Adam for Transformers: Why and Why Not

Yushun Zhang

The Chinese University of Hong Kong, Shenzhen, China

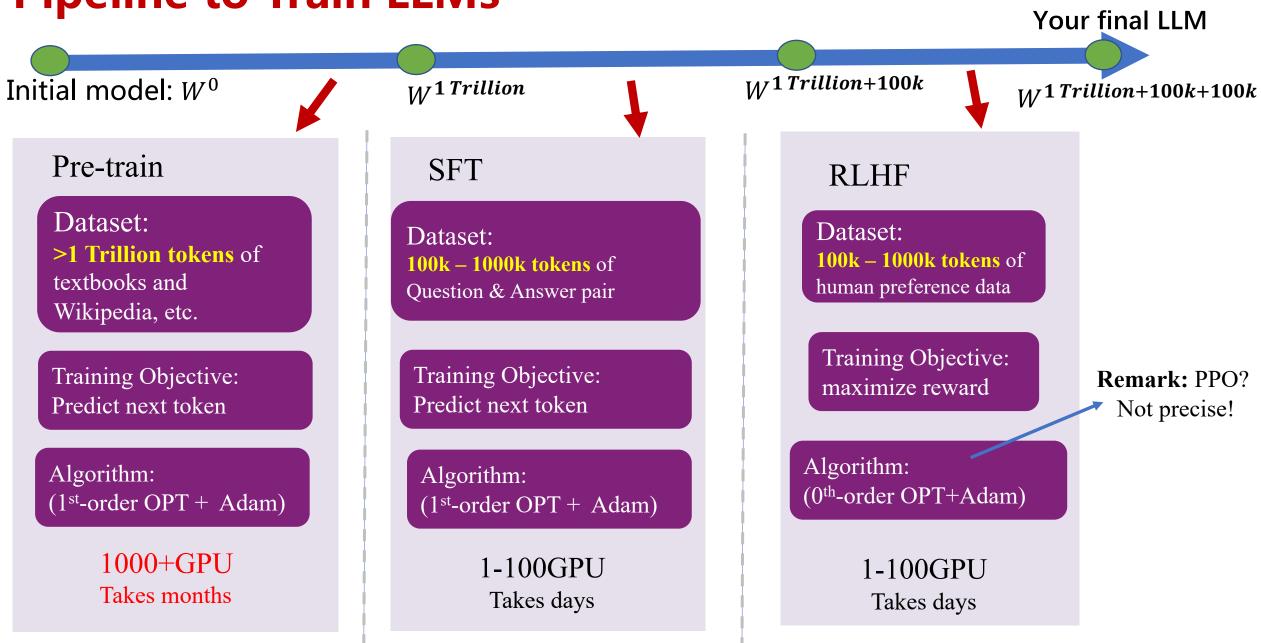
NeurIPS 2024

Presented at Tsinghua, Dec 2024 Thanks Kaifeng for the invitation!



Total page: 58

Pipeline to Train LLMs



Pre-training is EXPENSIVE

	Model size	Data size	# A800	Train Time	Rent price (RMB)	Purchase price (RMB)	Remark
预训练 (pre-training)	13B	1T tokens	80 张	约 45 days	691K	16M	Entry-level model
预训练 (pre-training)	130B	10T tokens	8000 张	约 140 days	21B	16B	Average-level model
领域增量预训练 (continue- training)	13B	200B tokens	80 张	约 9 days	140K	16M	Average-level domain-specific model

Remark:

1) 租赁价格, 按单卡 8 元/hr计算. 购买价格按1 台 A800 8 卡 160 万计算.

2) 如果是千卡租赁 , 可以谈到 3.3 元/hr 的价格 , 130B 模型可以降到 8600 万左右, 仍然很高。 Massage:

Message:

- a)从头开始预训练13B模型,80张A100,一次训练需要一个半月
- b) 增量预训练 13B的模型, 只用 1/5 的 tokens (200B tokens), 一次训练的时间也很长。

Background

- Adam becomes the most popular algorithms in deep learning (DL). (>170,000 citations, by May 2024, >198k citations, by Oct 2024)
- **Default in LLM** (large language models)

为了提升大模型训练, 需要理解 Adam

Overview of this talk

Part I:

> Why LLM training requires Adam, not SGD?

> We explain it from Hessian spectrum perspective

Part II:

Adam-mini: A "mini" version of Adam

Saves memory by 45%-50%; same loss curve as Adam

Can achieve 49.6% higher throughput on Llama2-7B pre-training (saves 30% training time)

Contents

Part I Why Transformers need Adam?

Part II Adam-mini: A lightweight version of Adam

Let us start with SGD...

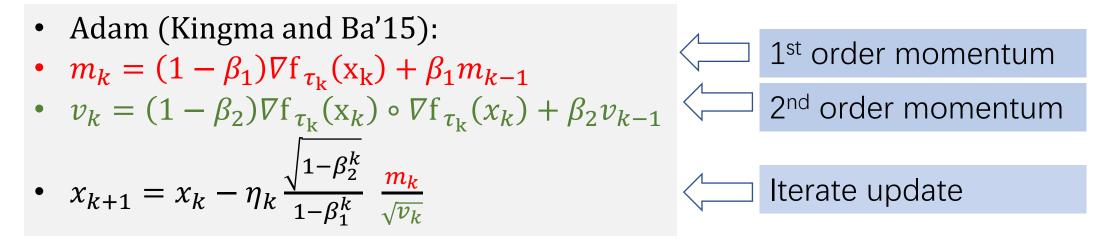
- Consider $\min_{x} f(x) \coloneqq \sum_{i=1}^{n} f_i(x)$. *n*: number of samples (or mini-batches of samples) *x*: trainable parameters
- In the *k*-th iteration: Randomly sample τ_k from $\{1, 2, ..., n\}$

SGD (Stochastic gradient descent): $x_{k+1} = x_k - \eta_k \nabla f_{\tau_k}(x_k)$

SGD with momentum (SGDM): $m_{k} = (1 - \beta_{1})\nabla f_{\tau_{k}}(x_{k}) + \beta_{1}m_{k-1}$ $x_{k+1} = x_{k} - \eta_{k}m_{k}$

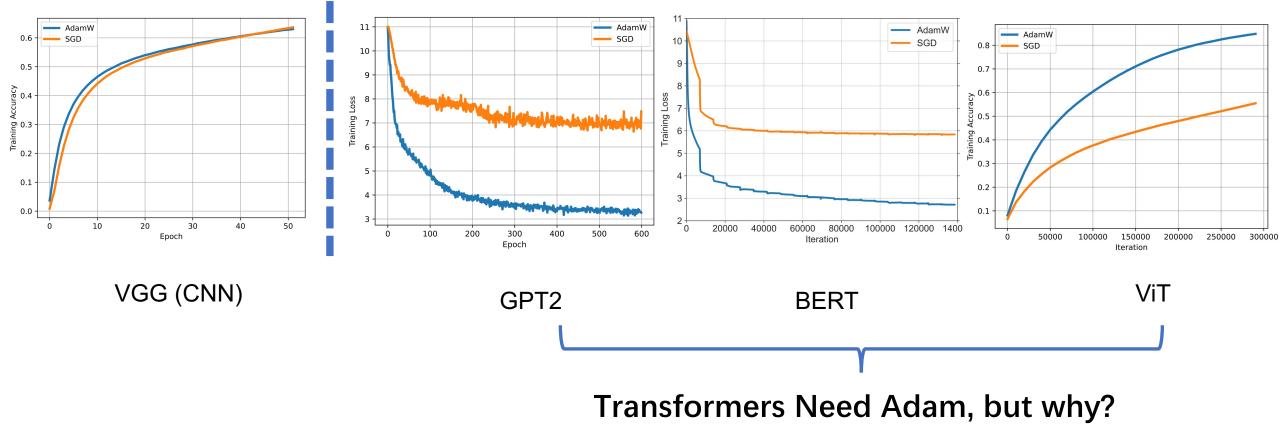
Adam

• $\min_{x} f(x) \coloneqq \sum_{i=1}^{n} f_i(x)$. In the *k*-th iteration: Randomly sample τ_k from {1,2, ..., n}



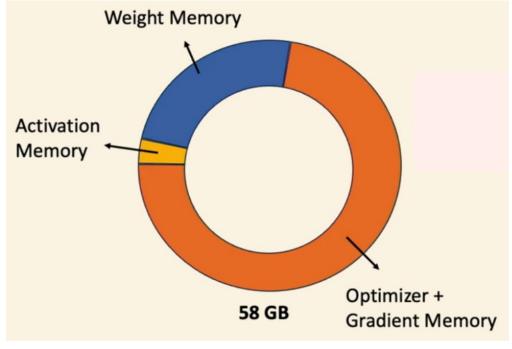
- β_1 : Controls the 1st-order momentum m_k . Default setting: $\beta_1 = 0.9$
- β_2 : Controls the 2nd-order momentum v_k . Default setting: $\beta_2 = 0.999$
- One important difference with SGD:
 - -- Adam use coordinate-wise Ir $\frac{\eta}{v_i}$
 - -- SGD uses single $\ln\eta$ for all

SGD works well on CNN, largely underperforms Adam on Transformers



However, Adam is expensive to use...

