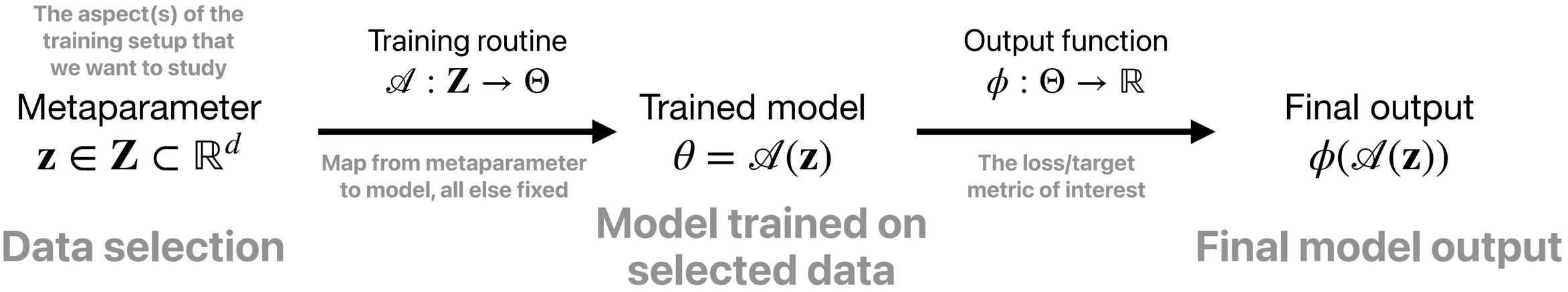

Goal (Data curation)

Find the selection $\mathbf{z}$ that minimizes the resulting model’s test loss

Goal (Data attribution)

Predict how changing the selection $\mathbf{z}$ will change resulting model’s output

Roadmap

Main idea: The metagradient

Prequel: Two challenges

Looking forward

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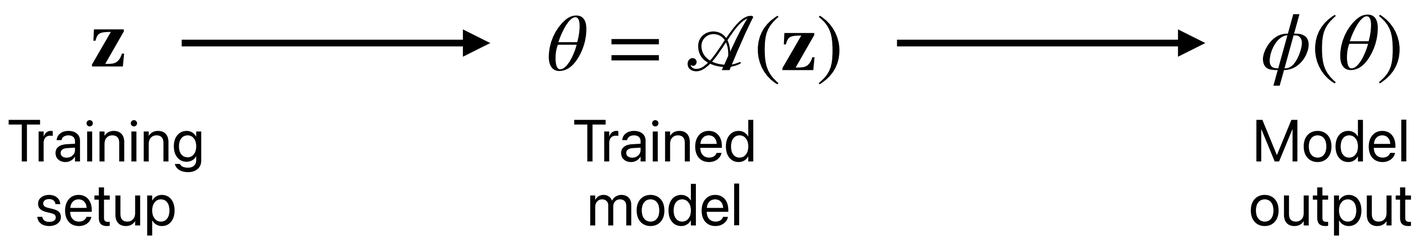
Prequel: Two challenges

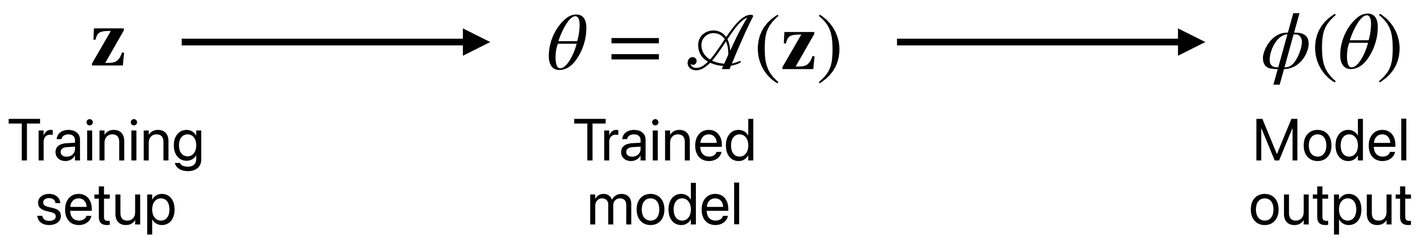
Looking forward

Main idea: The metagradient



Main idea: The metagradient

In many cases, metaparameter $\mathbf{z}$ is a continuous variable (or can be relaxed to one)



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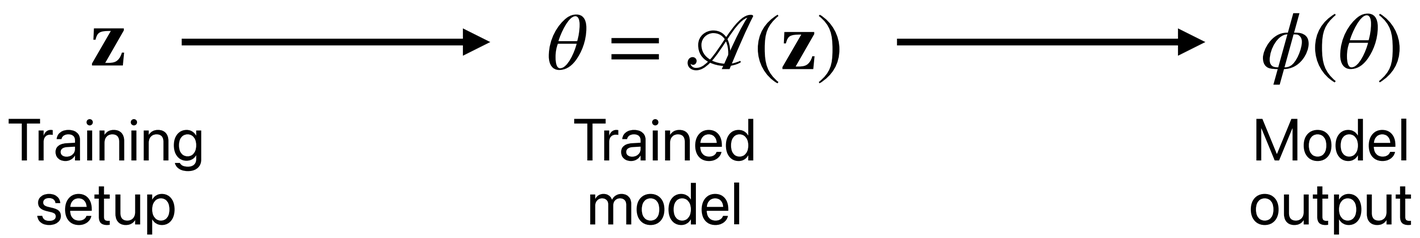
We will show how to **compute** and **use** the *metagradient*:



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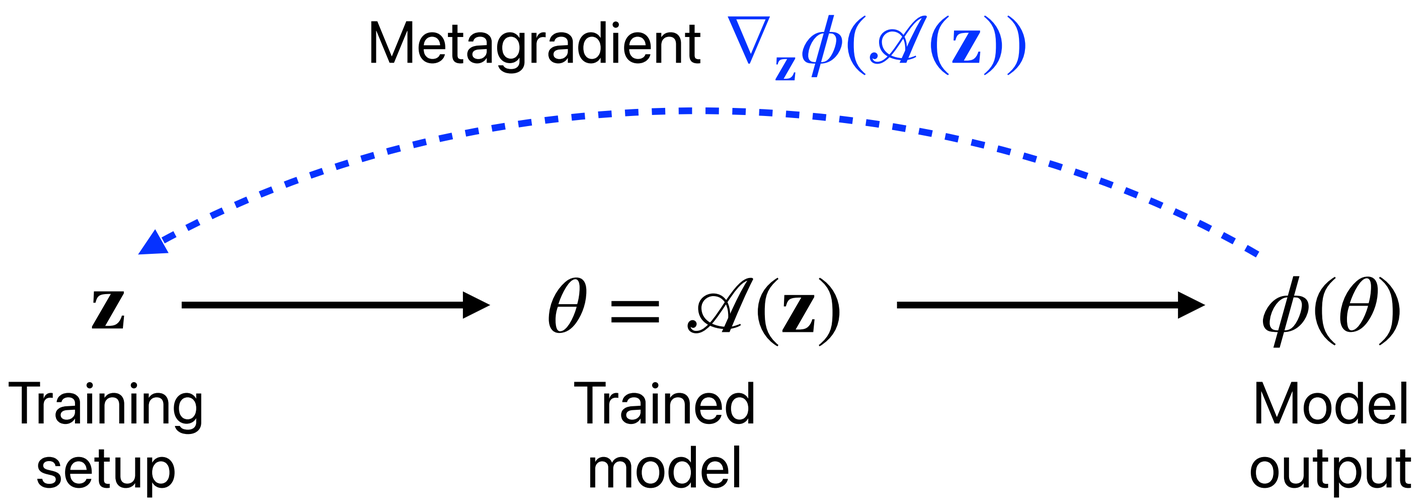

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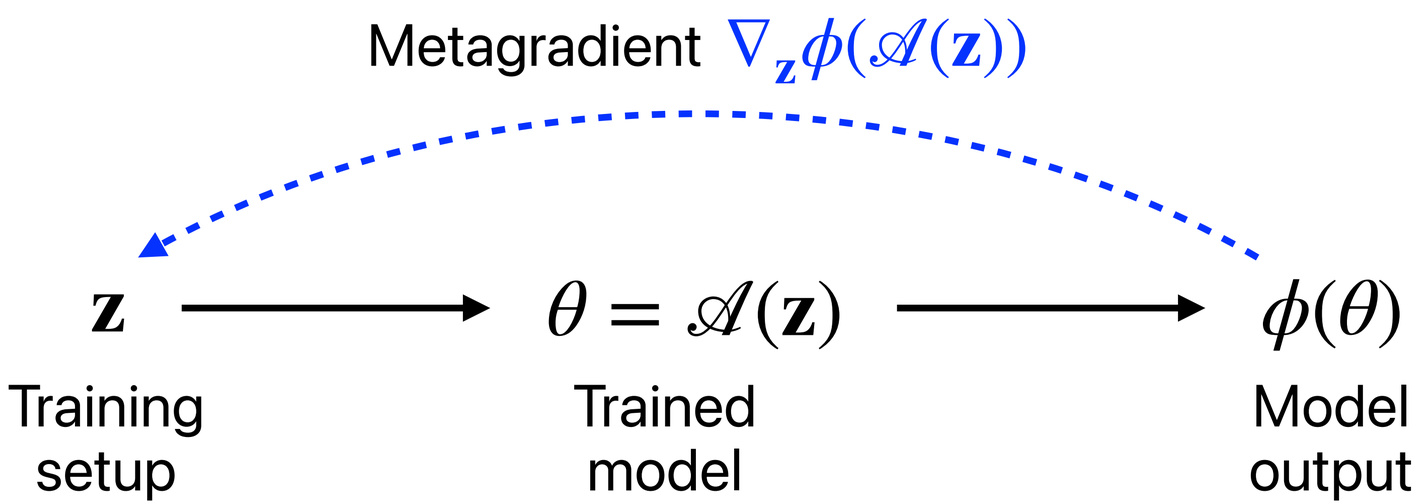

Cost: In practice, "only" 3-5x the cost of model training!

Main idea: The metagradient

Metagradients offer a powerful way to optimize and predict (aspects of) model behavior

Optimizing with metagradients

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      Requires T total metagradient calculations

Task: Data selection

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Choose train subset

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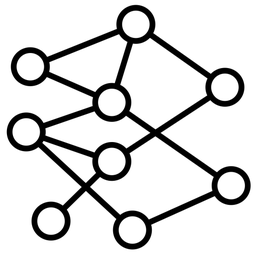
Train a model



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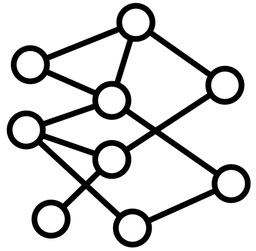

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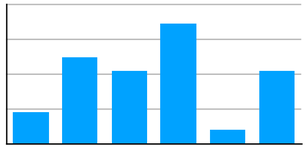

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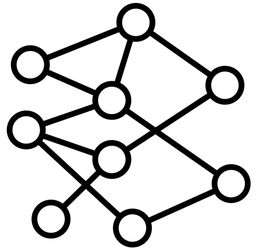

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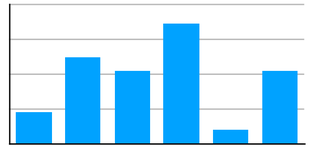

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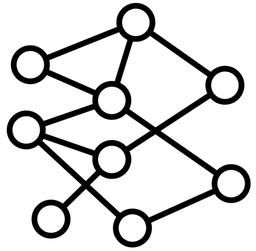

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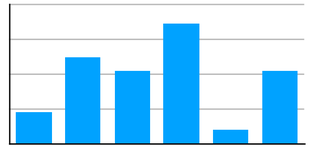

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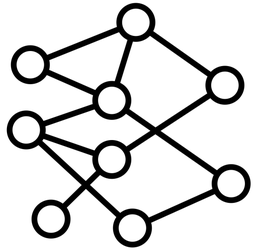

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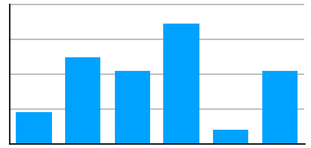

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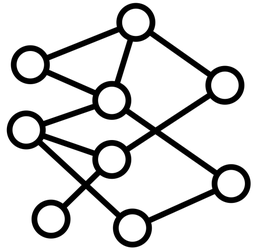

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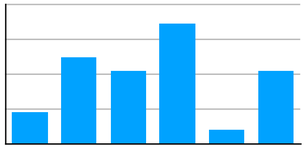

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Increasingly recognized as a critical step in large-scale ML pipeline

Task: Selecting CLIP data

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*simplified

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DATACOMP:
In search of the next generation of multimodal datasets

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Data selection task where the learning algorithm (CLIP training) and evaluation (zero-shot classification) are **fixed**

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Data selection task where the learning algorithm (CLIP training) and evaluation (zero-shot classification) are **fixed**

Goal: Curate the best possible dataset

Task: Selecting CLIP data

Setup

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Example leaderboard (small):

Rank	Created	Submission	ImageNet acc.	Average perf.
1	03-14-2025	M-FLYT + SCS (alpha=0.5)	0.080	0.185
2	08-18-2024	EcoDatum	0.053	0.182
3	08-12-2023	> w <	0.056	0.180
4	11-04-2023	Hype Sampler	0.063	0.180
5	01-08-2024	Content Alignment Model ∩ Flipped CLIP Score	0.064	0.178
6	09-07-2023	Detection ∩ CLIP score	0.053	0.178
7	09-06-2023	BLIP2-COCO-finetuned_similarity_top-35%	0.053	0.177
8	08-03-2023	WS (baselines)	0.059	0.175
9	04-28-2023	Baseline: CLIP score (L/14 30%)	0.051	0.173
10	09-07-2023	OCR and Naive english filtering	0.057	0.173
11	08-05-2024	MoDO	0.051	0.173
12	08-25-2023	Fondant baseline, CLIP score (L/14 1%-30%), ascii > 4	0.053	0.168
13	08-25-2023	text masked CLIP 30%	0.048	0.164
14	08-02-2023	CLIP score (L/14 30%) baseline	0.049	0.164
15	04-28-2023	Baseline: Image-based	0.043	0.159

⋮

Task: Selecting CLIP data

Results (DataComp-small)

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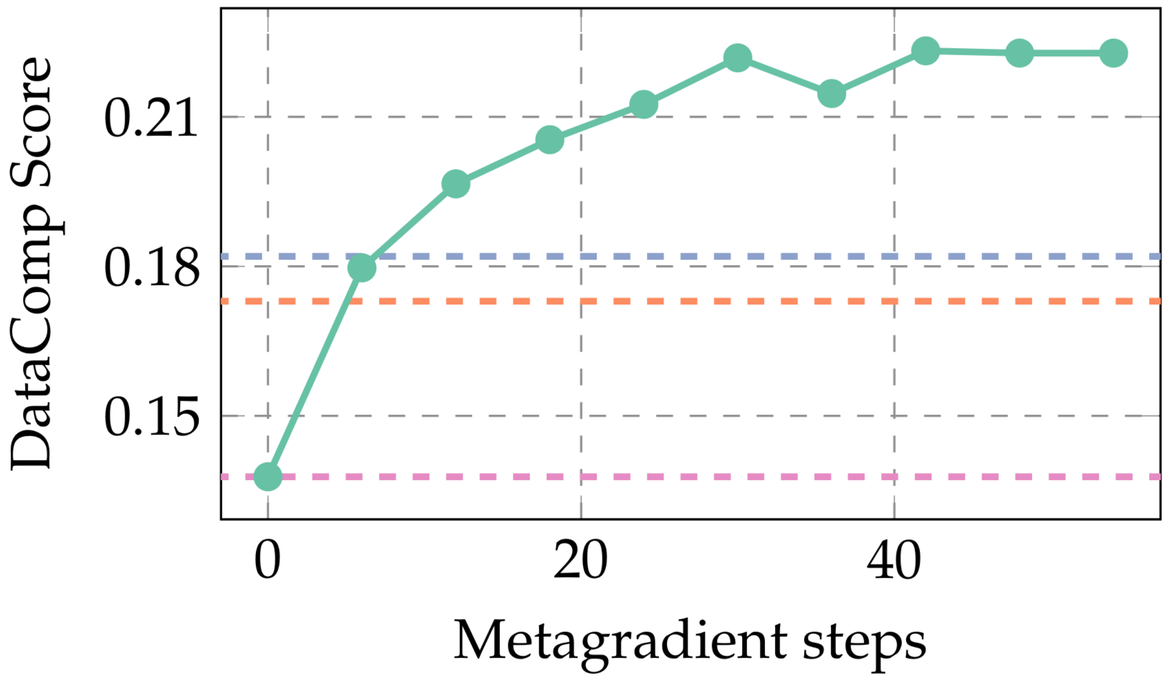

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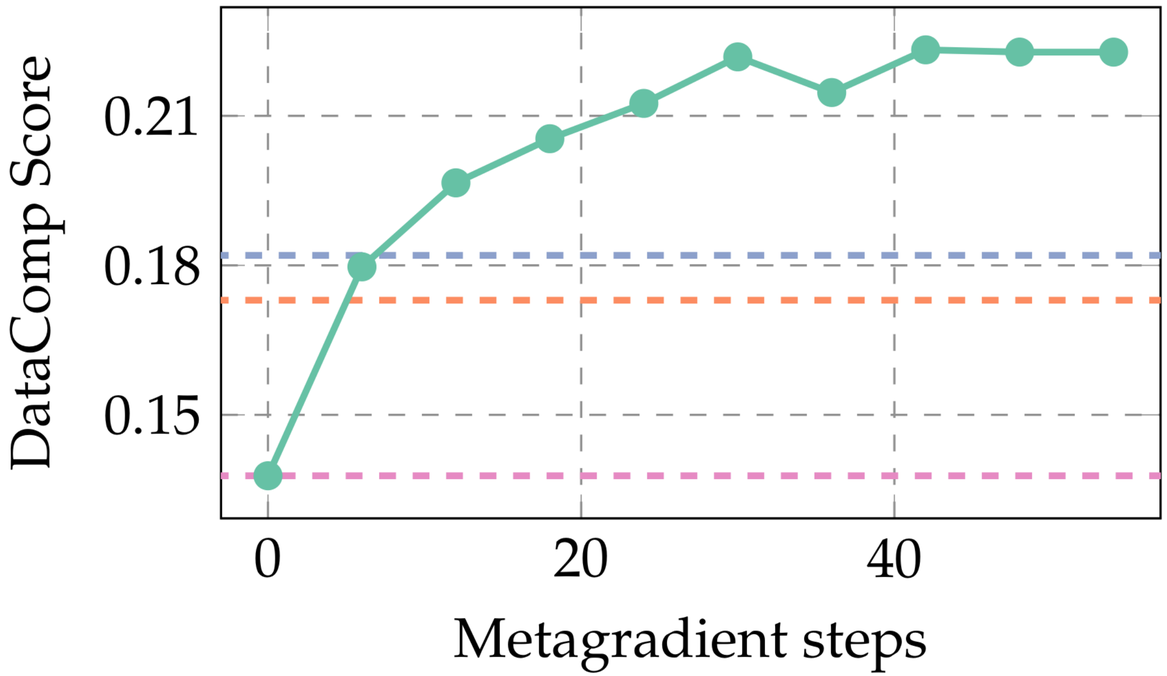

Method	Score	Δ
Baseline: No filtering	0.13	–
Best baseline from [GIF+24]	0.17	+0.04
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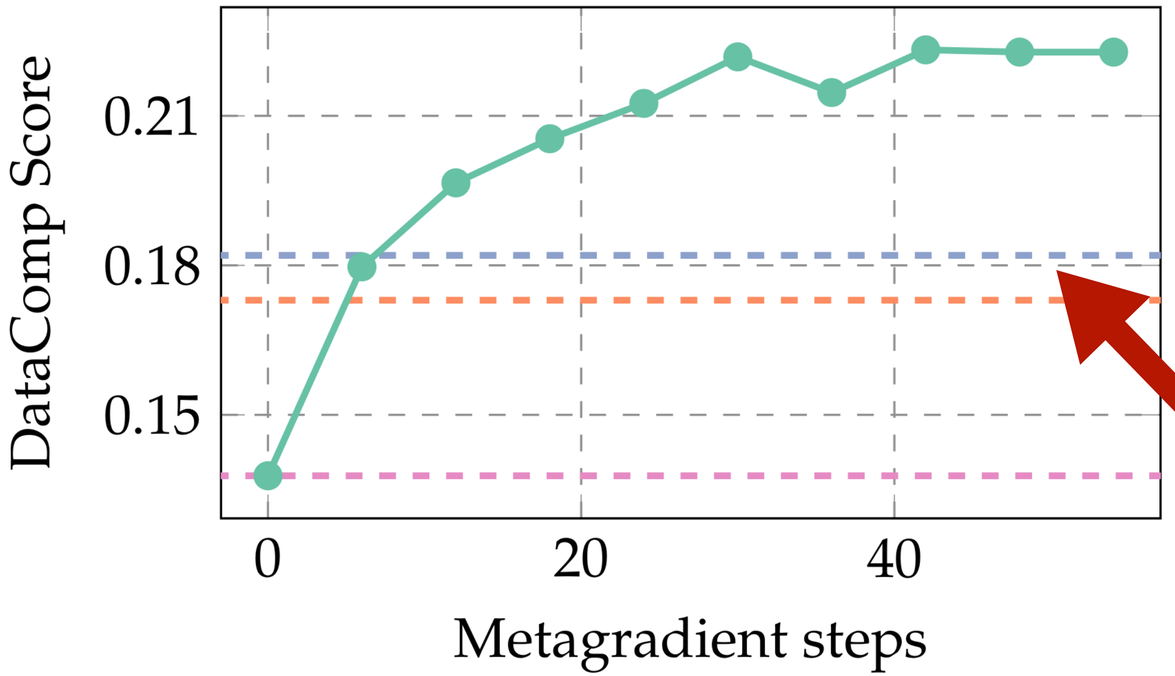