- Adam needs memory for $m \mbox{ and } v$
 - -- In total: 2x model size
 - -- becomes a major overhead for LLMs: e.g., for 7B models



[Figure from a recent talk by Meta]

• Palm-540B: Adam alone takes 50x A100-80GB GPUs ...

Literature on Why Adam better than SGD

- However, [Chen, Kunstner, Schmidt'21] provides negative evidence: SGD is worse than Adam on Transformers, even in full-batch case (with no stochasticity)

Heavy-tailed noise does not explain the gap between SGD and Adam on Transformers

> Jacques Chen, Frederik Kunstner, Mark Schmidt University of British Columbia

• So there shall be other reasons...

What problem structure might hamper SGD?

- Hessian eigenvalues largely decides behavior of gradient methods [Nocedal & Wright'99, Nesterov'13, Goh'17, Sun'2019]
- For instance: ill-conditioning slow down GD
- Can Hessian spectrum explain the gap of SGD and Adam?
- Unfortunately, no (not directly)...

Preliminary: Hessian spectrum

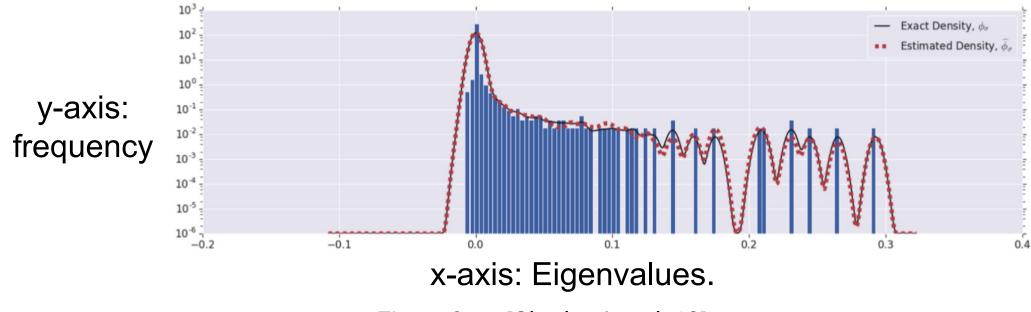


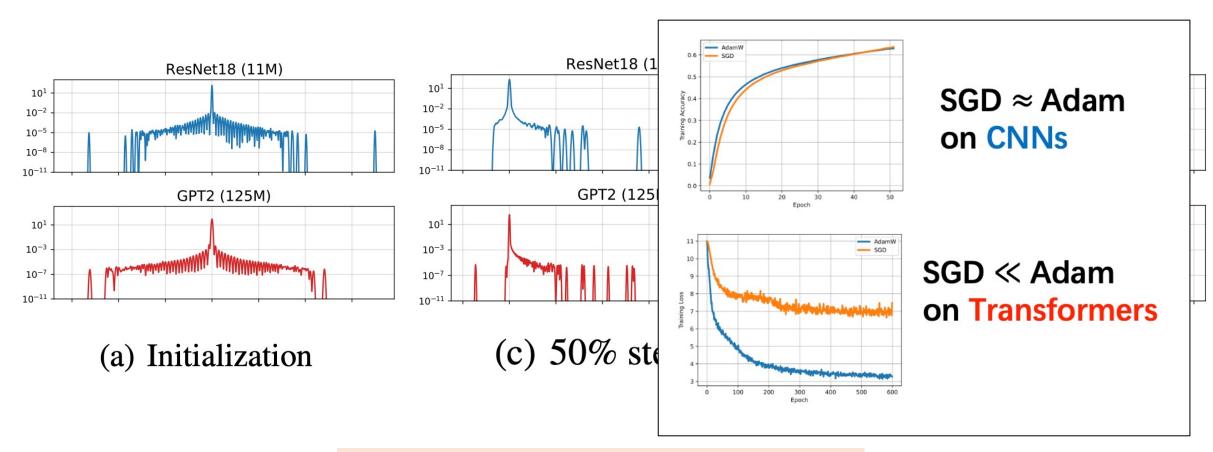
Figure from [Ghorbani et al. 19]

What is spectrum: histogram of eigenvalues

Remark: How to plot Hessian spectrum? We use Stochastic Lanczos Quadrature (SQL) [Bai, Fahey, and Golub 1996] (will take >10 pages to explain, omitted today)

We will compute the Hessian spectrum for a wide range of neural networks

Hessian spectrum cannot explain the gap



CNN and Transformers: Spectrum looks quite similar! (see more figures in the paper)

Something must be overlooked...

- Full hessian spectrum does not seem informative enough
- What else?
- We find one important features that are overlooked: The build-up rules of the architecture

-- Transformers are stacked up by different kinds of layers

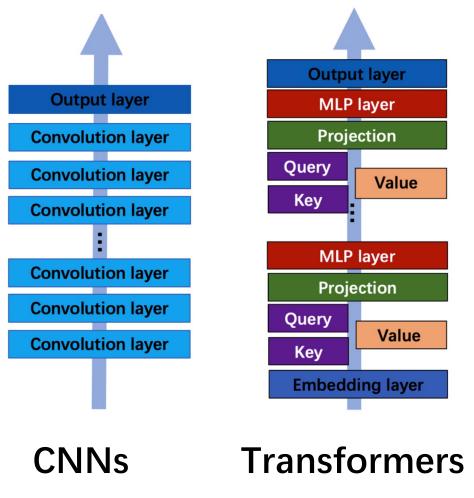
Build-up rules of architectures



CNNs: repetitive stack of similar layers

each block follow different design (e.g., Q, K, V, MLP) Total page: 58 16

Build-up rules of architectures



We hypothesize:

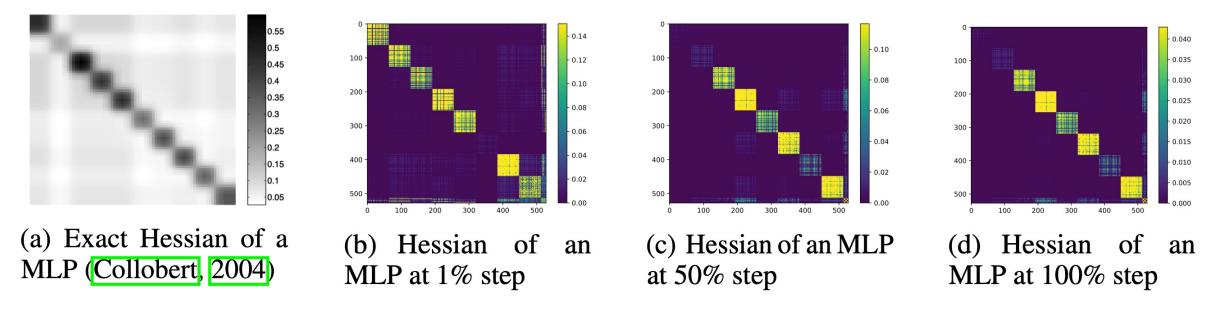
Different designs among parameter blocks

will affect

Hessian of these parameter blocks.

This inspires us to investigate the **blockwise Hessian spectra** (i.e., principle diag blocks in Hessian) Total page: 58

Another reason for studying blockwise Hessian near Block Diagonal structure



Proof (from Collobert 2004): for 1-hidden-layer network $f(\theta, x) +$ **Cross Entropy loss**, we have

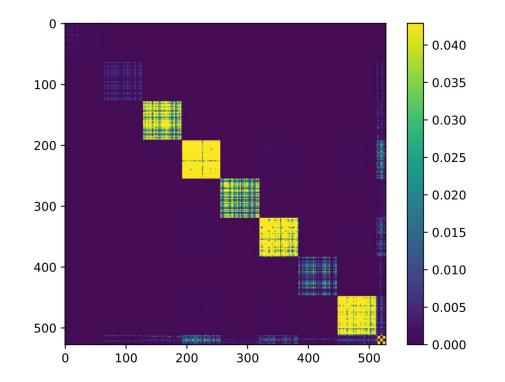
$$\frac{\partial^2 \ell(f(\theta, x), y)}{\partial w_i \partial w_j} = p_{\theta}(y|x) \left(1 - p_{\theta}(y|x)\right) v_i v_j \phi'\left(w_i^{\top} x\right) \phi'\left(w_j^{\top} x\right) x x^{\top} \quad \text{for } i \neq j,$$

where $w_i \in R^{data dimension}$: the weight associated with the *i*-th output neuron

When we maximize $p_{\theta}(y|x)$, $p_{\theta}(y|x) (1 - p_{\theta}(y|x))$ will quickly shrink to zero

But this structure is largely overlooked for both opt & DL community (sadly...)

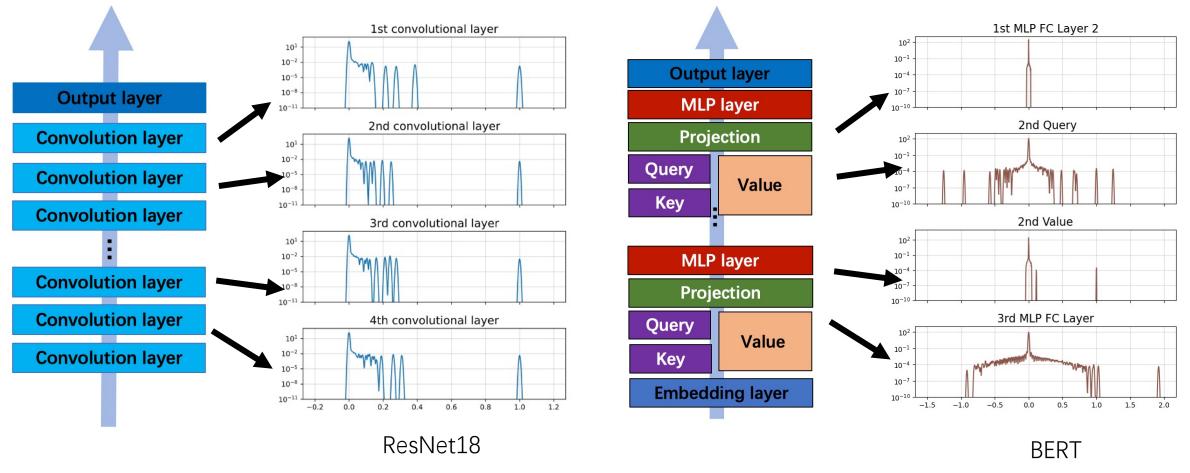
Blockwise Hessian spectrum might matters



Conjecture: Eigenvalues in each block (e.g., Q, K, V) could be important

- > What extra info over full spectrum?
- > By linear algebra: **location** of eigenvalues

Blockwise Hessian spectrum



CNNs: blockwise spectrum are quite similar We call it ``homogeneity" Transformers: blockwise spectrum are largely different We call it ``heterogeneity"

Total page: 58

JS-distance among blocks

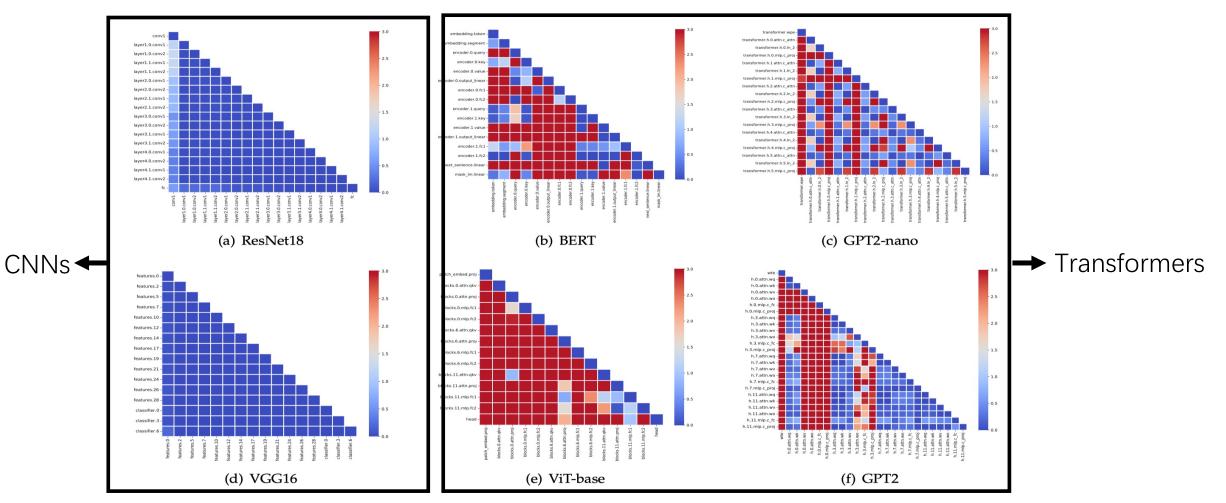
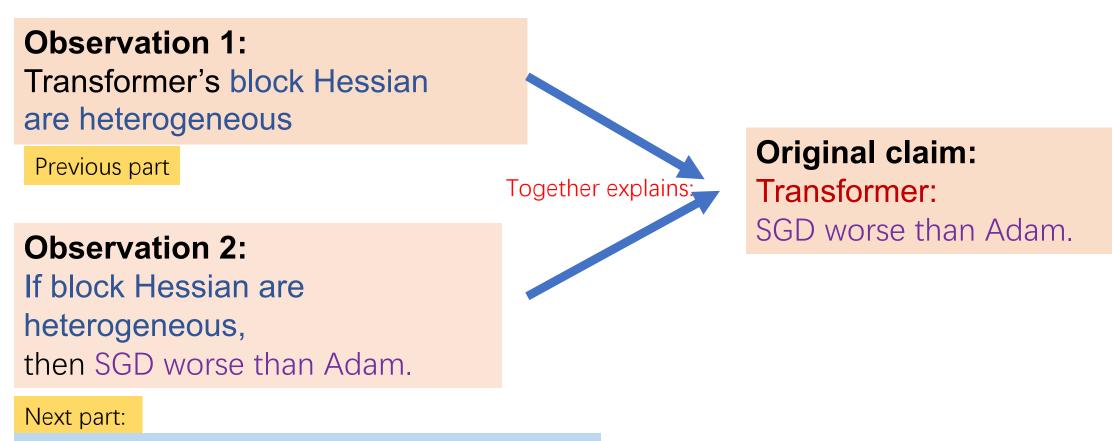


Figure 4: The JS distance among blockwise Hessian spectra for different models at initialization.

Observation 1: Heterogeneity is widely observed in Transformers, but not on CNNs!

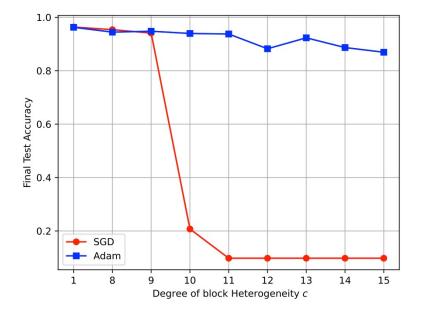
Our Explanation: Why Transformer Needs Adam



Claim 2: Hetereogeneity causes SGD worse than Adam.