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Task: Selecting CLIP data

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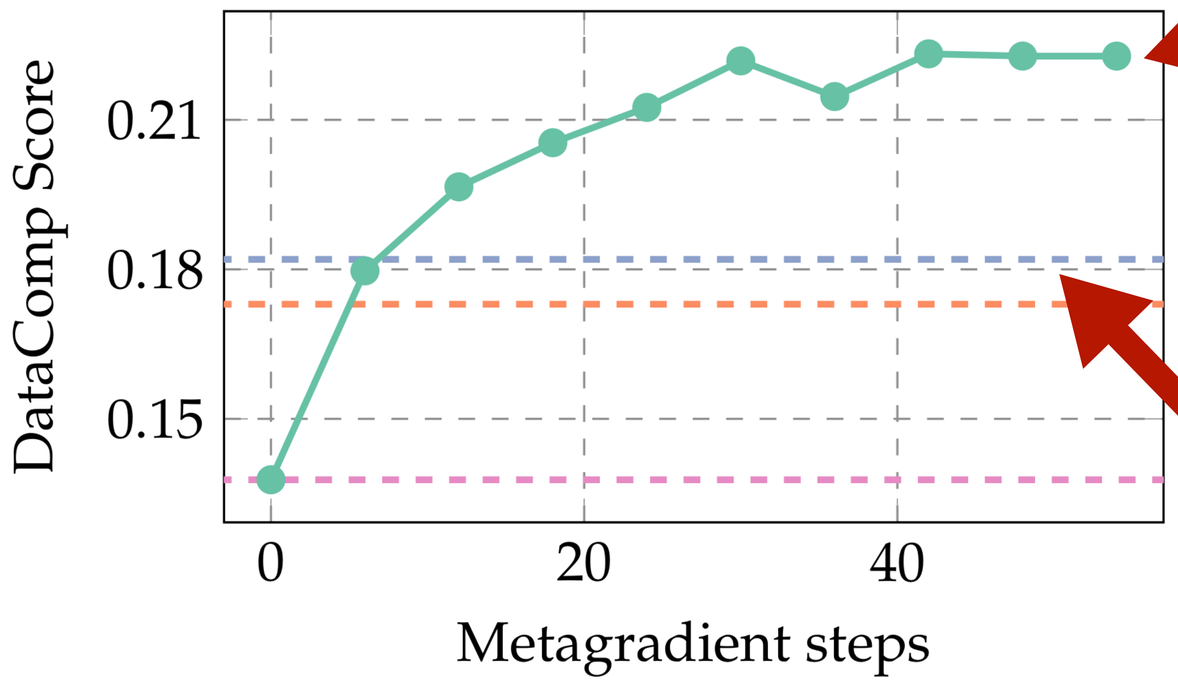

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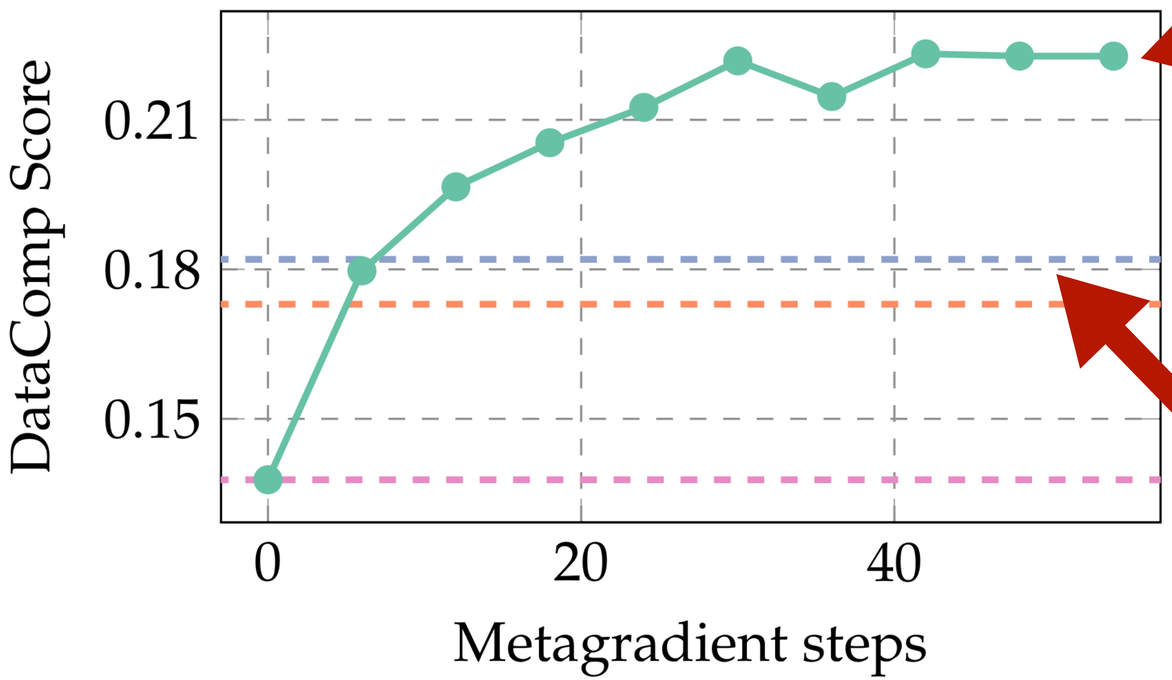

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Now working on DataComp-medium (already #1!)

Task: Selecting instruction fine-tuning data

Results (LESS IFT setting)

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Results (LESS IFT setting)

New goal: Select instruction fine-tuning data for LM benchmarks (2B param model)

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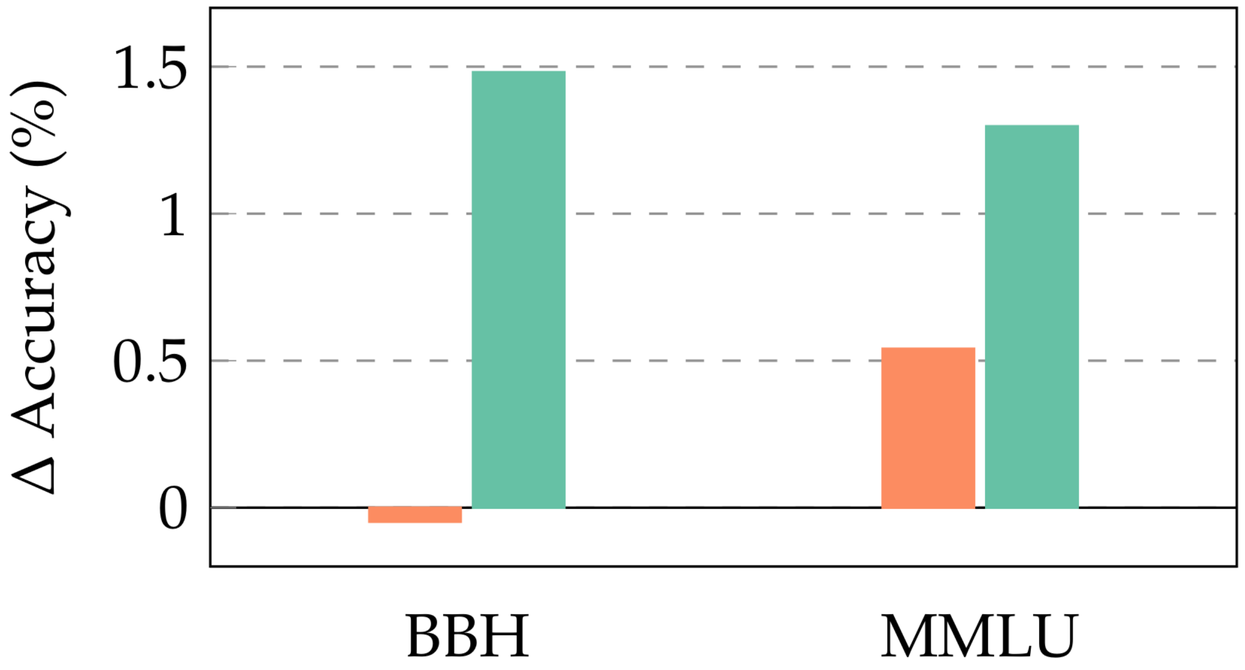

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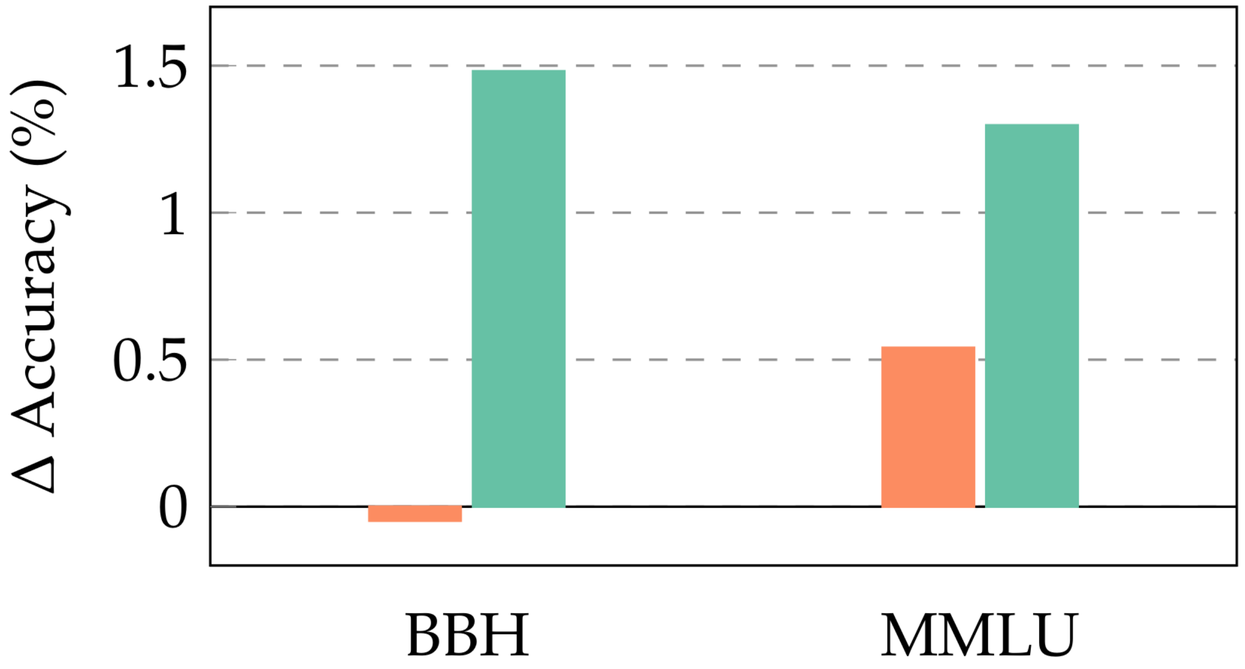

	BBH [SSS+22]		**MMLU** [HBB+20]	
	Acc.	Δ	Acc.	Δ
All Data	35.2%	–	41.2%	–
LESS	35.2%	−0.0%	41.8%	+0.5%
MGD-DS	**36.7%**	**+1.5%**	**42.5%**	**+1.3%**

Task: Selecting instruction fine-tuning data

Results (LESS IFT setting)

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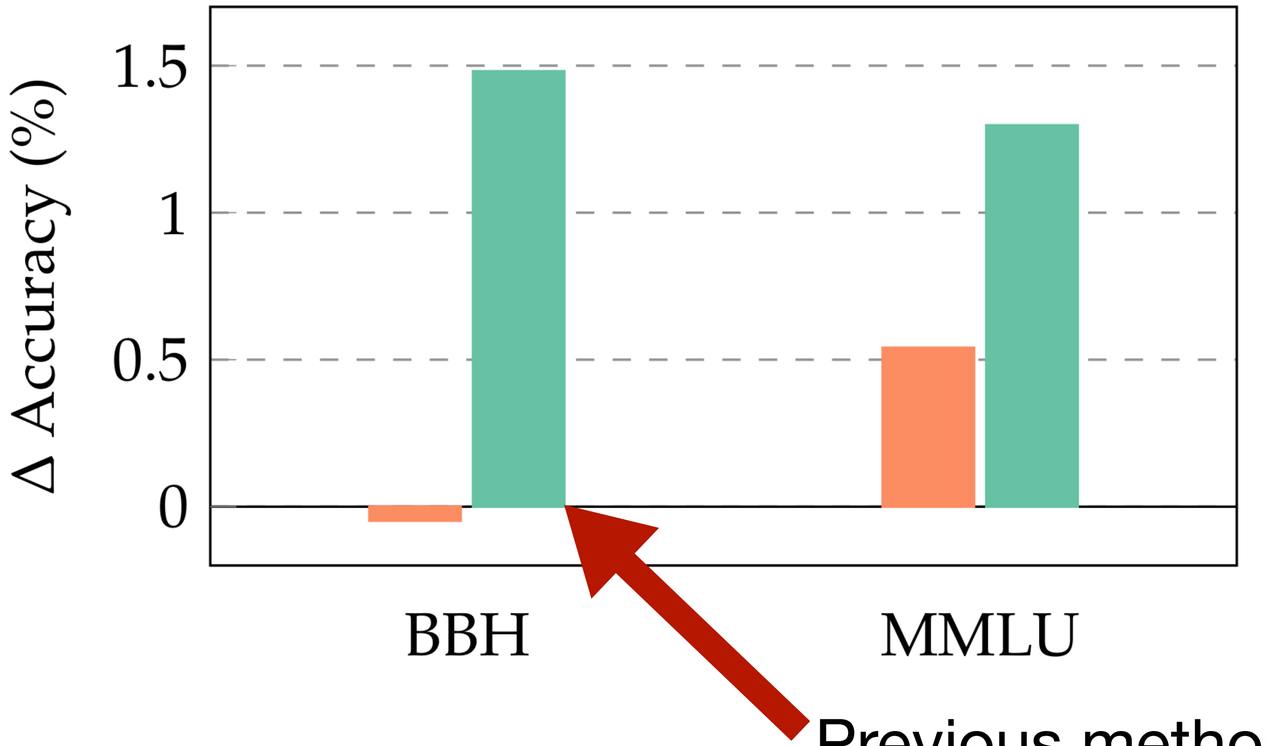

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Previous methods **harm** performance in BBH

Task: Selecting instruction fine-tuning data

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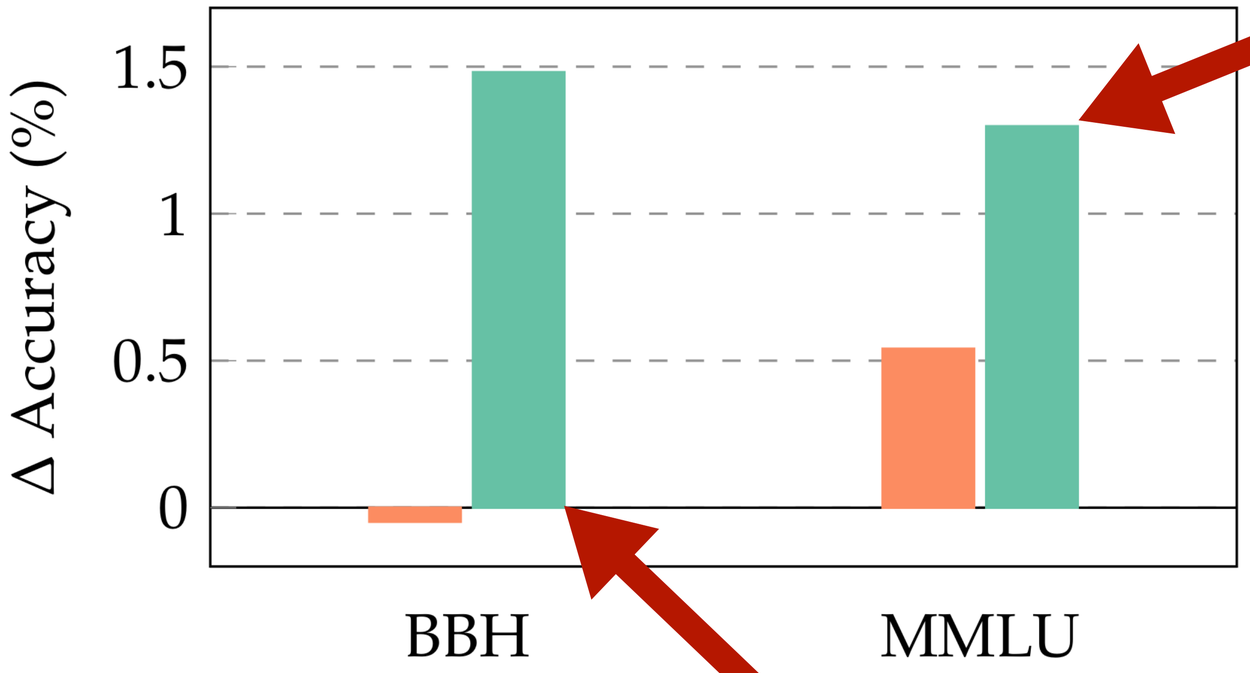

2x the improvement in MMLU

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Task: Poisoning CIFAR-10 training data

Setup

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Setup

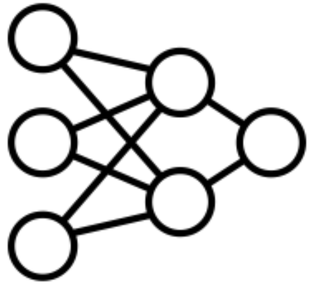
Insert poison data $\mathbf{z}$

Task: Poisoning CIFAR-10 training data

Setup

Insert poison data $\mathbf{z}$

Train model using fixed learning algorithm



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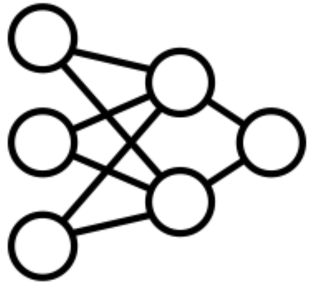

Goal: reduce overall test accuracy

CIFAR10: 85%

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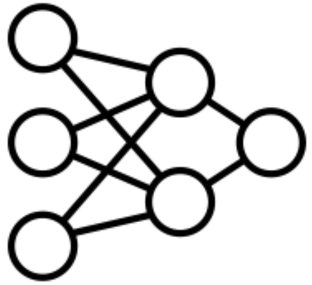

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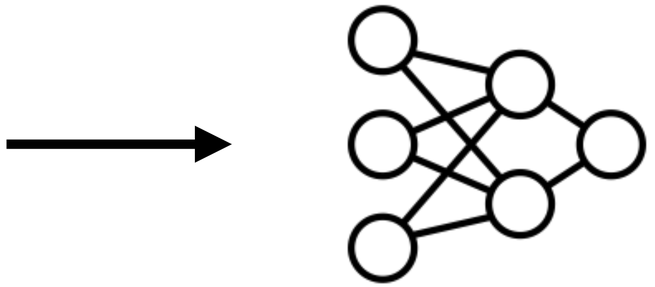

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> "However, in the setting of *indiscriminate* data poisoning, where an attacker aims to decrease the overall test accuracy by adding a small fraction of corrupted data, the effectiveness of existing attacks remains underwhelming."