Hetereogeneity makes SGD worse: Example 2 (pure MLP)

- Q: Is Transformer the only architecture that is heterogeneous & SGD worse?
- A: No! We provide a few more heterogeneous examples that SGD is worse.



x-axis: degree of Heterogeneity y-axis: final converged accuracy

Example 2:

A man-made MLP on MNIST: We exert heterogeneity by scaling each layer differently

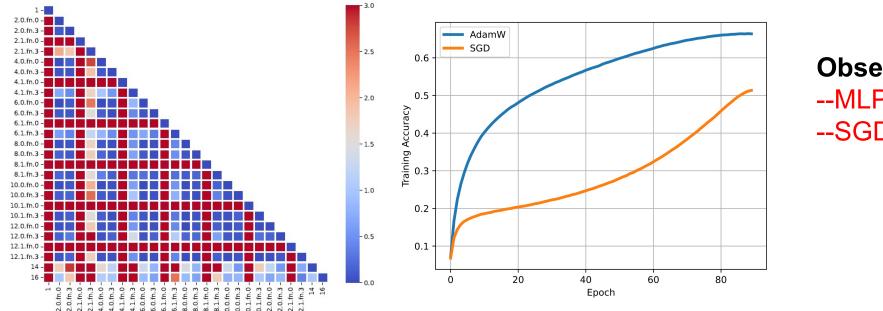
Observation:

SGD fails as heterogeneity grows while Adam remains unaffected

Hetereogeneity makes SGD worse: Example 3 (MLP-mixer)

Example 3: MLP-mixer [1]

A pure MLP architecture that outperforms CNNs on ImageNet



Observation:

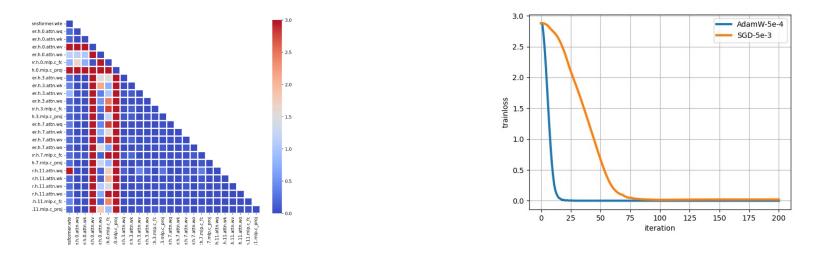
--MLP mixer is heterogeneous

--SGD performs worse than Adam

[1] MLP-mixer: An All-MLP Architecture for Vision. Tolstikhin et al., NeurIPS 2021

Heterogeneity is redued after training

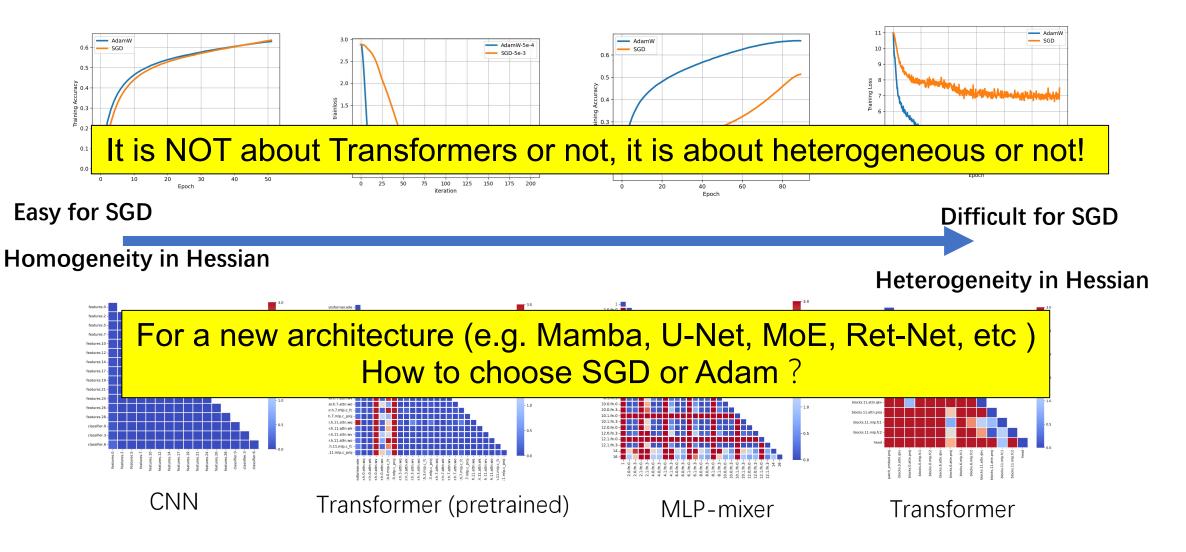
- We find **pretrained Transformers** suffer less heterogeneity
- May explain why fine-tuning is easier
- SGD could work here: still slower, but can reach similar loss as Adam
- Similar phenomena also holds for ViT-base



GPT2-125M (pretrained on 25B tokens): finetuning on a subset of Alpaca

Observation 3: Heterogeneity tends to reduce after (pre)-training

SGD performance v.s. Heterogeneity in Hessian



Empirical guidance: choose SGD or Adam?

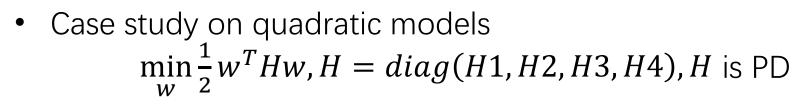
- Introduce metric to predict the failure of SGD before launching the training
- Our metric: average JS distance of spectrum among blocks at step = 0, called JS^0
- This metric could be efficiently computed using Stochastic Lanczos Quadrature Our PyTorch implementation: <u>https://github.com/zyushun/hessian-spectrum</u>

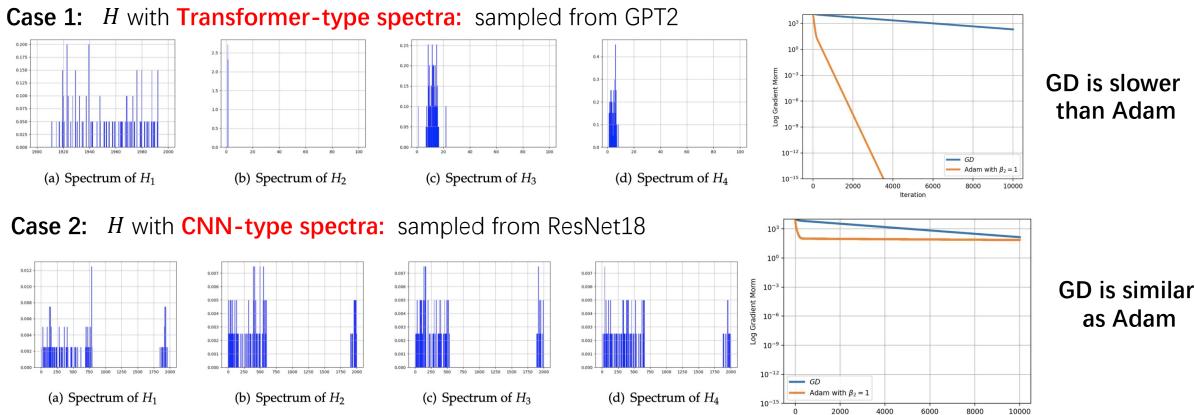
Model	ResNet18	VGG16	GPT2 (pretrained)	MLP-mixer	BERT	GPT2	ViT-base
JS^0	0.10	0.09	18.84	34.90	53.38	83.23	286.41

For CNNs: 100x smaller than Transformers!

Initial theory

Hetereogeneity makes SGD worse: Quadratic Prob





Remark:

Same condition number for case 1 & 2

but the performance is different, due to homo & heterogeneity

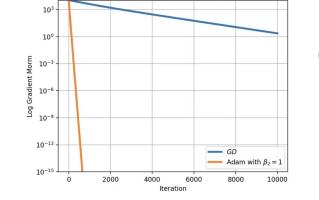
Iteration

Hetereogeneity makes SGD worse: Quadratic Prob

 $\min_{w} \frac{1}{2} w^{T} H w, H = diag(H1, H2, H3), H \text{ is PD}, \quad H_{l} \in \mathbb{R}^{3 \times 3}, l = 1, 2, 3$

Case 3: H with simplified heterogeneous spectra

Eigenvalues of H_l : { 1, 2, 3 }, { 99, 100, 101 }, { 1998, 1999, 2000 }



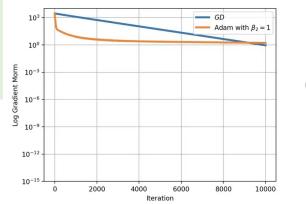
GD is slower than Adam

Case 4: *H* with simplified **homogeneous** spectra

Eigenvalues of H_l : { 1, 99, 1998 } , { 2, 100, 1999 } , { 3, 101, 2000 }

Remark:

All eigenvalues are the same for case 3 & 4 but the performance is different, due to homo & heterogeneity Total page: 58



GD is similar as Adam

Theoretical results

A well-known result for GD: Consider $\min_{w} f(w) = \frac{1}{2} w^{T} H w$, where H is PD, then there exits a H and w^{0} : $f(w_{GD}^{t+1}) - f^{*} \ge \left(1 - \frac{2}{\kappa}\right) (f(w_{GD}^{t}) - f^{*})$

where $\boldsymbol{\kappa}$ is the condition number of H

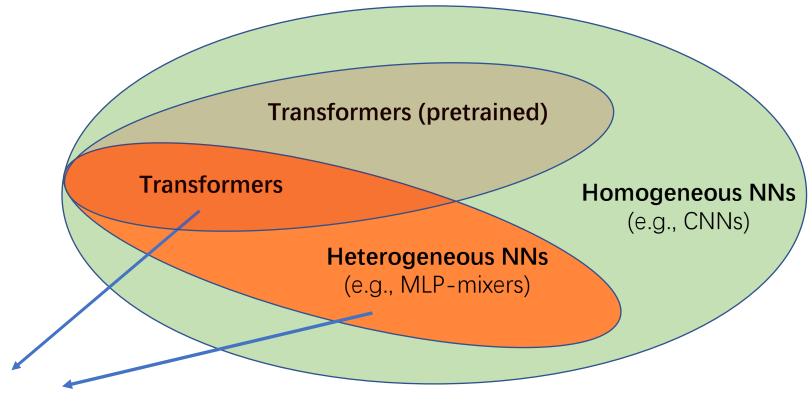
Theorem 1(Adam): Consider $\min_{w} f(w) = \frac{1}{2} w^{T} H w$, where H a block-diagonal PD matrix with L blocks, then: $f(w_{Adam}^{t+1}) - f^{*} \leq \max_{l \in [L]} \left(1 - \frac{1}{\kappa_{Adam,l}}\right) (f(w_{Adam}^{t+1}) - f^{*})$

where $\kappa_{Adam,l} = r \kappa_l$, κ_l is the condition number of H_l ; r is a constant related to initialization w^0

Comparing Two Results

- Compare GD vs Adam: Adam is faster than GD when $r \max_{l} \kappa_{l} \leq \kappa$,
- Happens in the heterogeneous quadratic examples
 Quantity of Adam ~20x smaller, and Adam is also 20x faster
- This provides a partial theoretical explanation why Adam works better than SGD on Heterogeneous case

Summarize in one figure



SGD < Adam here!

Why is SGD slow?

- -- SGD assigns one Ir for all parameter blocks
- -- Cannot handle heterogeneity across blocks

Why Adam?

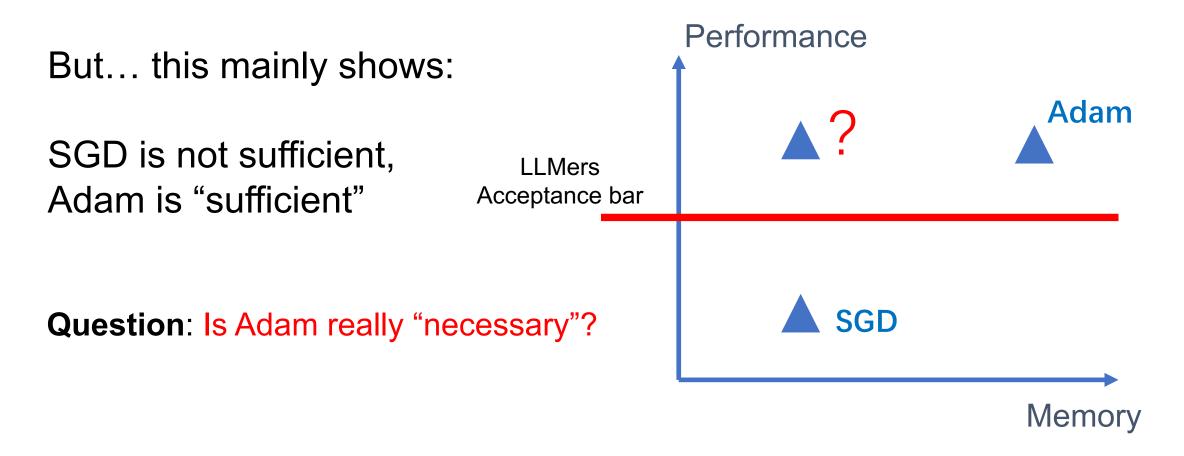
- --Each block needs (at least) one customized Ir
- -- could be provided by $\boldsymbol{\nu}$

Contents

Part I Why Transformers need Adam?

Part II Adam-mini: A lightweight version of Adam

Is Adam really "necessary"?



How to slim down Adam?

Major difference of Adam with SGD: its diagonal preconditioner

$$w \leftarrow w - \eta \ D \ \circ m$$

-- SGD:
$$D_{SGD} = I$$

-- Adam: $D_{Adam} = Diag(\frac{1}{\sqrt{v_1}}, \frac{1}{\sqrt{v_2}}, \dots, \frac{1}{\sqrt{v_2}})$

- Why D_{Adam} helps: D_{Adam} assigns different Irs for each parameters
- In optimization theory: converges faster when $\kappa(D_{Adam}H) \leq \kappa(H)$
- Caveat:

D_{Adam} is not always effective! Related to an old topic in linear algebra

A bit of history: diagonal preconditioner

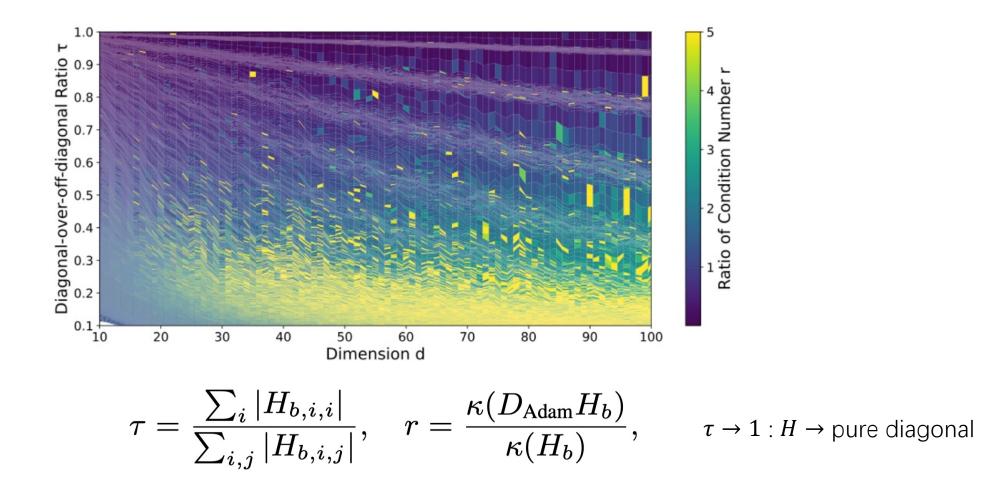
Q1: For what kind of Hessian *H* do we have $\kappa(D_{Adam}H) \leq \kappa(H)$?