[Lu Kamath Yu '23]

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Task: Poisoning CIFAR-10 training data

Approach

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(this is the full algorithm)

Task: Poisoning CIFAR-10 training data

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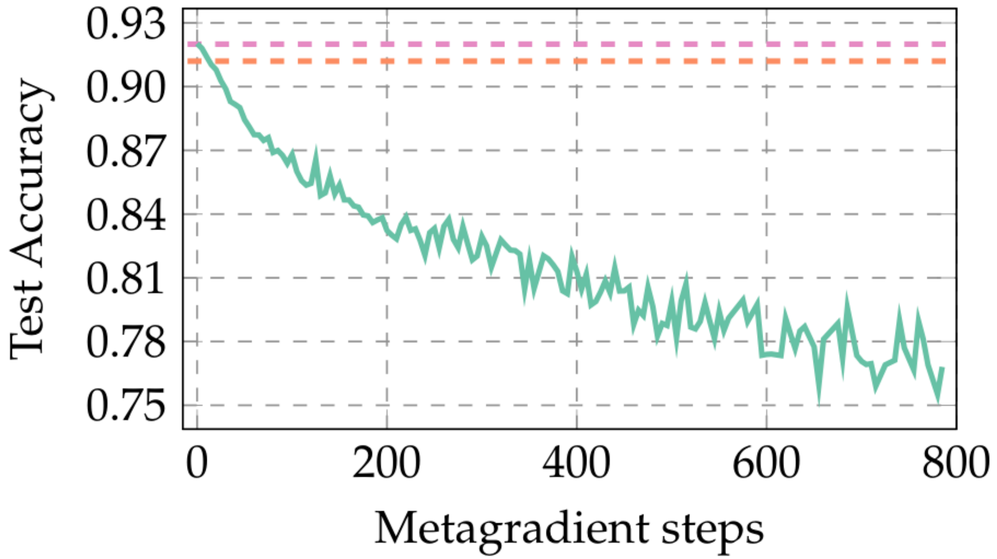

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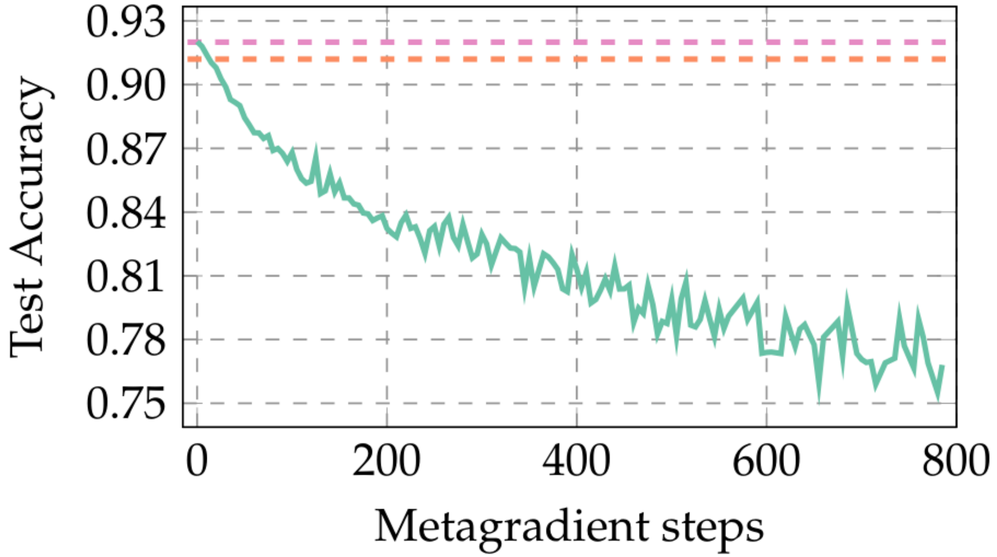

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MGD-DP (ours)	**78.1%**	**−13.9%**

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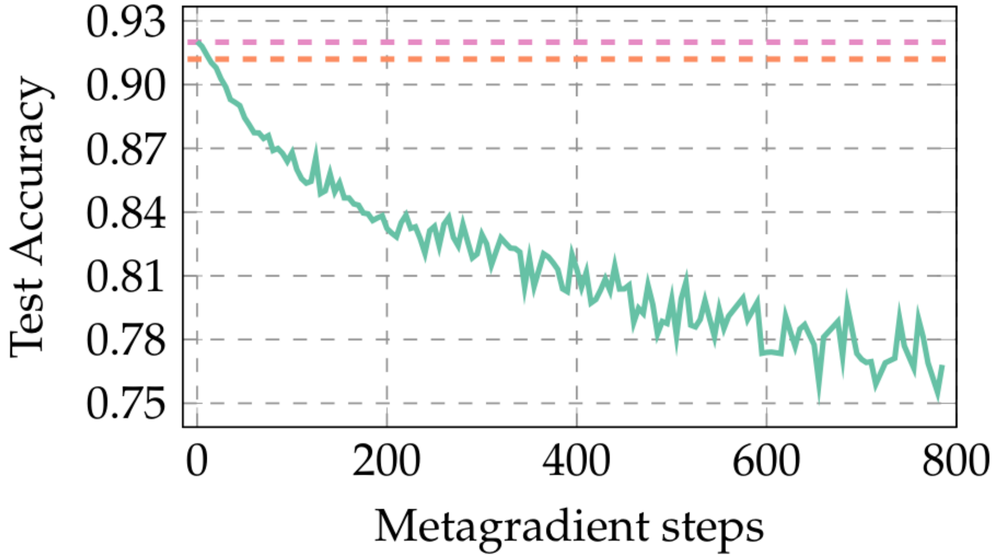

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Task: Poisoning CIFAR-10 training data

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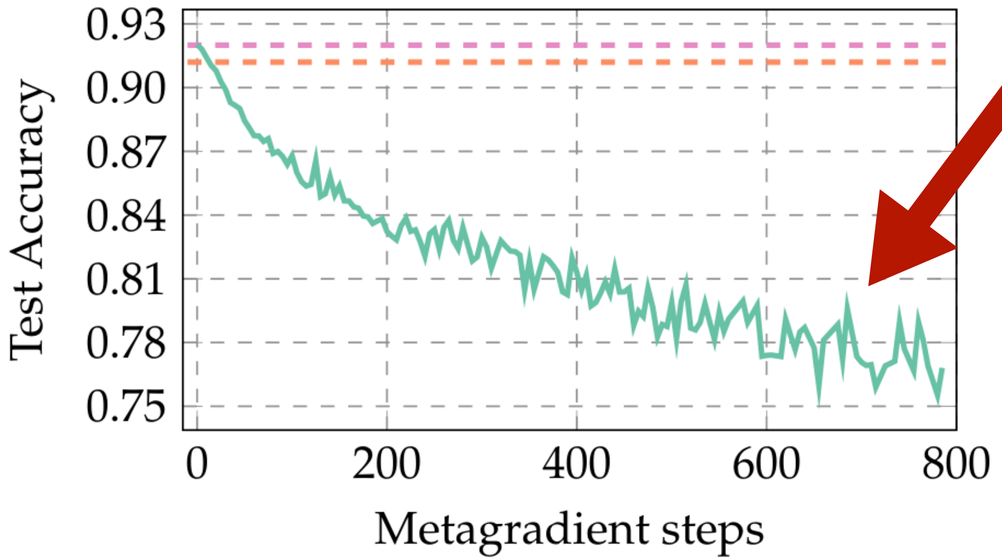

We induce 17x the accuracy drop vs. existing methods

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   This is just a linear function of $\mathbf{z}$, no “extra computation” beyond $\mathbf{z}_0$

Task: Training data attribution

Setup

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Setup

Choose train subset

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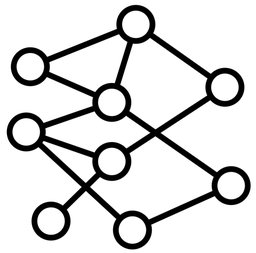
Train a model



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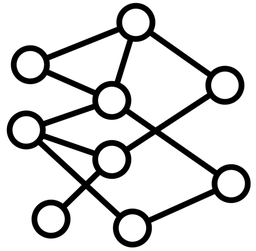
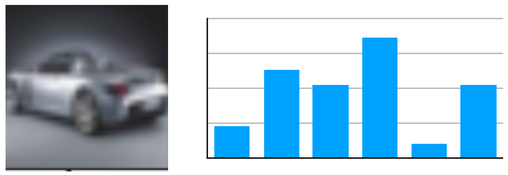


Measure loss on test example x:



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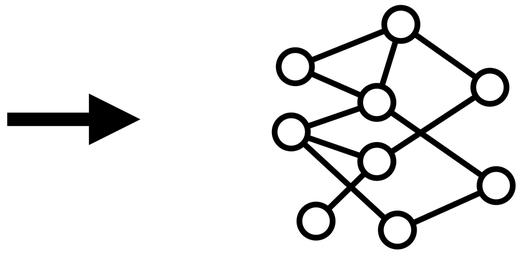

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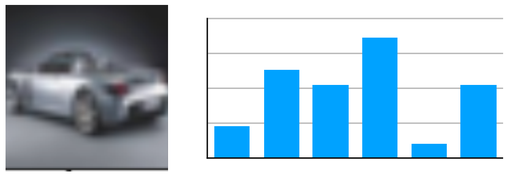

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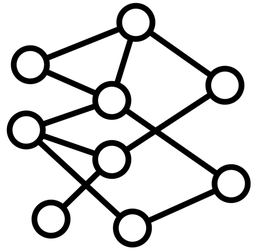

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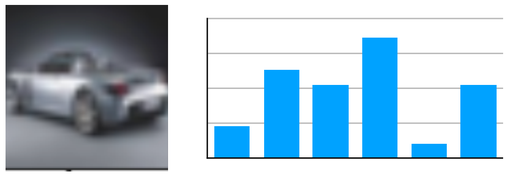

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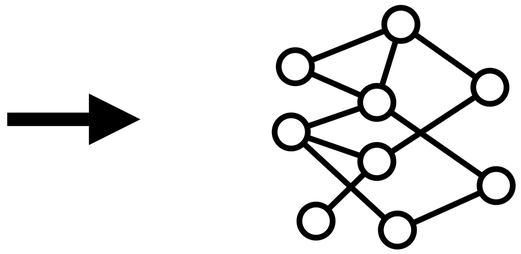

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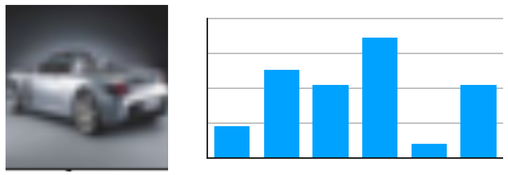

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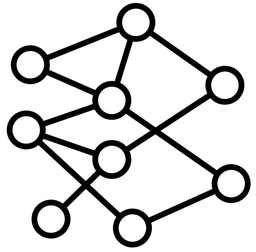

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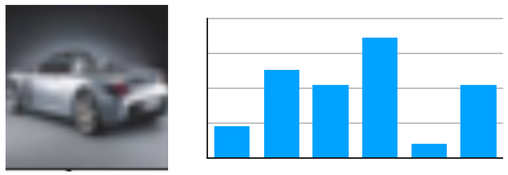

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[Park Georgiev | Leclerc Madry '24; Grosse Bae Anil et al. '24; many others]

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Metaparameter $\mathbf{z}$: vector $\mathbf{z} \in \mathbb{R}^n$ s.t., $\mathbf{z}_i$ is the weight on i-th training example

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AKA the exact influence function (Hampel ’47)

Task: Training data attribution

Results

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Deleting 1% random subsets from CIFAR-10 training:

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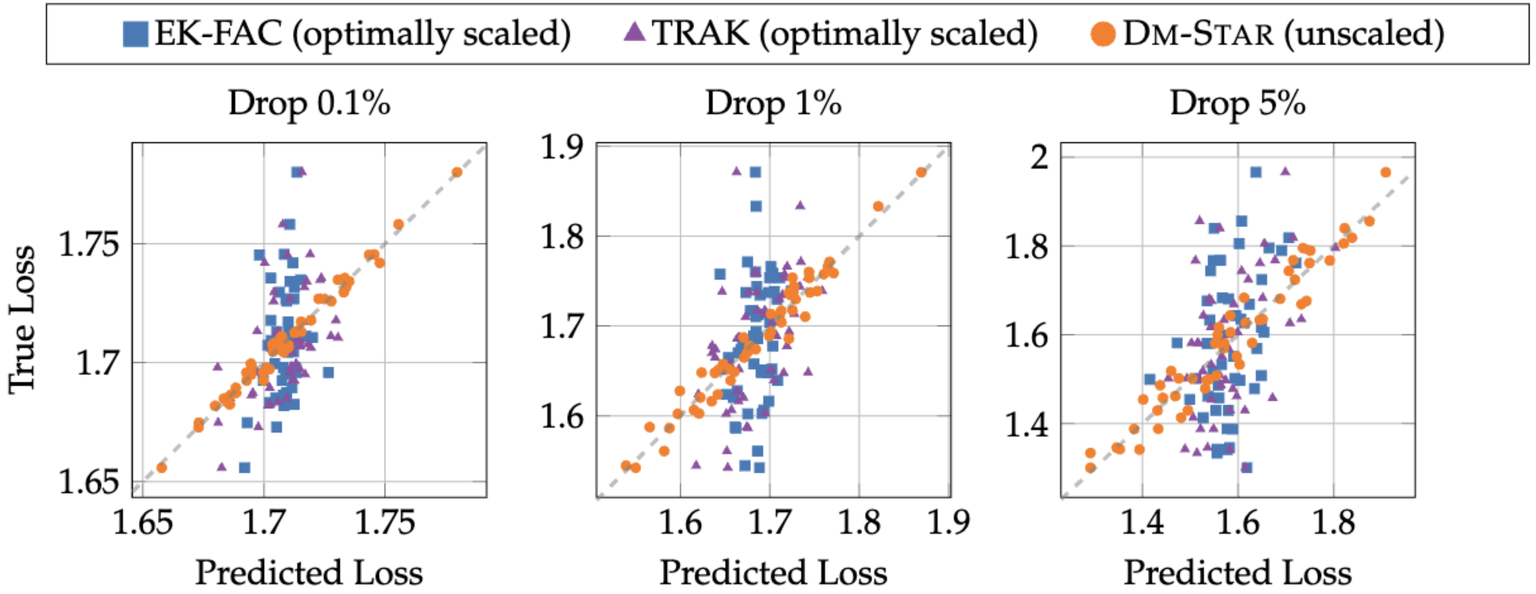

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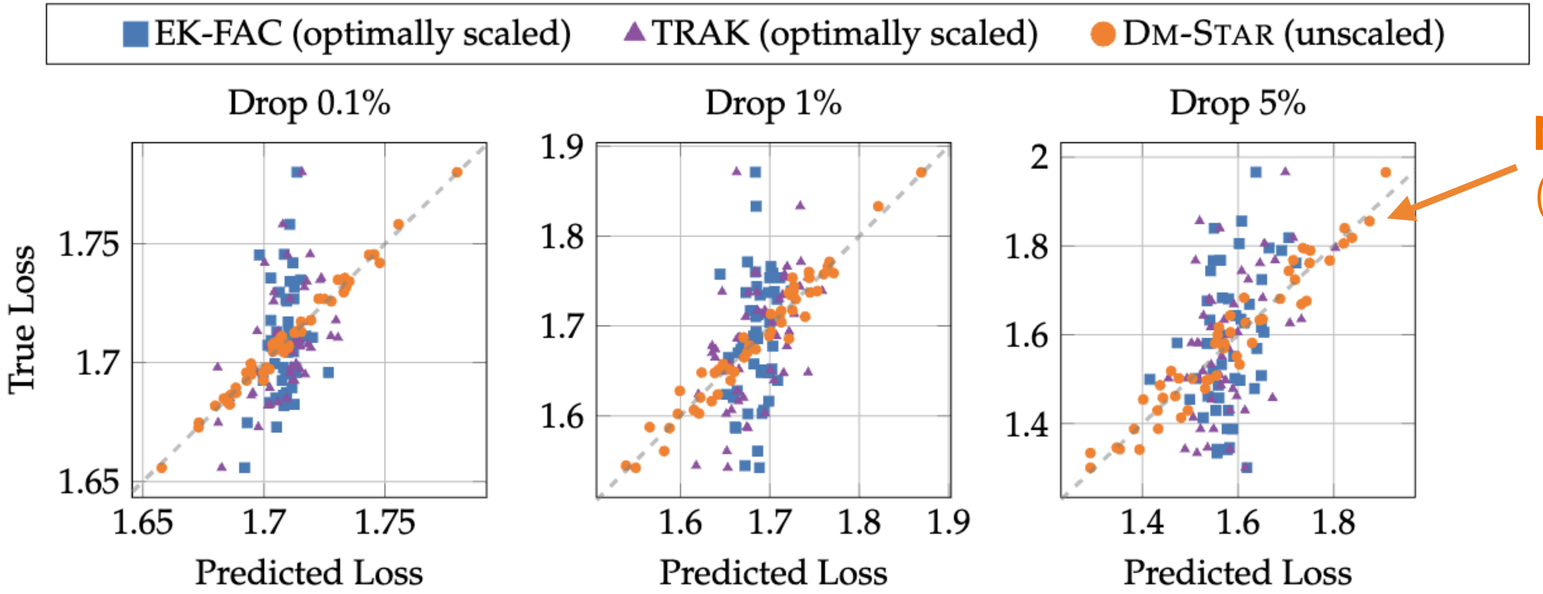

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($\rho = 0.9$, well-scaled)

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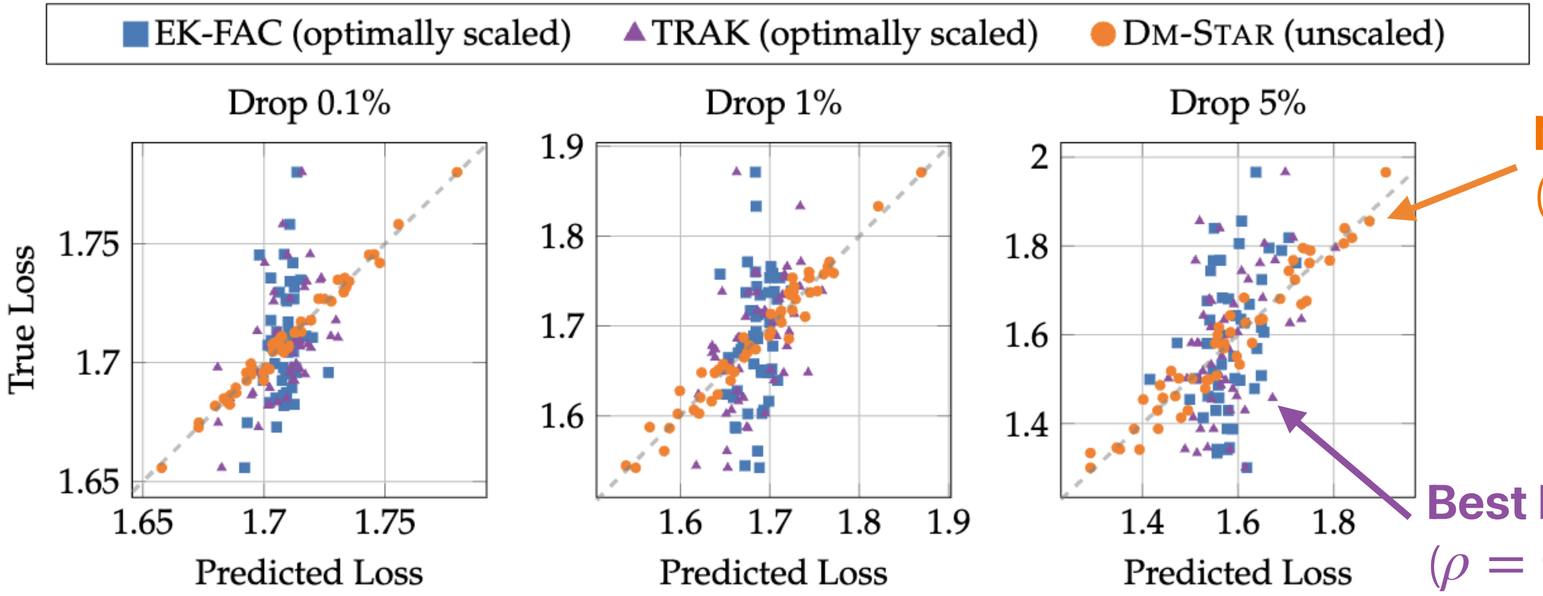

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Best baseline
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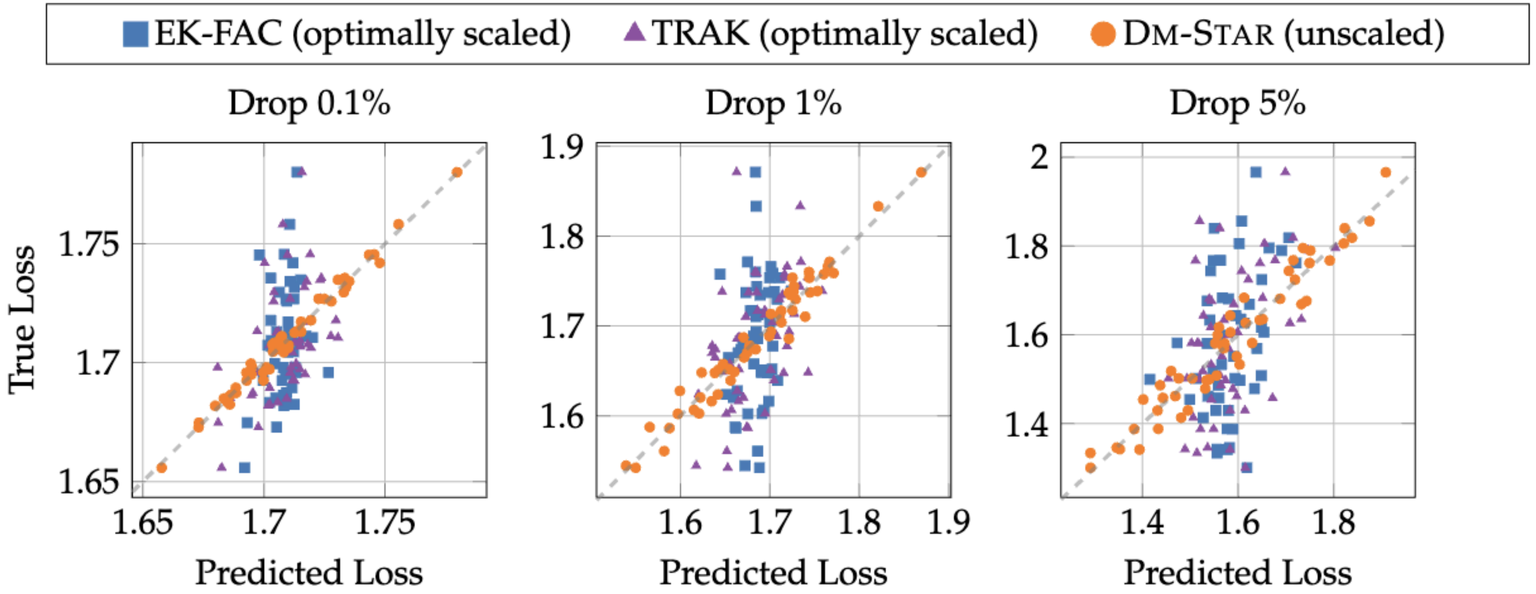
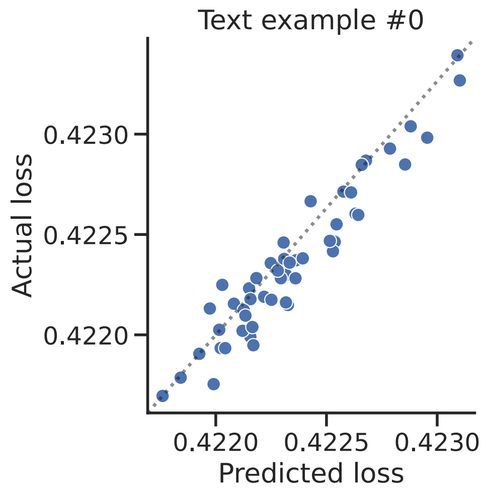


Also works for LMs!