- This is a pure linear algebra problem, but NOT easy to answer...
- In [1]: A similar question for $D_{Jacobi} = Diag(\frac{1}{h_{11}}, ..., \frac{1}{h_{nn}})$, not well answered so far
- We still lack theoretical understanding of *D_{Adam}*

Q1 (numerical-version): what Hessian structure does Neural Nets have? Is D_{Adam} effective on this class of *H*?

[1] Worst-case Complexity of Cyclic Coordinate Descent, Sun and Ye, 2017, Mathematical Programming

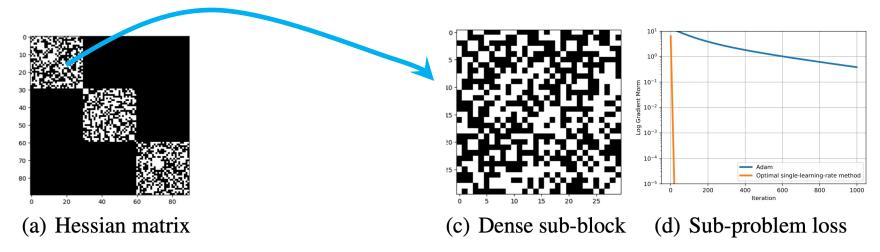
Numerical results on random *H* and **D**_{Adam}



Observation: D_{Adam} is NOT effective when H is dense

How effective is D_{Adam} on dense block?

 $\min_{x} \frac{1}{2} x^{T} H x$, where $H = Diag(H_1, H_2, H_3), H_i$ are random PD (dense) matrices

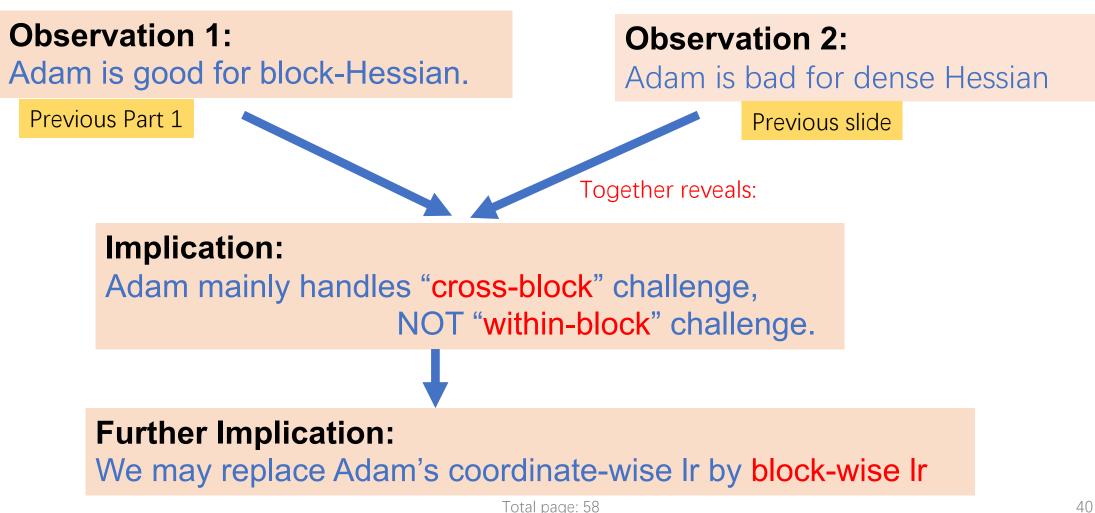


Another Case: Dense block.

We take the 1st sub-block H_1 in (a) and use it for a new problem (c)

- -- Figure (c): **GD with (a different) optimal Ir** outperforms **Adam**, even though Adam uses more Ir!
 - -- This means: D_{Adam} is NOT so effective on $H_1!$

Our Explanation: Why Transformer Needs Adam



How effective is D_{Adam} on this block-diagonal Hessian?

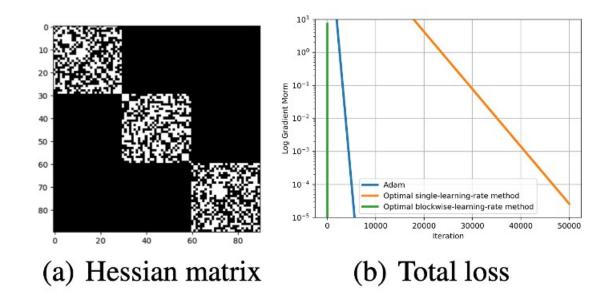
• We explore it numerically on quadratic functions:

 $\min_{x} \frac{1}{2} x^{T} H x$, where $H = Diag(H_1, H_2, H_3), H_i$ are random

Algorithm (block-wise optimal Ir method):

- -- Collect optimal Ir's for each block
- -- Apply them to "blockwise" version of GD,

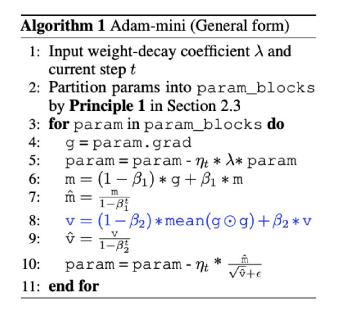
Observation: Figure (b): **blockwise GD** outperforms Adam with only 3 learning rates!



Using Fewer Learning Rates?

- More Irs do not neccessarily bring extra gain (This reveals a drawback of design in Adam)
- For each block, a single but good Ir can outperform Adam
- > But how to find these good Irs without grid-search?

Adam-mini (Framework)



Step 1: partition the gradient g into B sub-vectors according to the dense Hessian sub-block g_b, b = [B]
 Step 2: for each g_b, calculate:

$$v_b = (1 - \beta_2) * \texttt{mean}(g_b \circ g_b) + \beta_2 * v_b, \quad b = 1, \cdots B$$

- Step 3: then use $\frac{\eta}{\sqrt{v_b}}$ as the Ir for the parameters associated with g_b

• Step 1 is important, and will be discussed later.

Adam-mini: an illustration

- Illustration: For a problem with 5 parameters, $w \leftarrow w \eta \, u \circ m$ Adam: $u = (\frac{1}{\sqrt{v_1}}, \frac{1}{\sqrt{v_2}}, \frac{1}{\sqrt{v_3}}, \frac{1}{\sqrt{v_4}}, \frac{1}{\sqrt{v_5}})$ Adam-mini: if block partition is (1,2,3); (4,5), then $u = (\frac{1}{\sqrt{(v_1+v_2+v_3)/3}}, \frac{1}{\sqrt{(v_1+v_2+v_3)/3}}, \frac{1}{\sqrt{(v_1+v_2+v_3)/3}}, \frac{1}{\sqrt{(v_4+v_5)/2}}, \frac{1}{\sqrt{(v_4+v_5)/2}})$
- Benefits: reduce # learning rates: from # parameters to # blocks
- For LLMs, we will show that this would free \geq 99% elements in v
- **Remark:** Cheap way to find "good Irs", but might not be optimal
- Remaining question: How to partition parameters for a given problem, e.g., Transformers?

Parameter Partition: Failed Attempt

Failed Attempt:

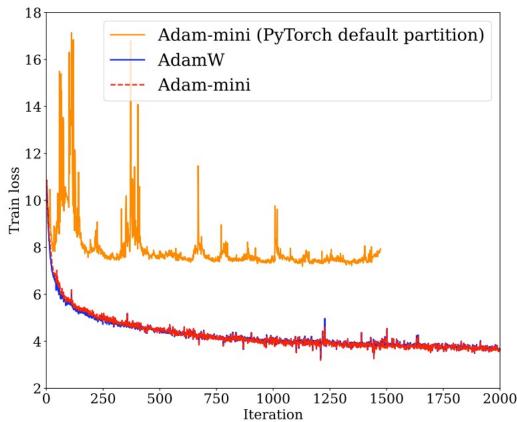
- Default PyTorch partition strategy (layer-by-laver) is a naive candidate

Total page: 58

- Unfortunately, this default strategy over-sim
- Observe training instability on 1B models

Why?