Deleting 1% of data from Gemma-2B fine-tuning



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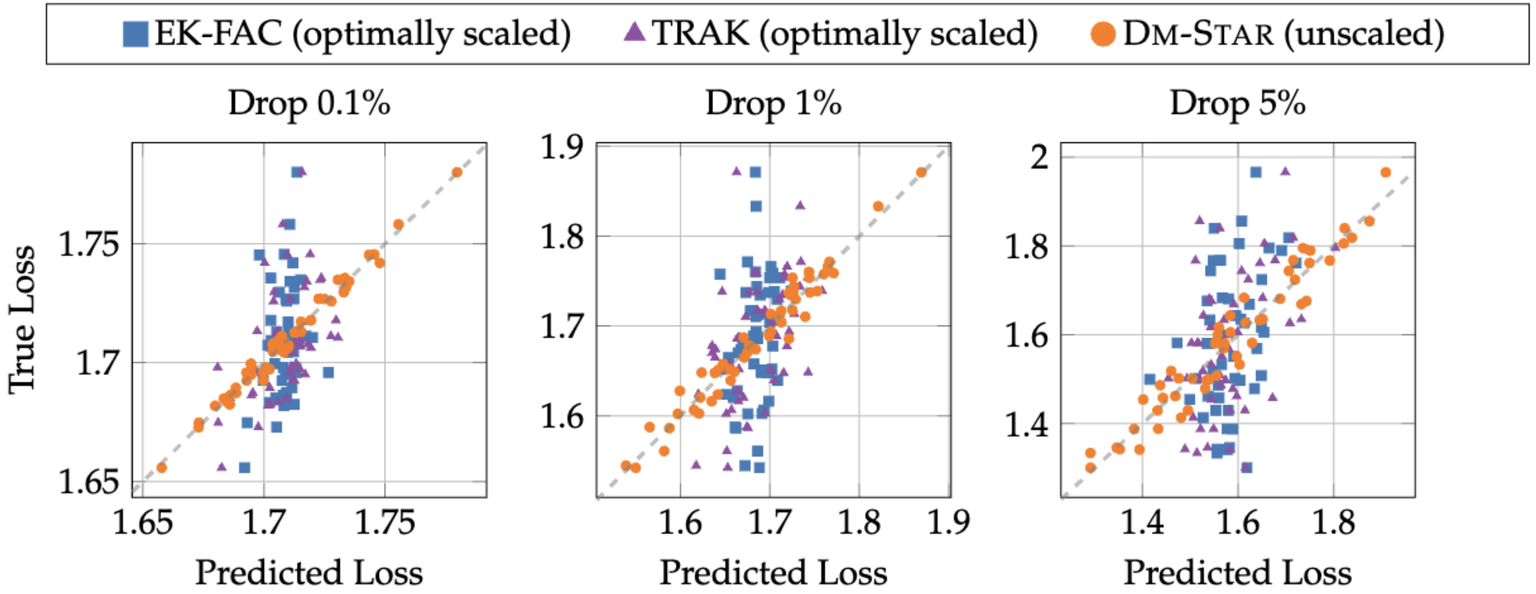

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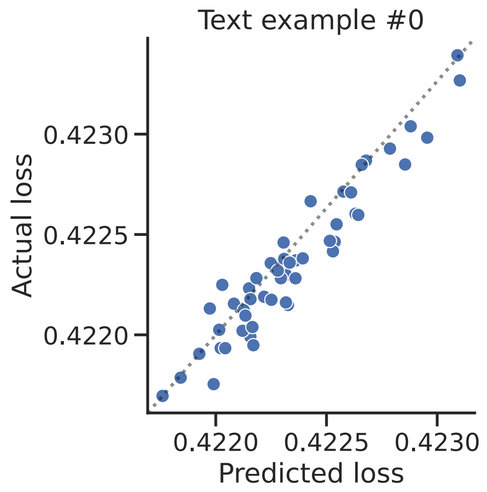

(From a different paper; online soon!)

Roadmap

~~Main idea: The metagradient~~

Prequel: Two challenges

Looking forward

A brief history of the metagradient

Why hasn't this been done before?

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Exact metagradients at small scale [Maclaurin Duvenaud Adams '15; Franceschi et al. '17; ...]

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Broadly, nothing has scaled to "medium"-size training (e.g., >10M params, >1k iters)

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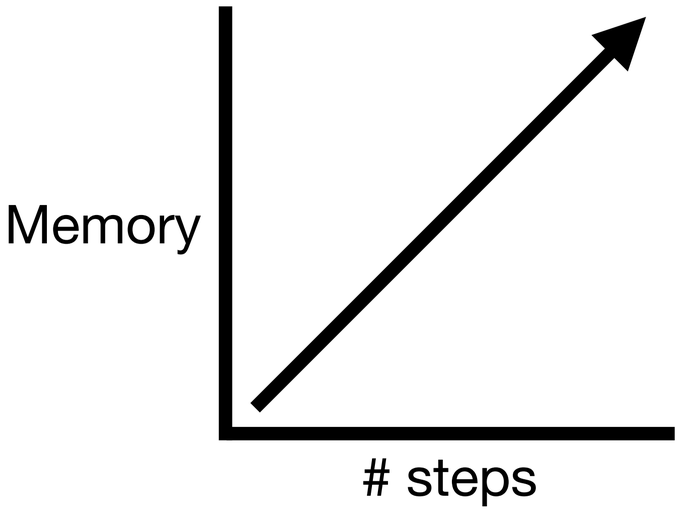

#1: Computational tractability

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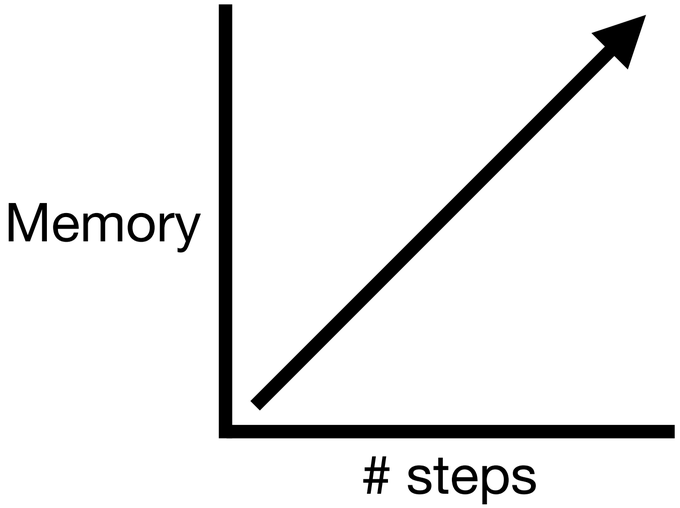

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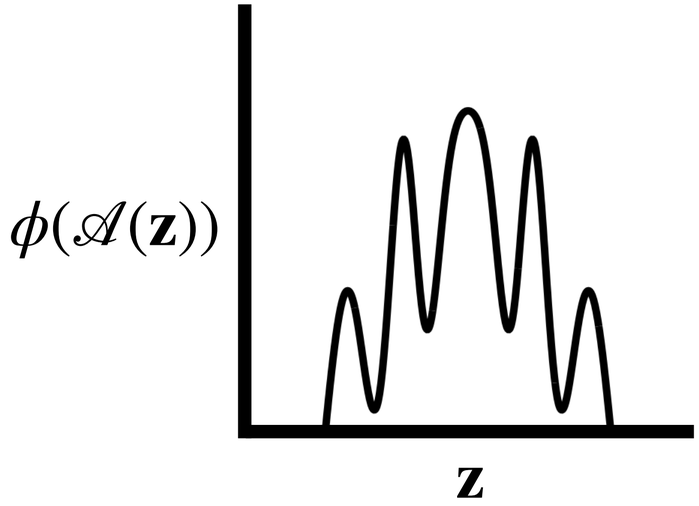

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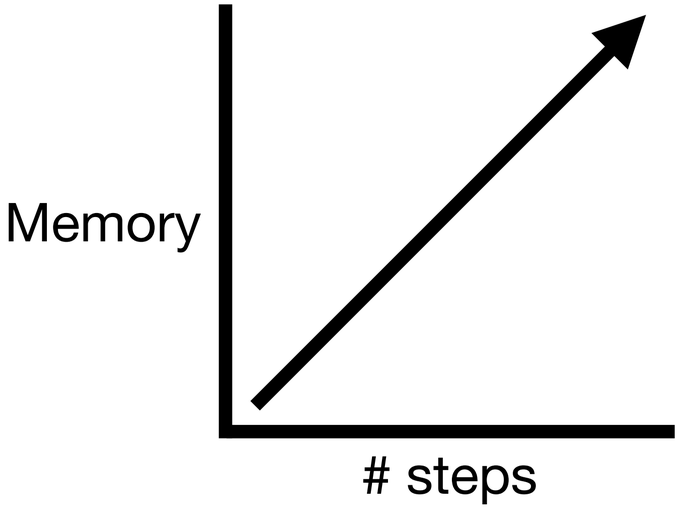

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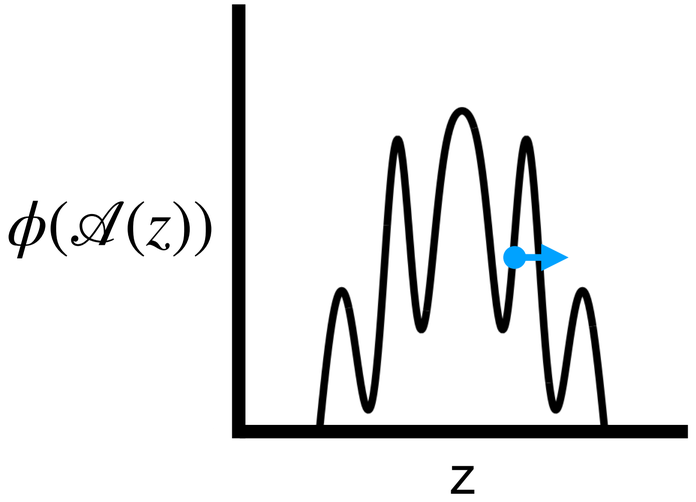

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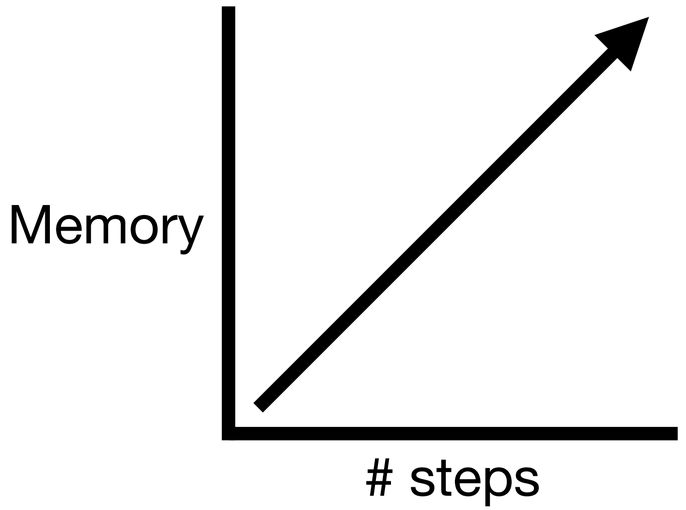

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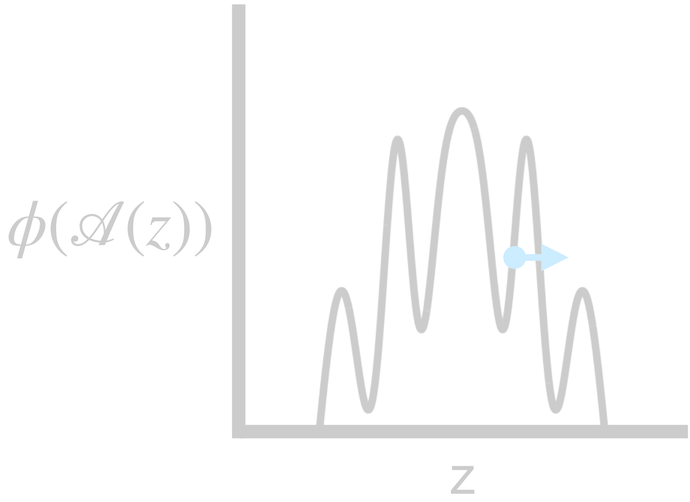

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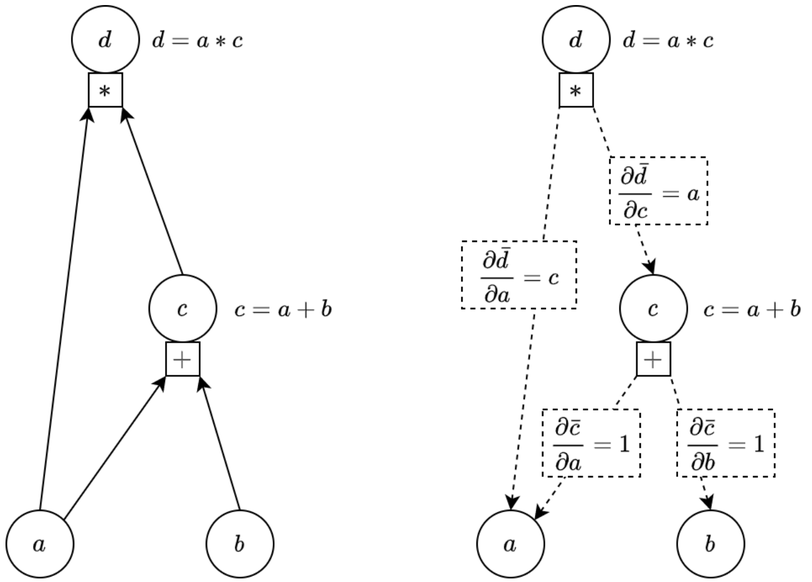

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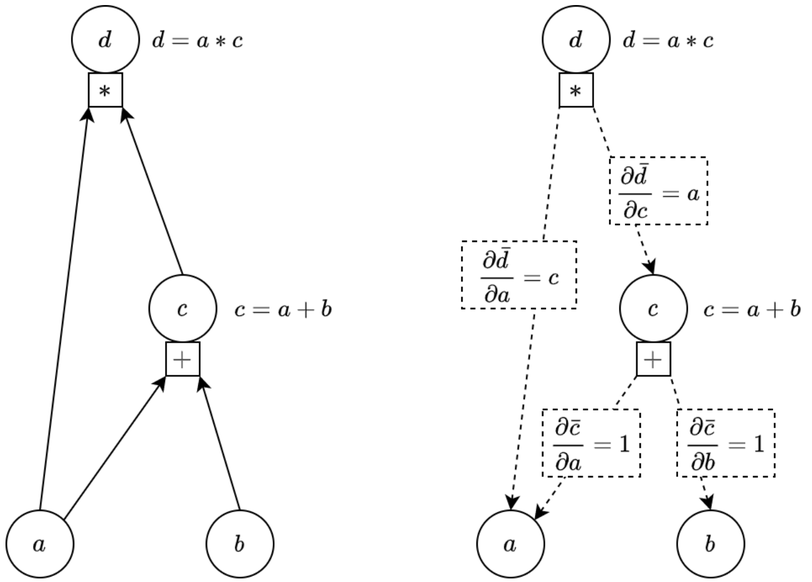
Key insight: Training an ML model is just a (very, very, very long) sequence of operations! Maybe we can just backprop through it?



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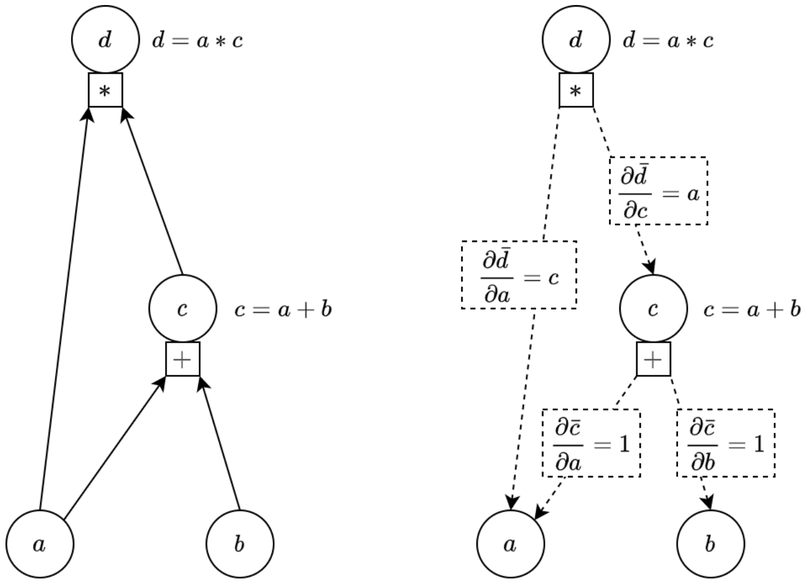

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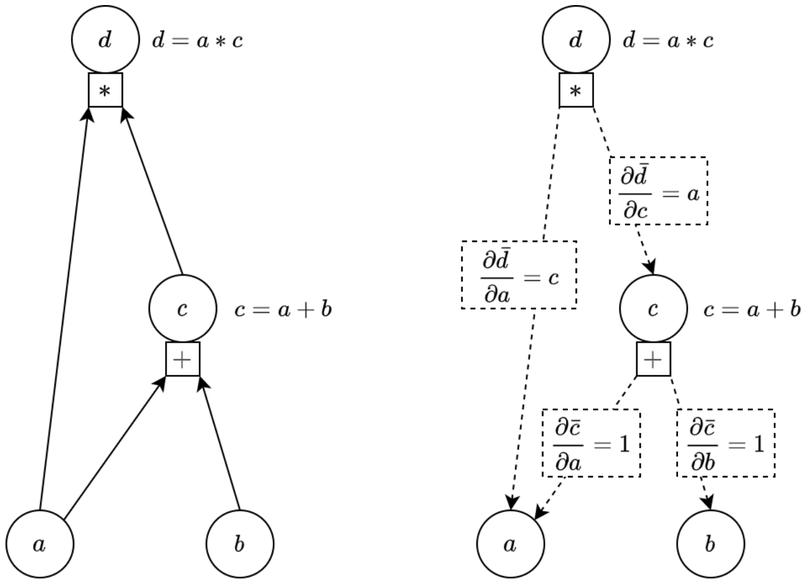

We will think of AD as a black box that can compute gradients of a many $\rightarrow$ one compute graph $O(\#\text{ edges})$ memory

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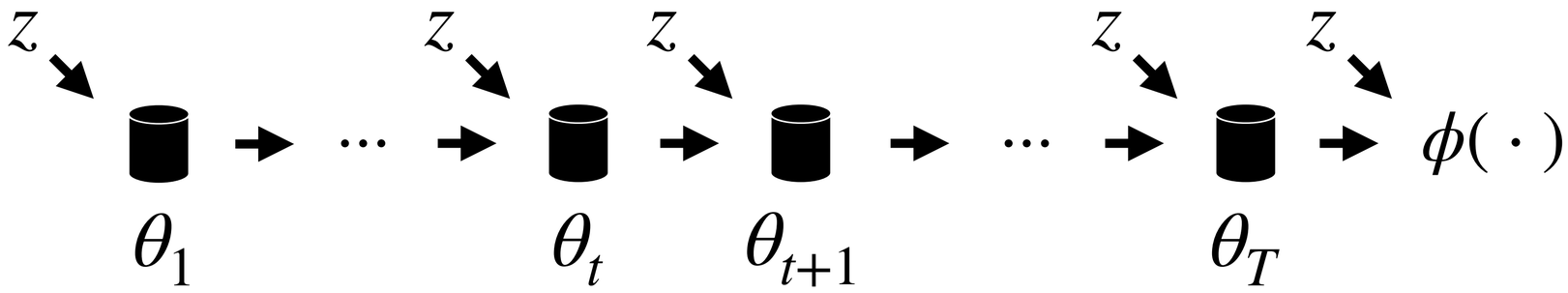

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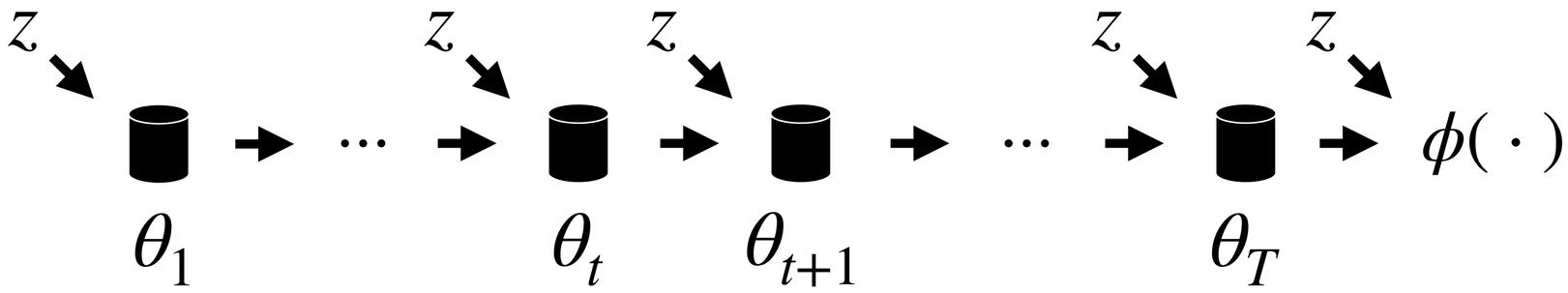