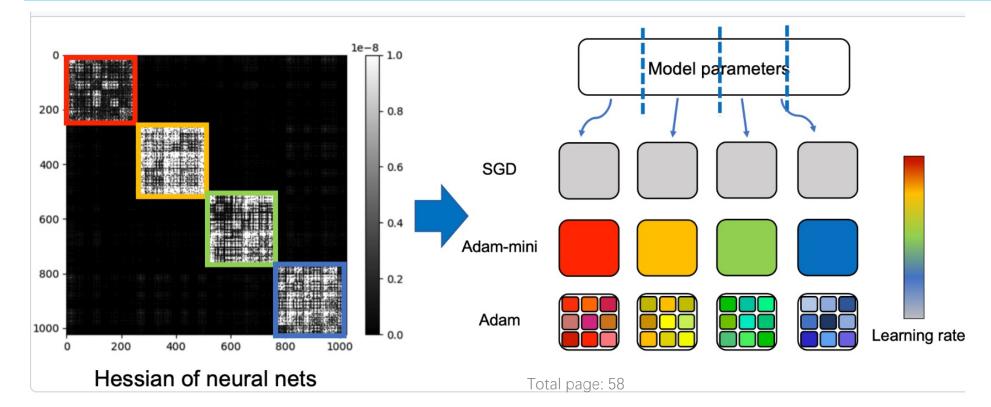
We suspect the default PyTorch partition did not fully capture the **Hessian structure**



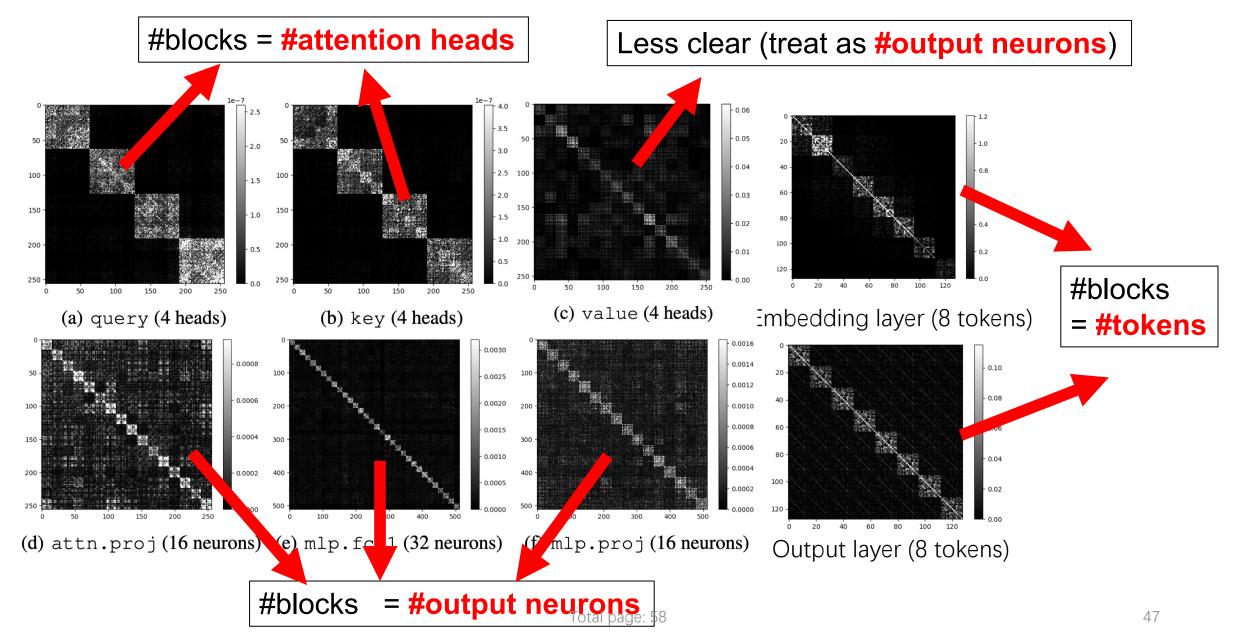
Partition Principle

Partition Principle:

Partition parameters into blocks s.t. each block is associated with a dense sub-block in Hessian.



Applying Principle to Transformer (non-equal sized blocks)



Side story: "Bug"

Remark: 和初版 (in May, 2024) 不同!

对 embedding & output layer:

初版

本版

根据 Hessian blocks划分

和理想划分策略不一致! NOT Principled enough!

和理想划分策略完全一致!

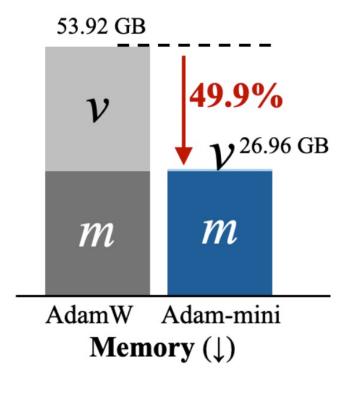
Due to "bug": In Pytorch, embedding layer is W^T , extra "transpose"!

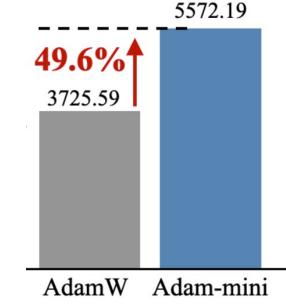
Complete form of Adam-mini

Partition for Transformer

	Algorithm 1 Adam-mini in Pytorch style	Algorithm 3 Partition for Transformers		
Adam-mini given	1: Input weight-decay coefficient λ and	1: param_blocks = {}		
the partition rule	current step t	2: for name, param in parameters do		
	2: Choose param_blocks from	3: if 'embed' or 'output' in name then		
Algorithm 2 or 3		4: Partition param by tokens		
	3: for param in param_blocks do	5: for $i = 0 \dots tokens - 1$ do		
	: g=param.grad	<pre>6: param_blocks[name+i]=param[i]</pre>		
	5: param = param - $\eta_t * \lambda *$ param			
	6: m = $(1-eta_1)* extsf{g}+eta_1* extsf{m}$	8: else if 'query' or 'key' in name then		
7: $\hat{\mathbf{m}} = \frac{\mathbf{m}}{1 - \beta_1^t}$ 8: $\mathbf{v} = (1 - \beta_2) * \operatorname{mean}(\mathbf{g} \odot \mathbf{g}) + \beta_2 * \mathbf{v}$		9: Partition param by heads		
		$\mathbf{r}_{\mathbf{v}}$ 10: for i = 0heads-1 do		
	9: $\hat{\mathbf{v}} = \frac{\mathbf{v}}{1-\beta_{1}^{t}}$	<pre>II: param_blocks[name+1]=param[1]</pre>		
	- /-2	12: end for		
10: param = param - $\eta_t * \frac{\hat{m}}{\sqrt{\hat{v}} + \epsilon}$		13: else if 'value', 'attn.proj', or 'mlp'		
11: end for		in name then		
Dertition for simple mod		14: Partition param by output neurons		
Partition for simple mod		15: for $i = 0output_neurons-1$ do		
(CNNs, GNNs, Diffusior	orithm 2 Partition for non-Transformer	<u>16:</u> param_blocks[name+i]=param[i]		
1: param_blocks = {}		18: else		
•	for name, param in parameters do			
	3. param_blocks[name]=param			
	4: end for	21: end for		
	5: return param_blocks	22: return param_blocks		

Memory cut down & Throughput enhancement





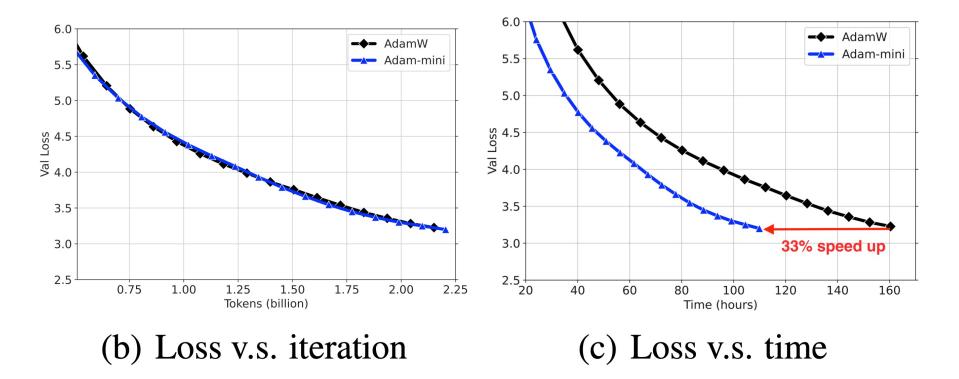
Throughput (†)