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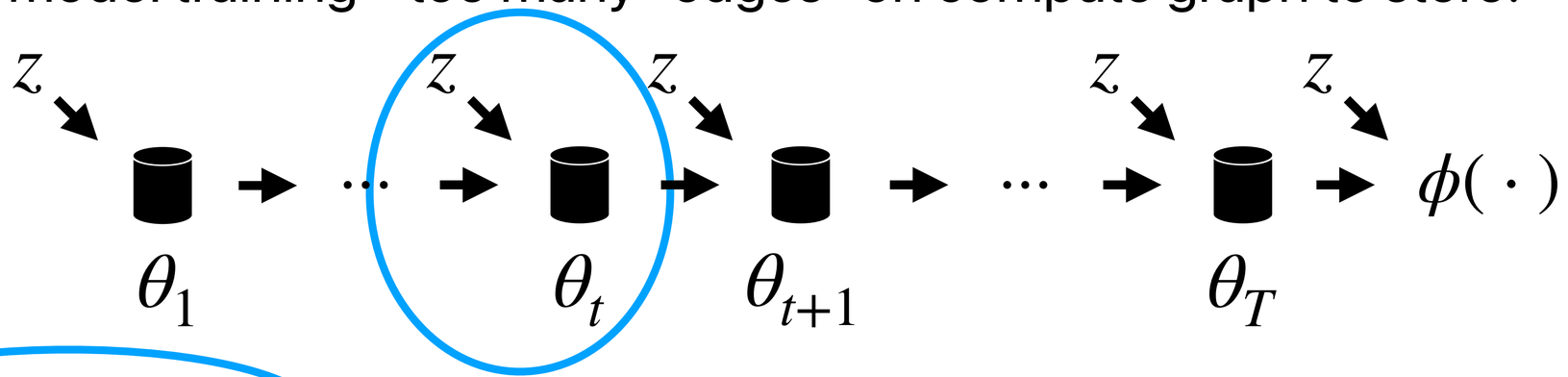

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$$\frac{df(z)}{dz} = \frac{df(z)}{d\theta_{t+1}} \cdot \frac{d\theta_{t+1}}{dz} \qquad \frac{df(z)}{d\theta_t} = \frac{df(z)}{d\theta_{t+1}} \cdot \frac{d\theta_{t+1}}{d\theta_t}$$

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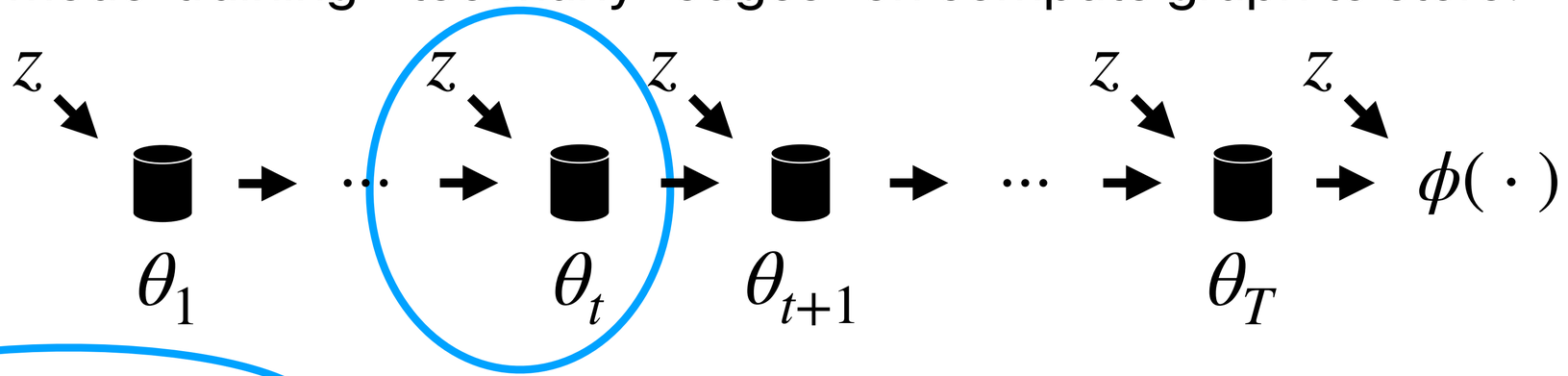

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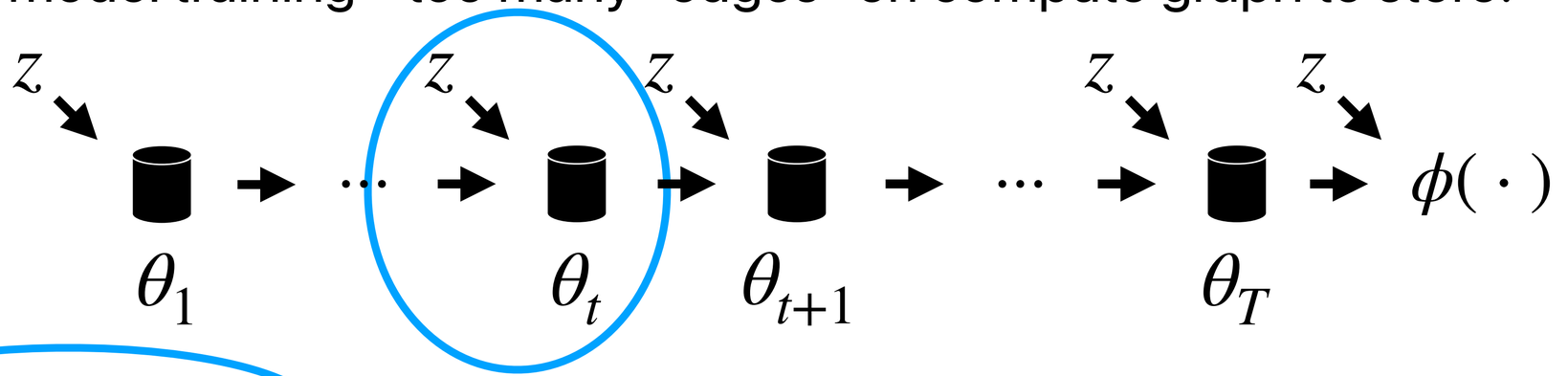

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Algorithm: save all states $\{\theta_i\}_{i=1}^{T}$, do autograd one step at a time from iterate T down to 1

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REPLAY: Efficiently calculating metagradients at scale

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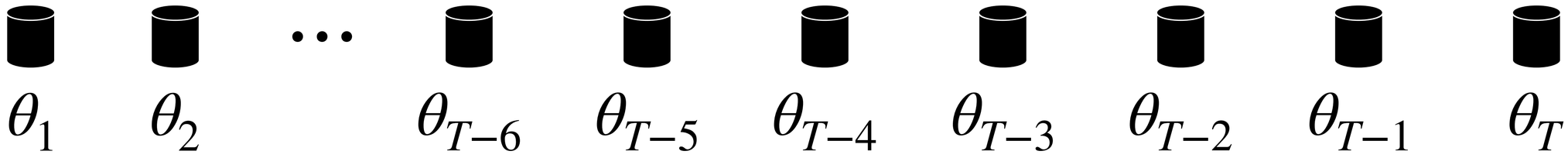

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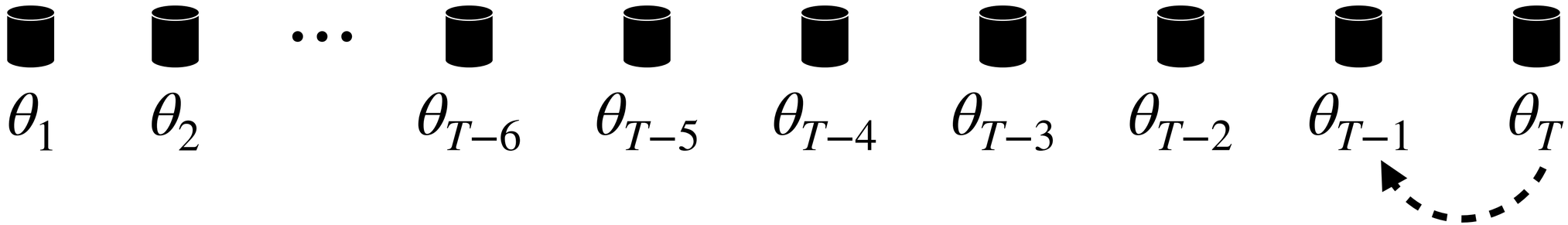

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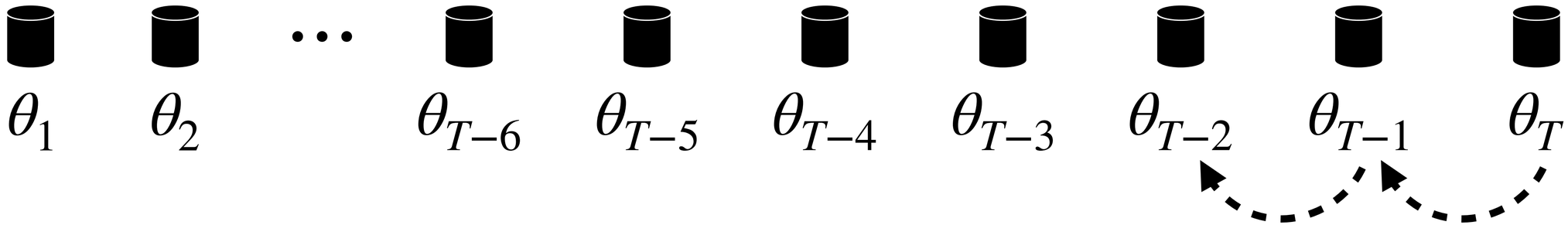

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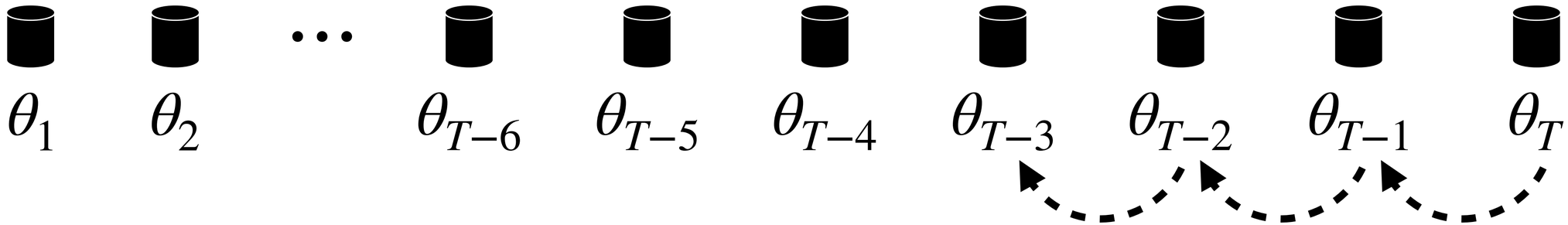

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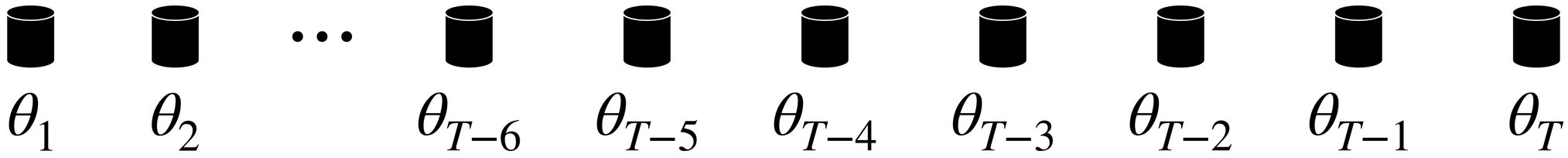

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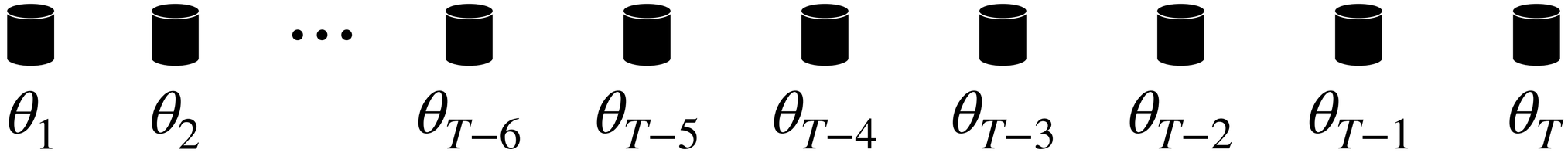

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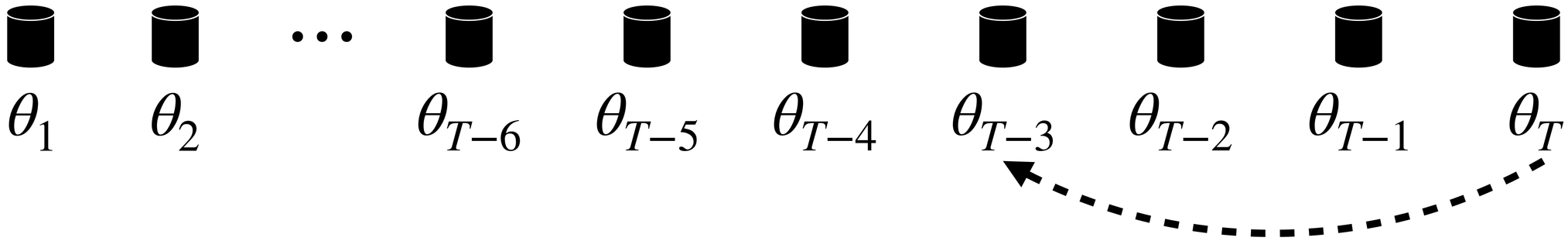

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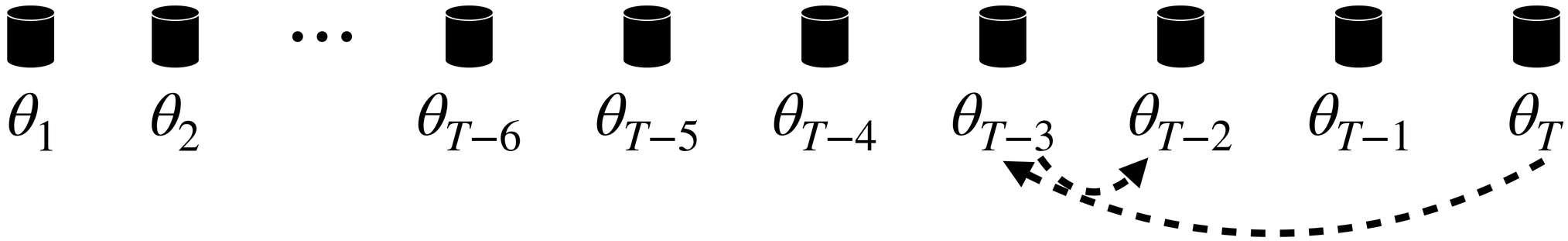

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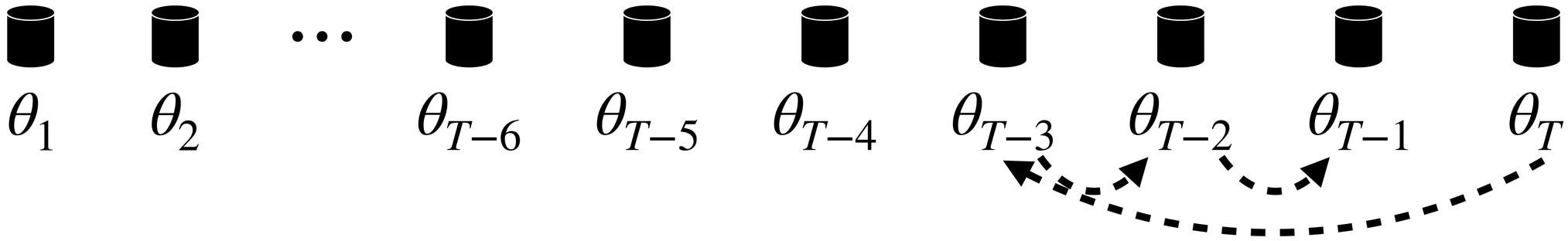

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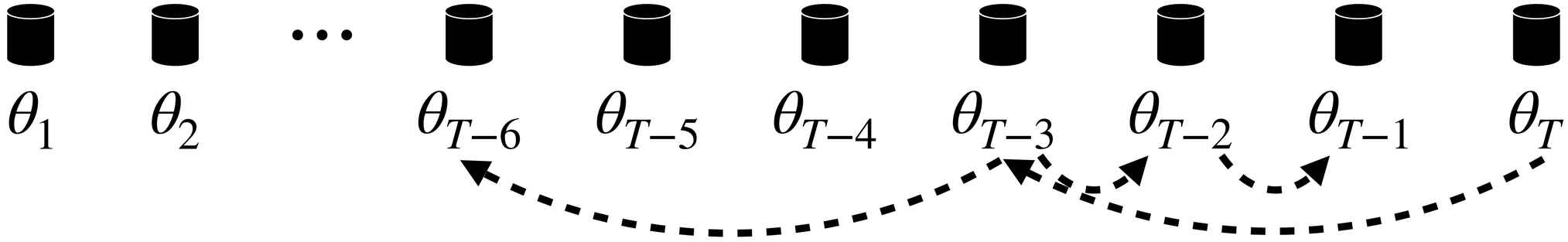

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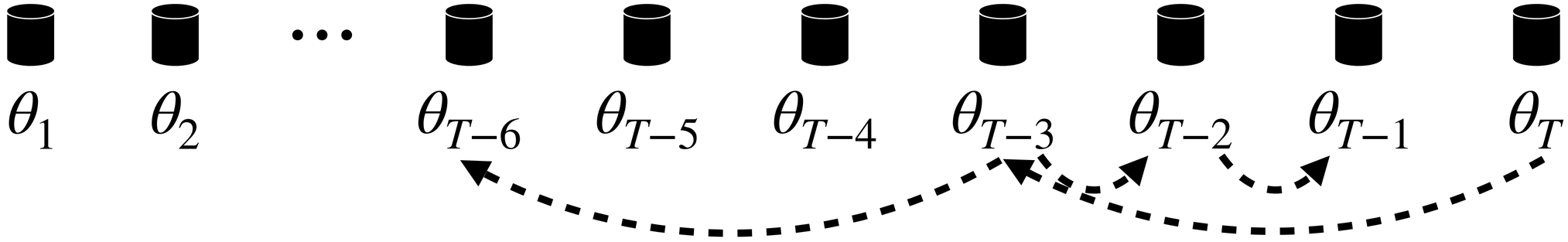

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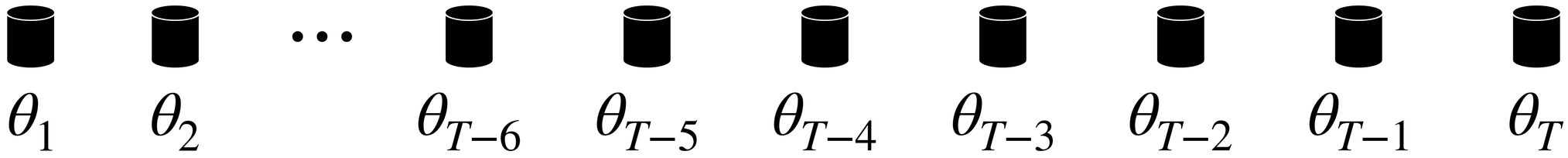

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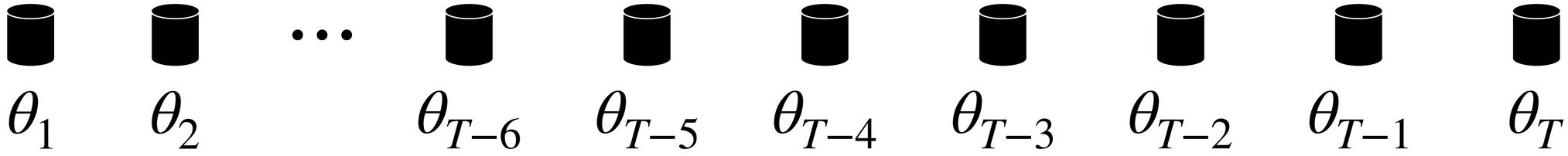

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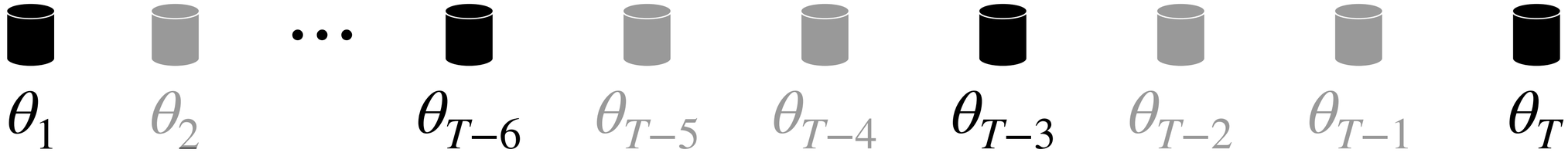

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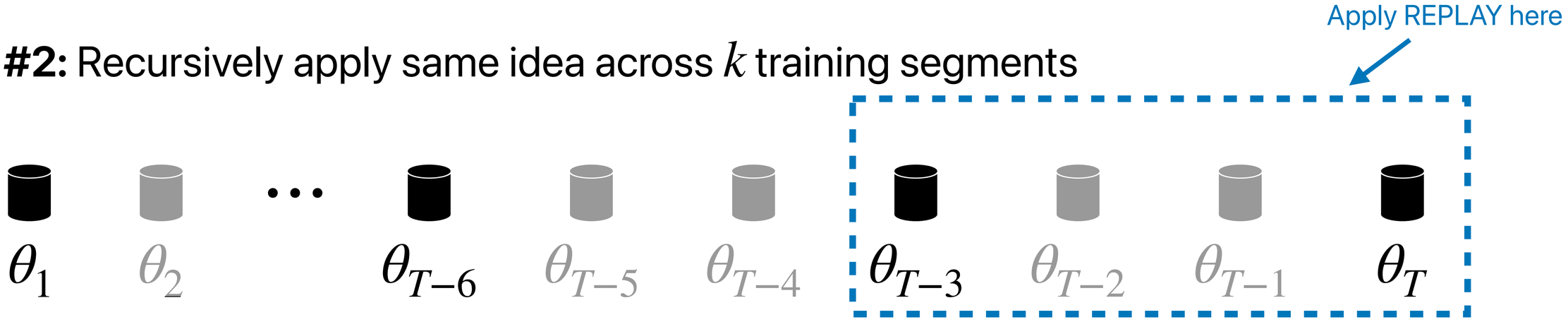

Problem #1: Calculating the gradient

REPLAY: Efficiently calculating metagradients at scale

A simple modification: REPLAY (Recursive rematerialization for metagradients)

Key primitive of step-wise AD: **traversing** the states $\theta_T \ldots \theta_1$ in reverse order
(Maclaurin Duvenaud & Adams, 2015)

Deterministic training allows us to "replay" from a previous state to rematerialize

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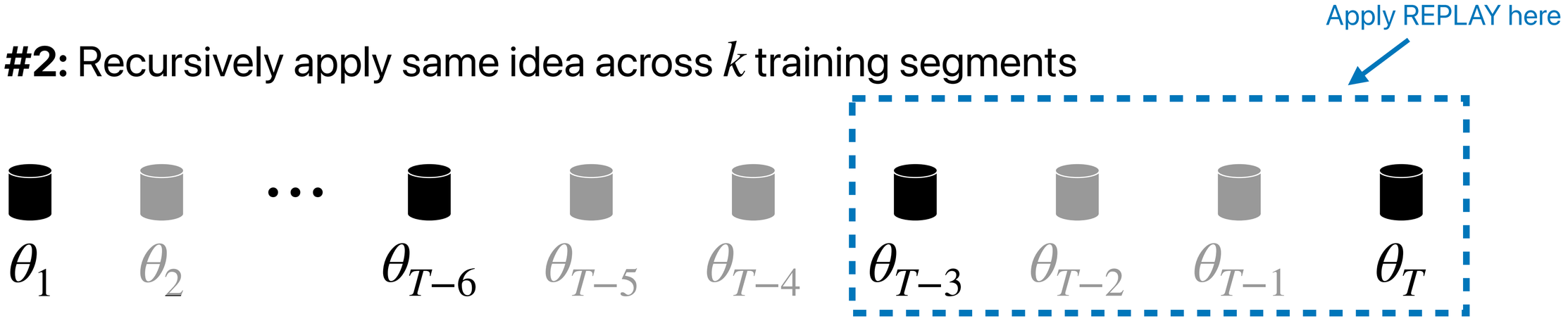

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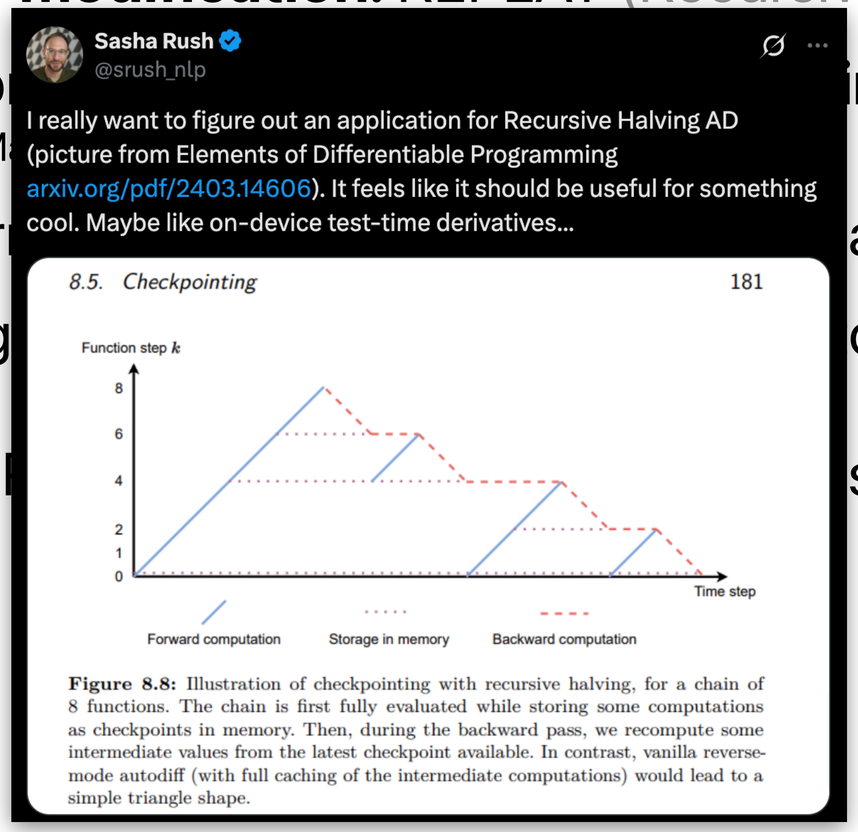

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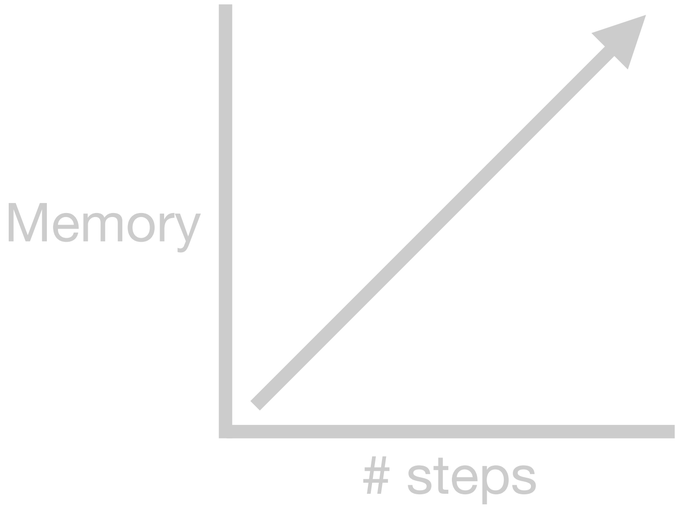
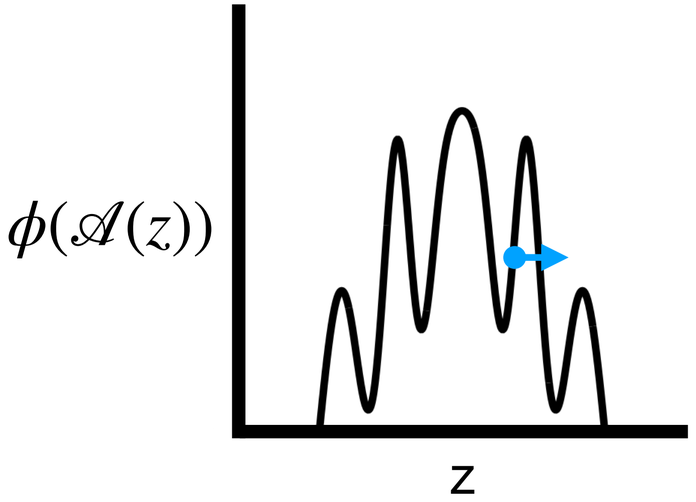
Metagradient roadmap: Two challenges

Two barriers to optimizing with the metagradient $\nabla_z \phi(\mathcal{A}(z))$



#1: Computational tractability



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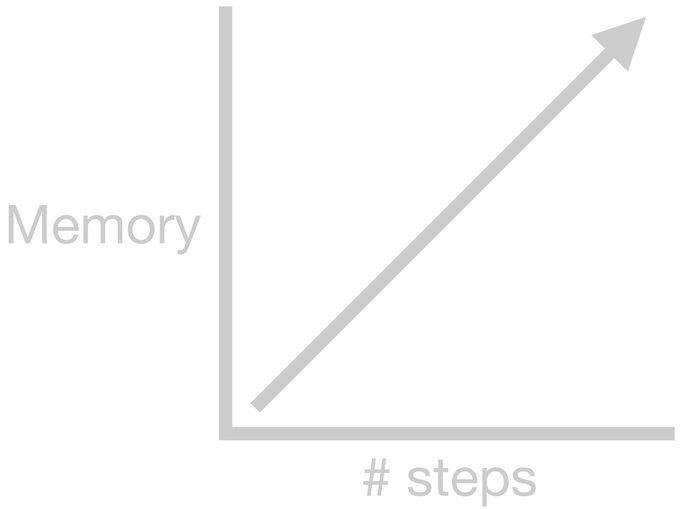

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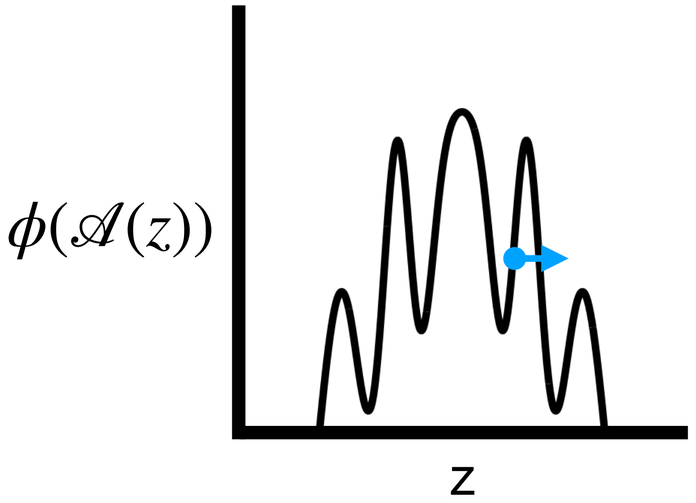

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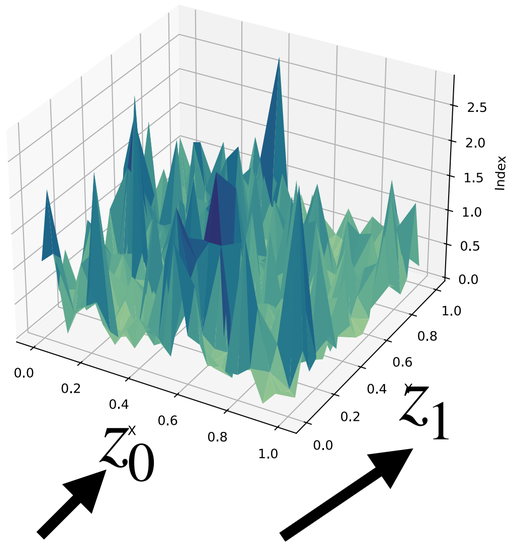

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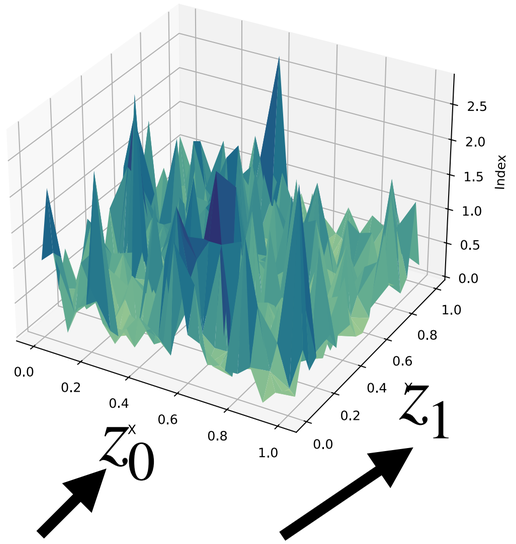

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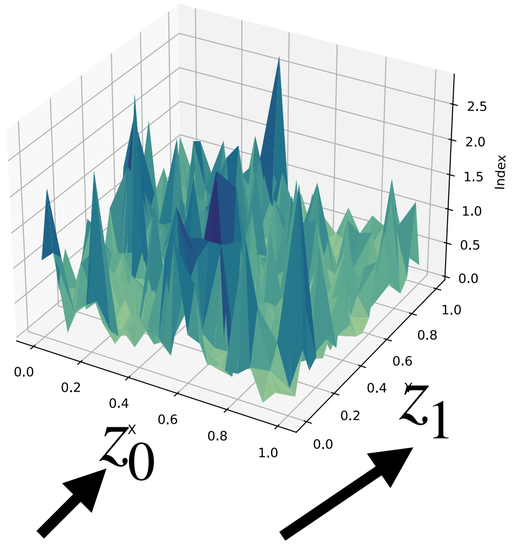

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Need to find "smooth" model training routines!

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We adapt this estimator to a new metric Metasmoothness$(\mathscr{A}) \in [-1,1]$

Our final estimator: feasible, interpretable, and accurate!

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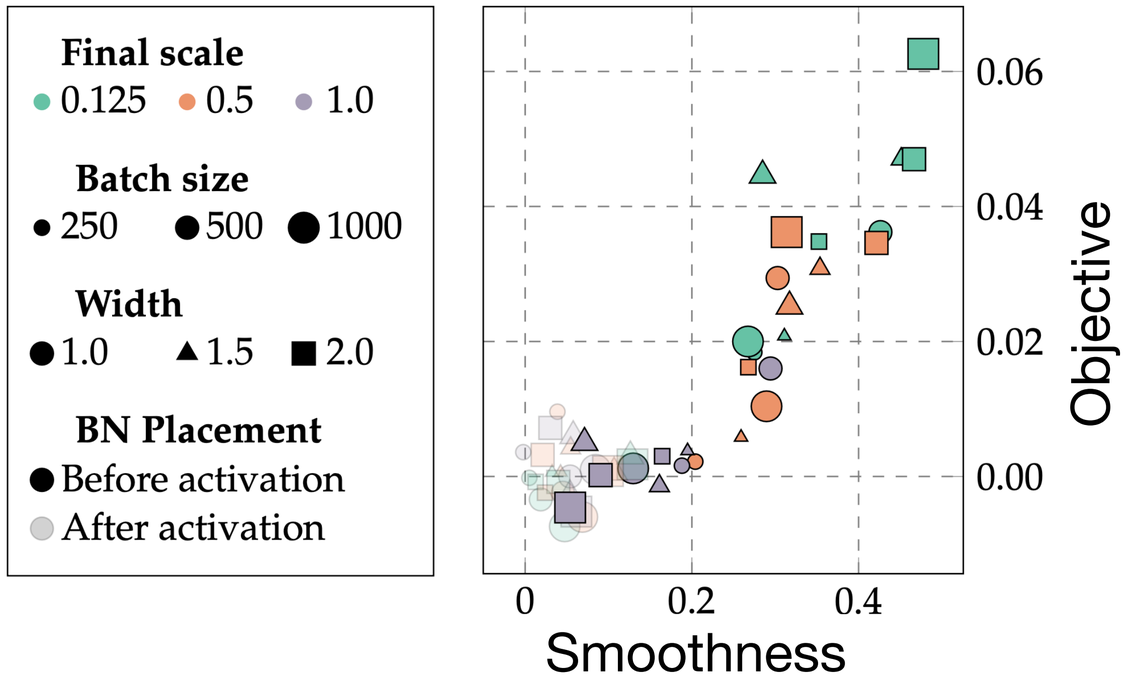

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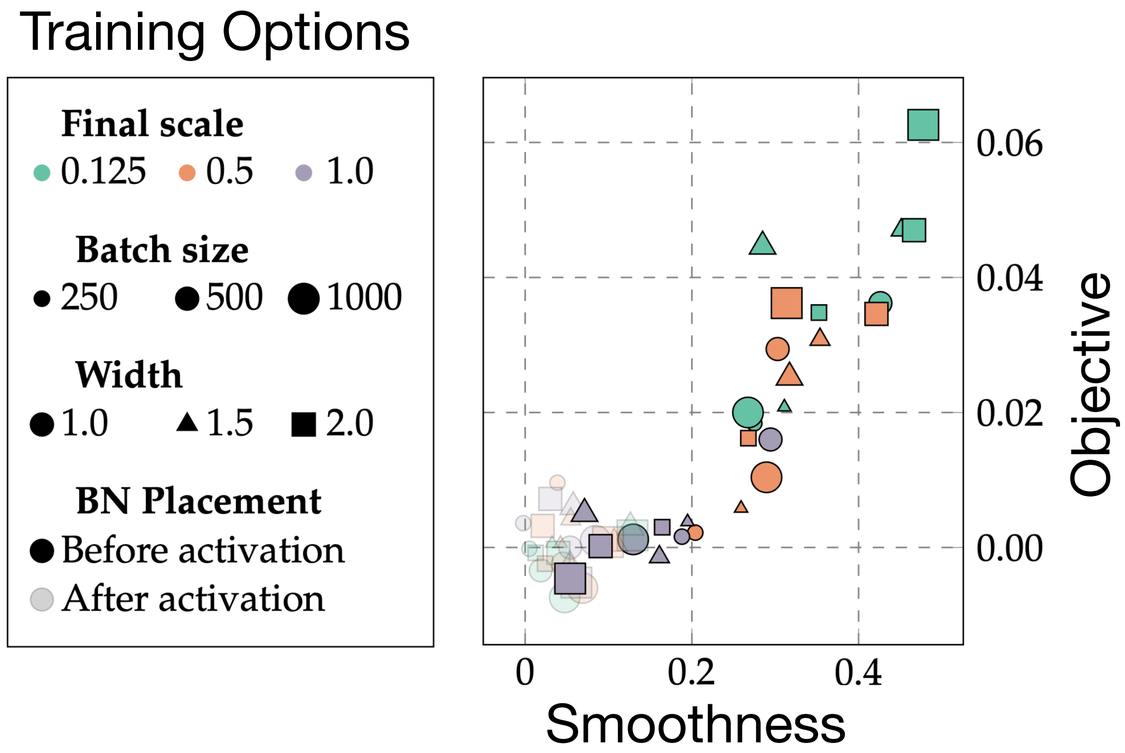

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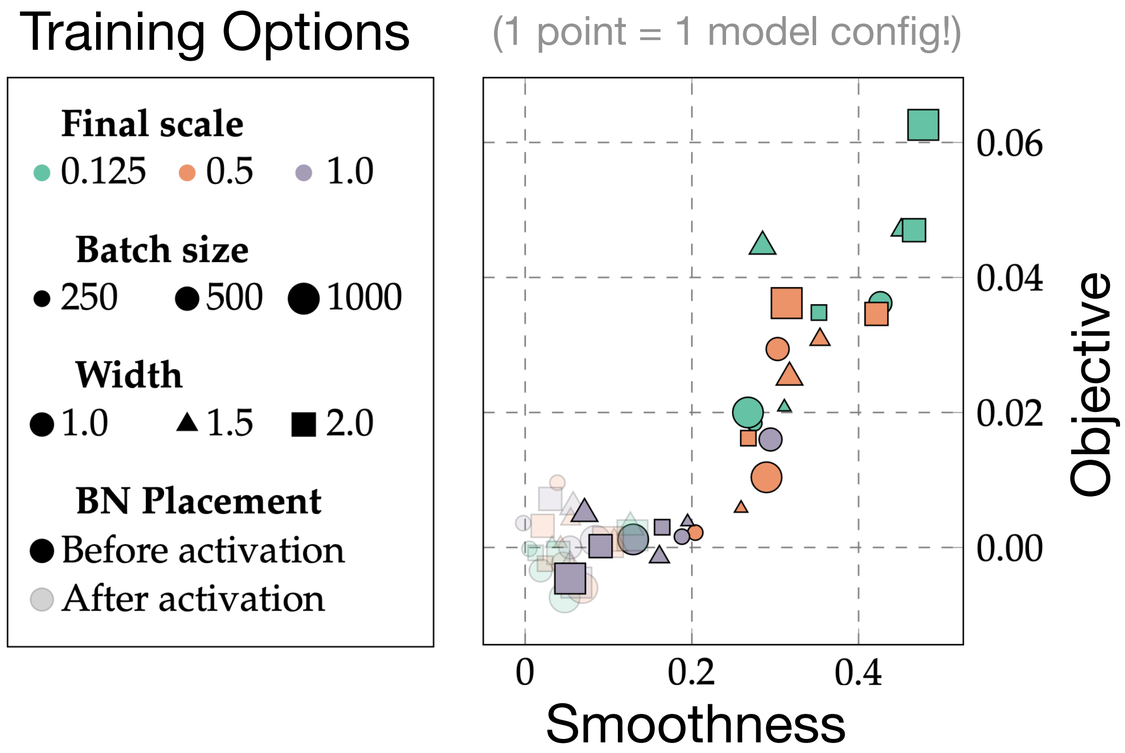

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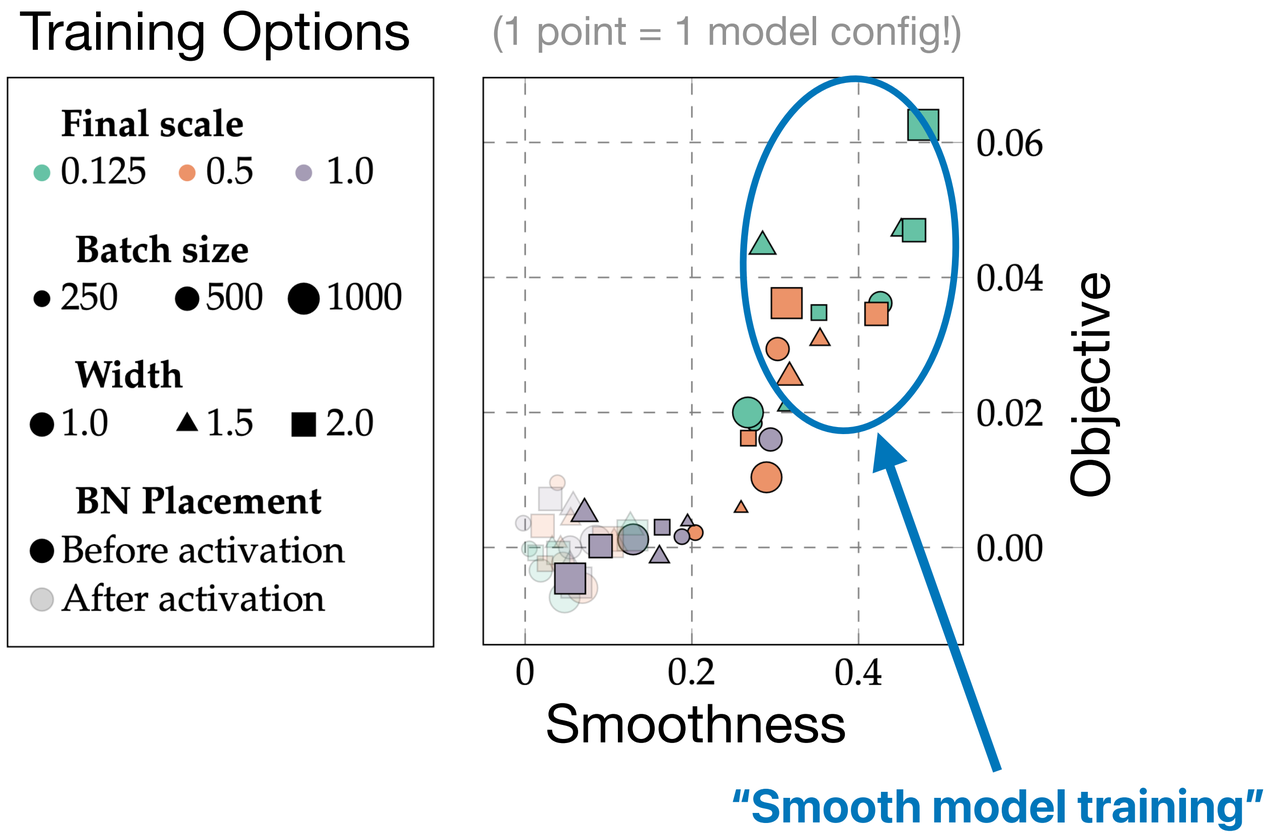

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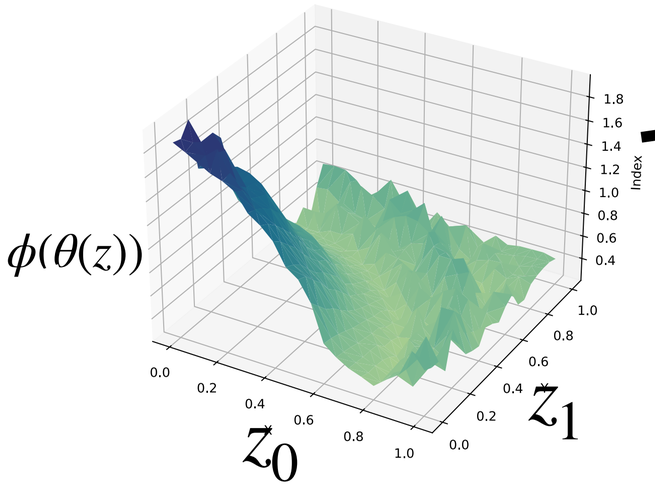

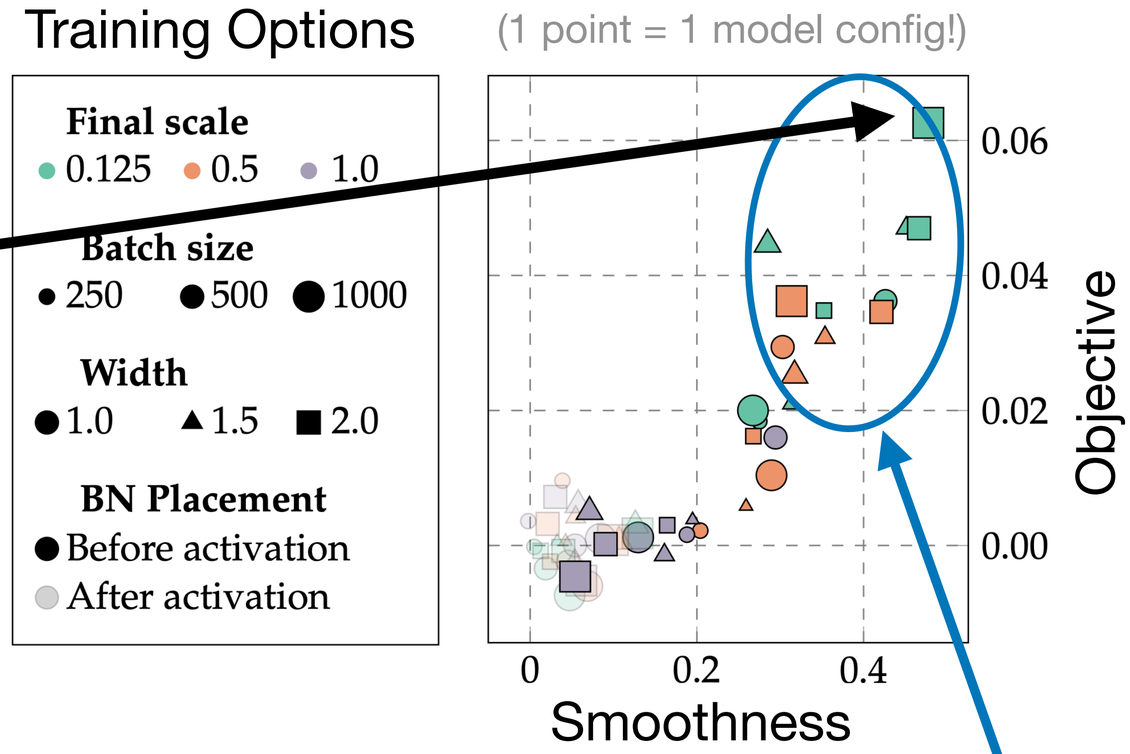

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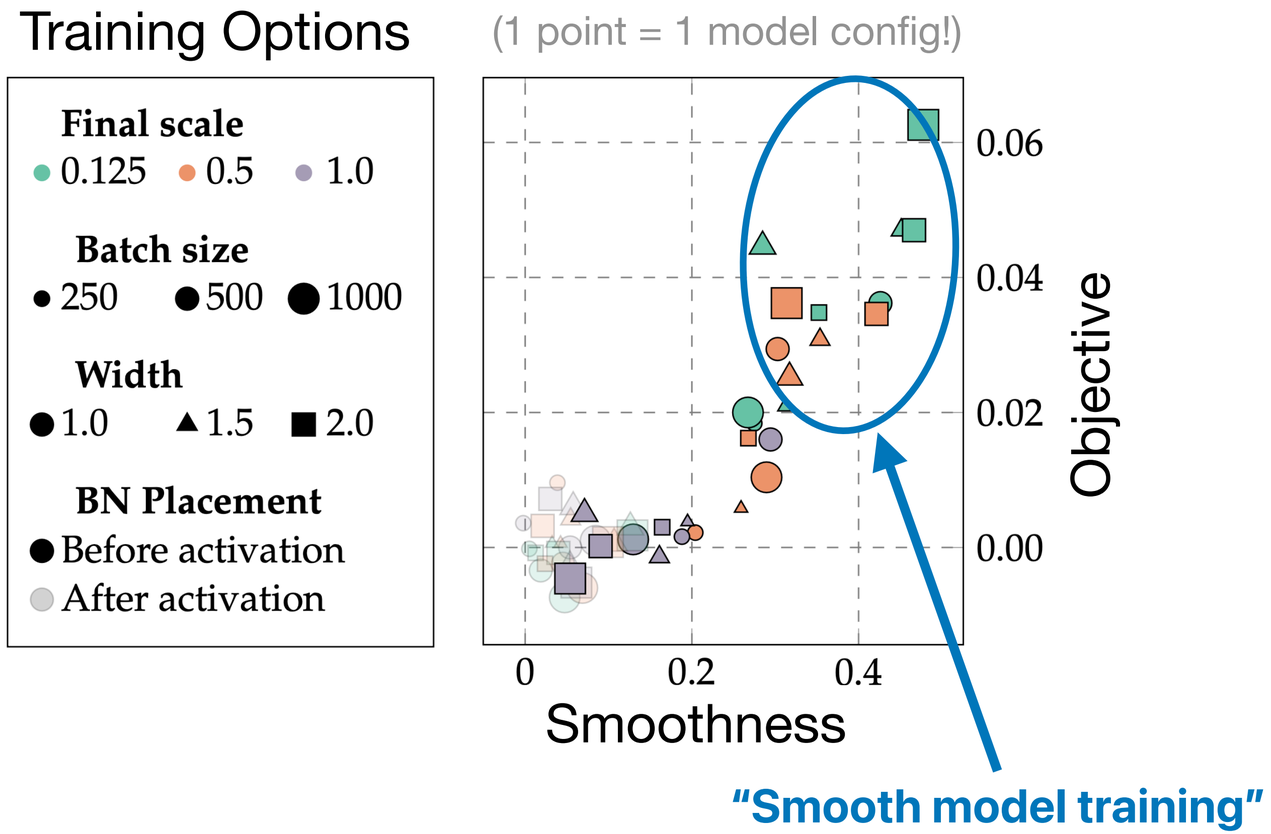

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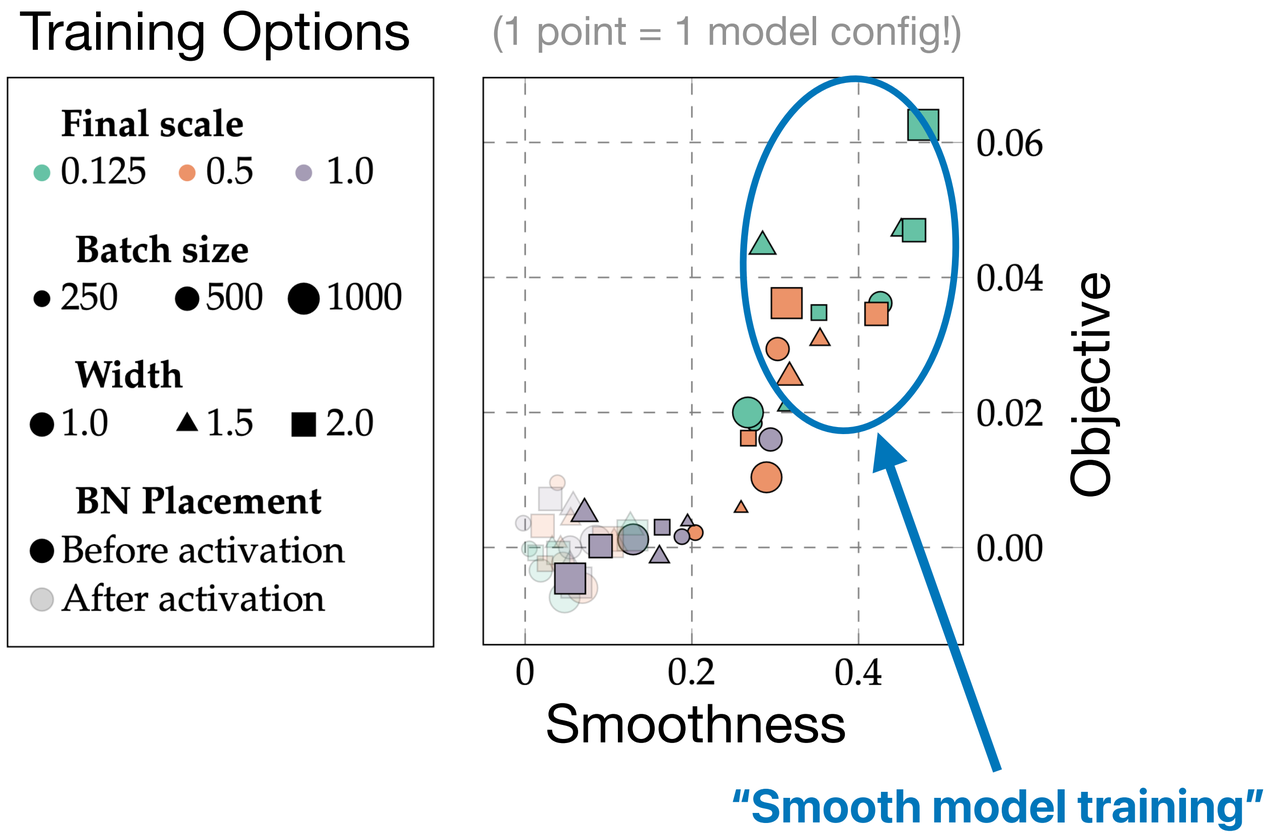

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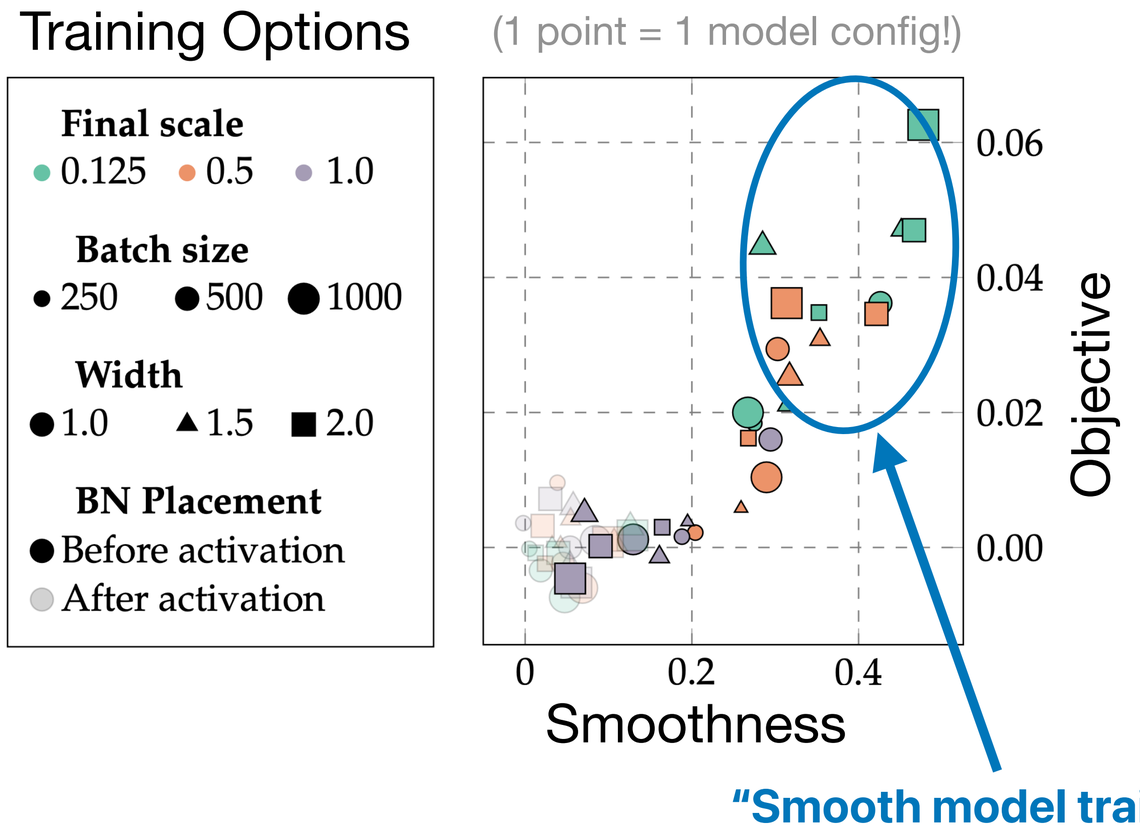

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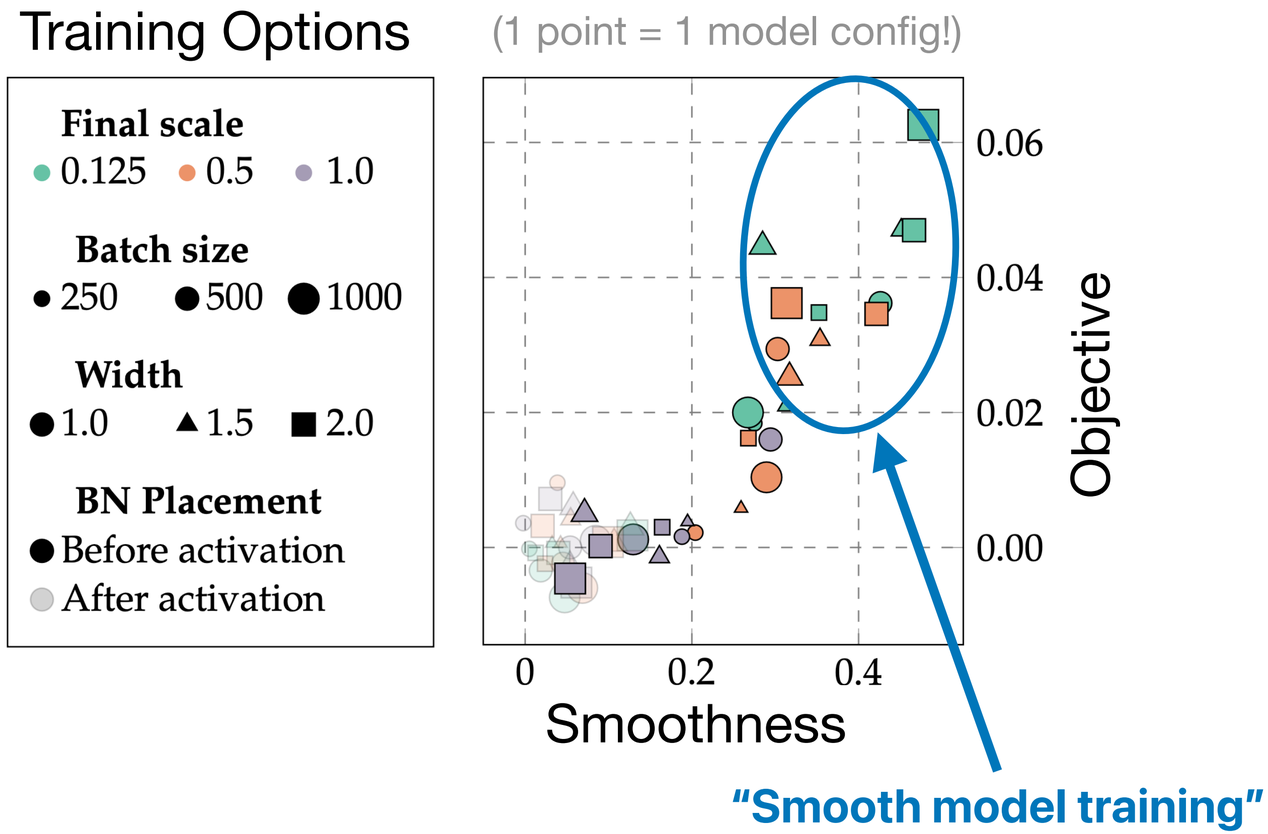

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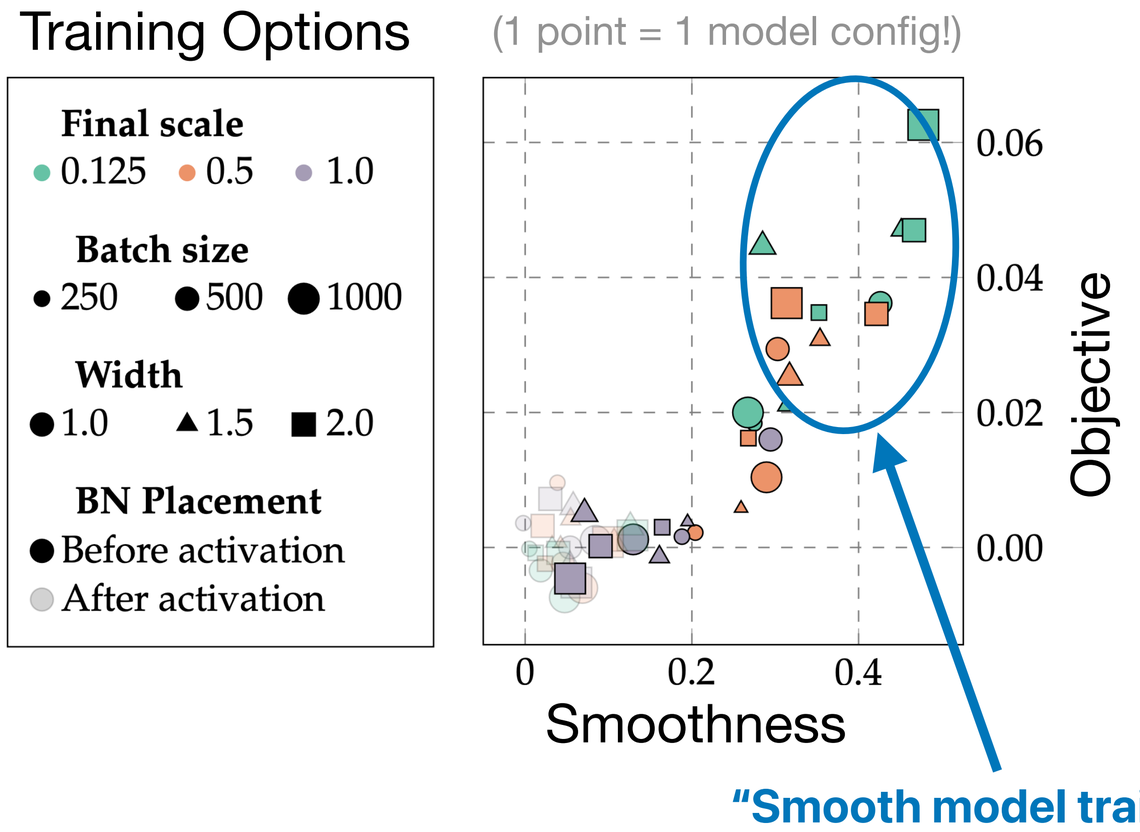

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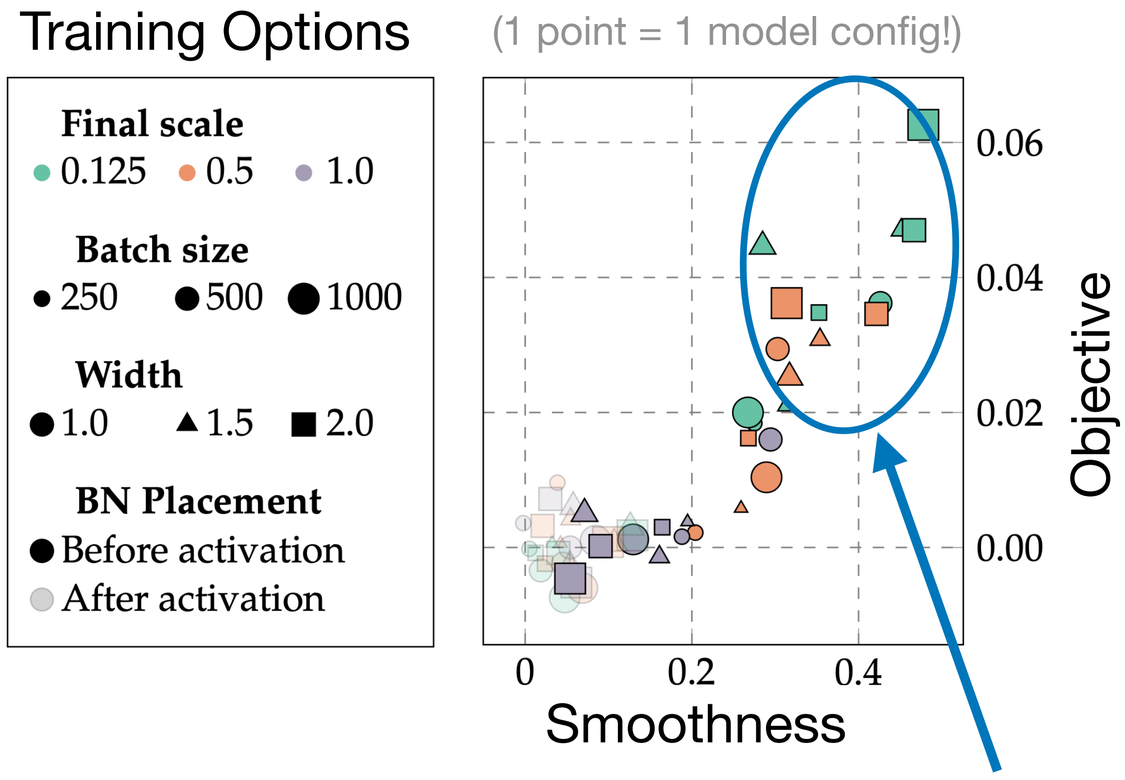

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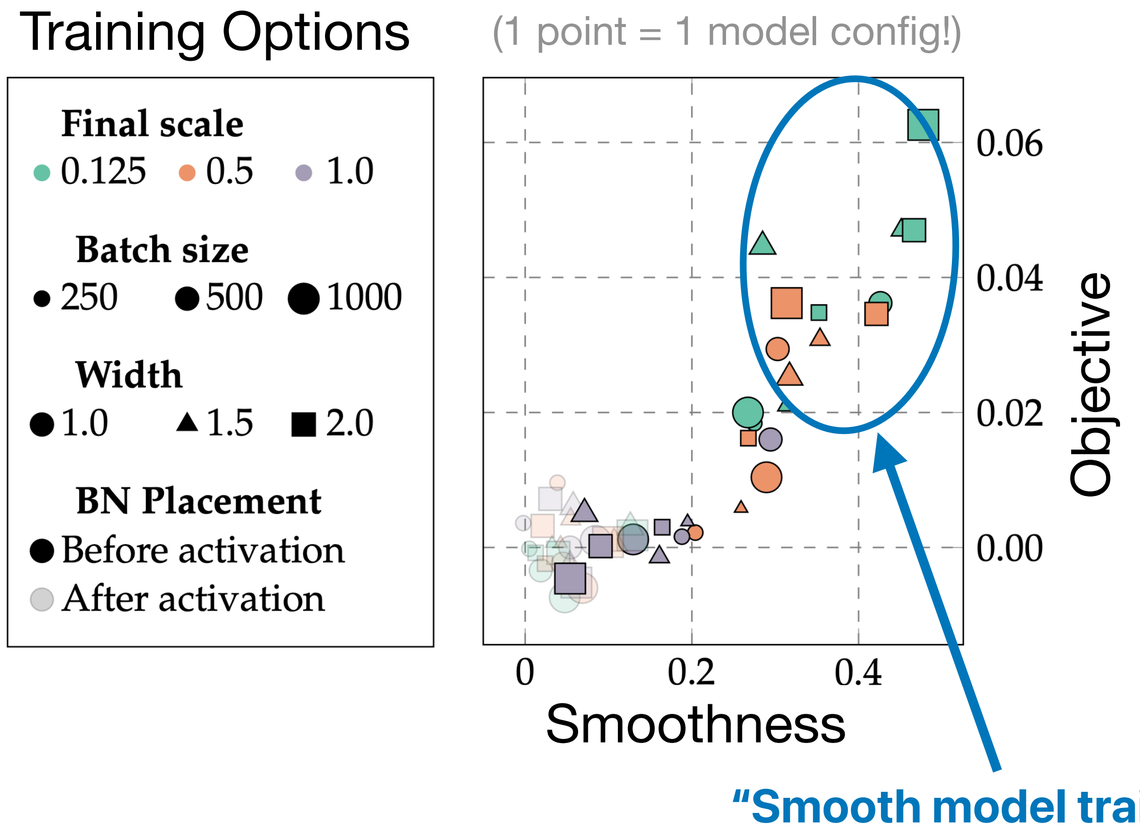

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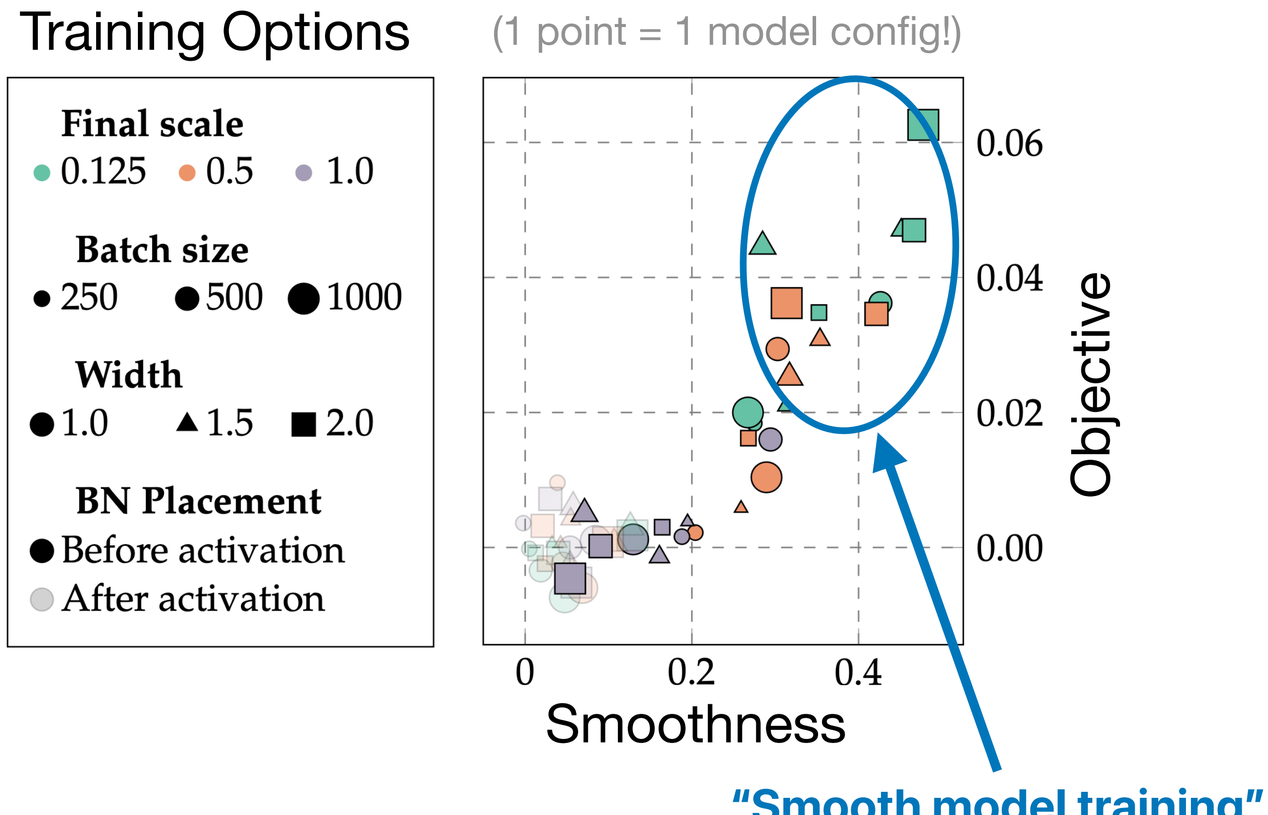

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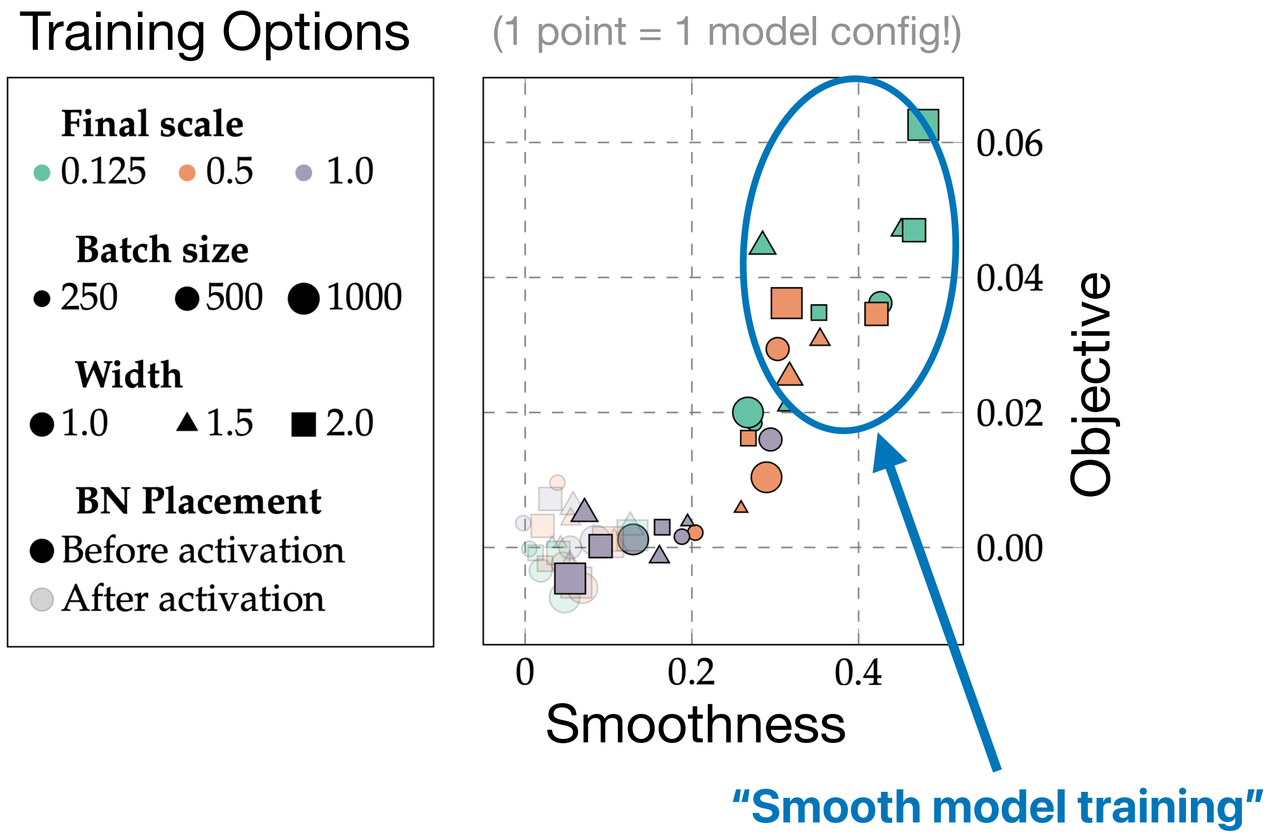

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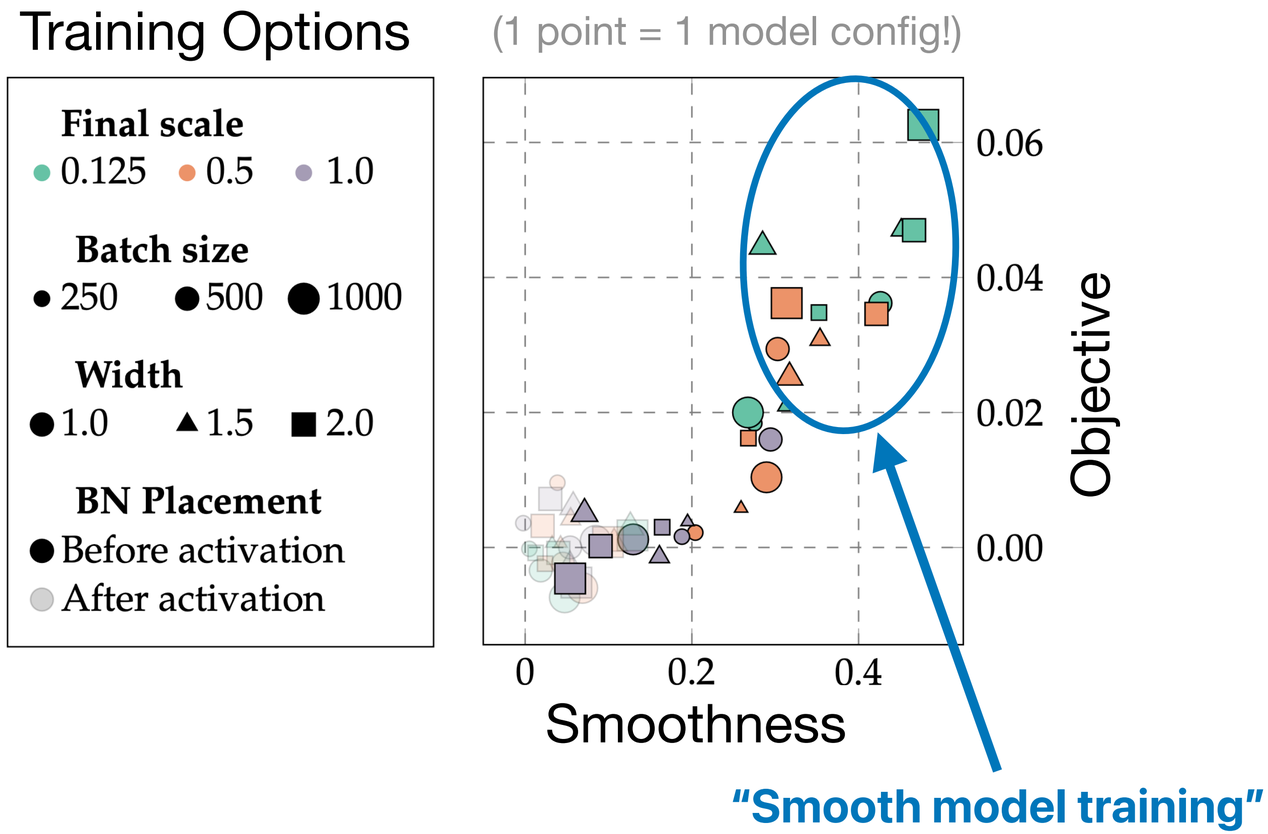

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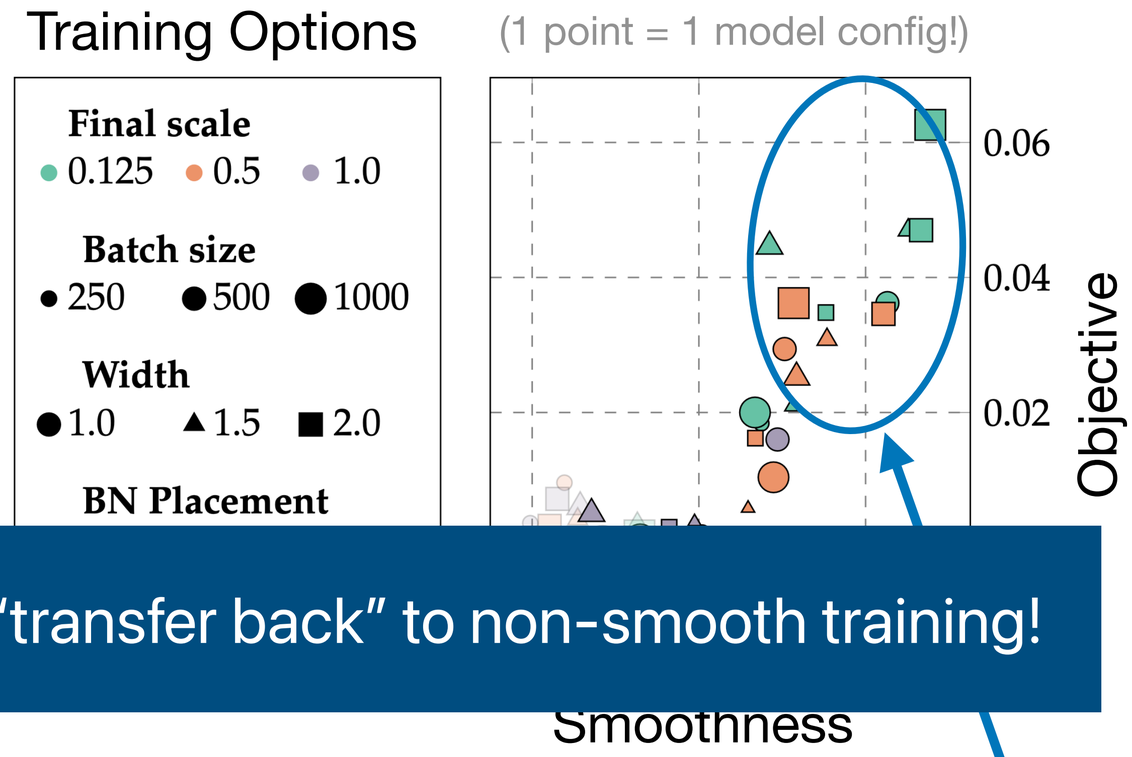

Key property: Optimized parameters "transfer back" to non-smooth training!

Roadmap

~~Main idea: The metagradient~~

~~Prequel: Two challenges~~

Looking forward

Future work

Our goal/hope is for the following recipe to be a general one:

1. Pick a design choice you're interested in optimizing/predicting
2. Write problem as a metaparameter prediction or optimization problem
3. Find a smooth training setup
4. Compute the metagradient
5. Apply gradient descent/Taylor approximation

What do we need to get there?

Future work

What do we need to get there?

1. A more systematic way of finding smooth models
2. More computational efficiency gains
3. More creative ways of applying metagradients
   - Hyperparameter optimization? (Simple example in the paper)
   - Data weighting *networks*?
   - Synthetic data generators?
   - Gradient pre-conditioners?

   "Anything we can continuously parameterize, we can (try to) optimize"

Conclusion

Design space of ML is too large to explore → how do we think about design choices?

Approach: Take the **gradient** of a model output with respect to metaparameters

Challenges:

- Computing the metagradient at scale
- Making the metagradient useful for optimization

Addressing these challenges unlocks:

- Data selection (> 2x more effective) & attribution
- Data poisoning (> 10x more effective)
- Gradient-based hyperparameter optimization
- **What next?**

See the paper for more!

🔗 https://arxiv.org/abs/2503.13751

📪 andrewi@stanford.edu

🌐 andrewilyas.com