Saves 50% memory of Adam

Can increase about **50**% throughput of Adam (# processed data per second)

Why? Reduce communication + larger batch size per GPU

Llama2-7B: pre-training



Same loss curve as Adam

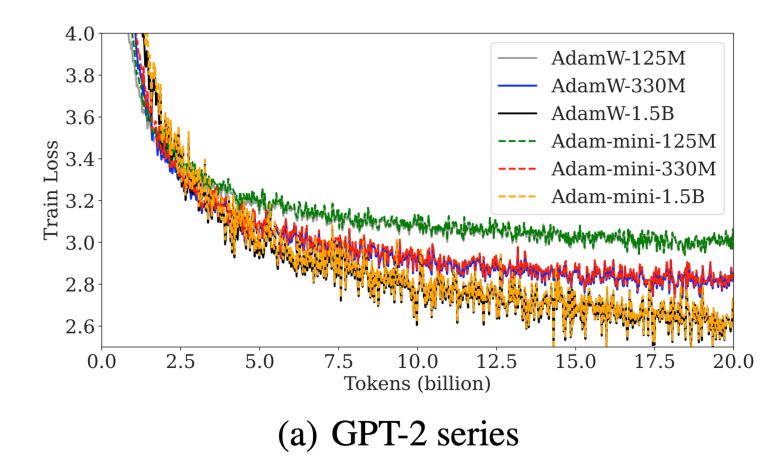
> 33% less time to process the same # tokens (tested on 2x A800-80GB GPUs)

Llama2-7B: pre-training

Optimizer	# Tokens (B)	GPU hours (h) (\downarrow)	
AdamW	1	74.56	
Adam-mini	1	49.85 (↓ 33 .1%)	
AdamW	70	5219.16	
Adam-mini	70	3489.55 (↓ 33 .1%)	
AdamW	140	10438.32	
Adam-mini	140	6979 .10 (↓ 33 .1%)	

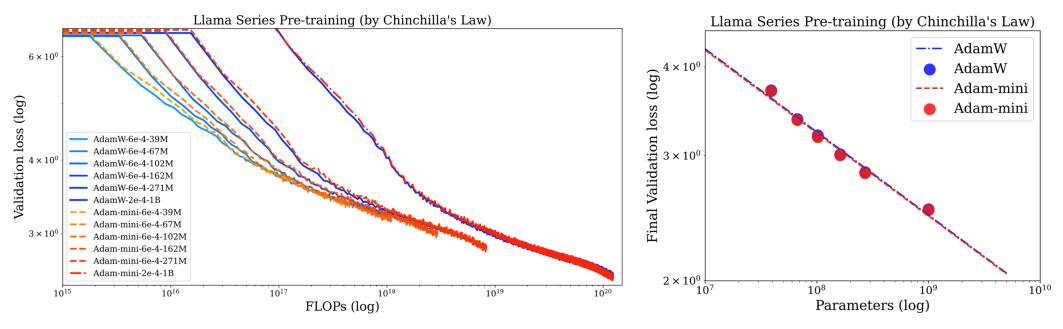
33% less time to process the same # tokens (tested on 2x A800-80GB GPUs)

GPT-2 pre-train (125M, 330M, 1.5B)



The curves of Adam-mini closely resemble the curves of AdamW

Scaling laws of Adam-mini from 39M to 1B



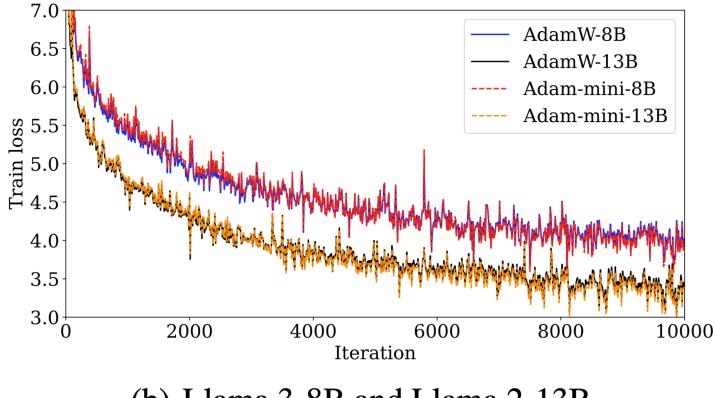
(a) Scaling laws in terms of compute

(b) Scaling laws in terms of parameters

- We train Llama series (from 39M to 1B) for complete pre-training runs ("complete" under the definition of Chinchila's law: # data= 20 * # parameters)
- For all models, Adam-mini performs similarly to AdamW

This serves as an evidence that Adam-mini can work on larger models, e.g., 30B, 100B (if the scaling law holds)

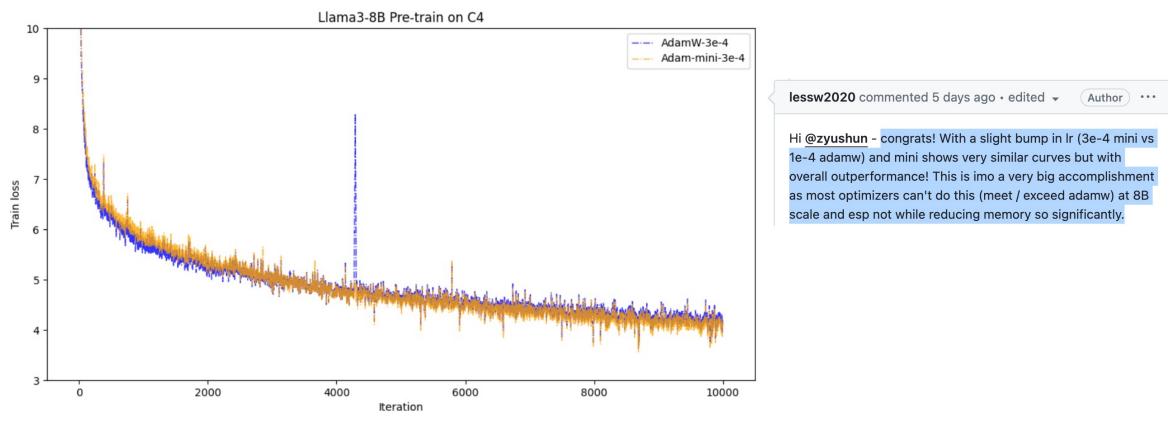
Llama 3-8B and Llama 2-13B



(b) Llama 3-8B and Llama 2-13B

The curves of Adam-mini closely resemble the curves of AdamW

Independent verifier from PyTorch team (Llama3-8B)



Highlight:

"This is imo a very big accomplishment as most optimizers can't do this (meet / exceed adamw) at 8B

... and especially not while reducing memory so significantly"

Total Pages: 59

Llama2-7B: SFT and RLHF

Finetuning tasks for Llama2-7B pre-trained model (released by Meta).

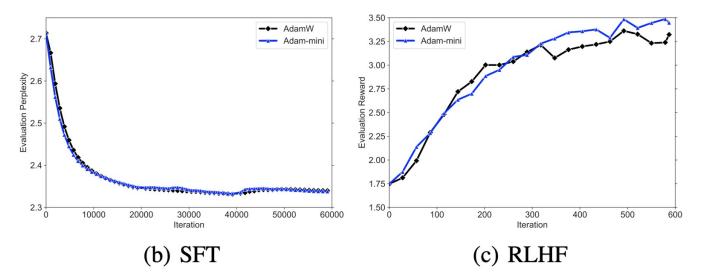
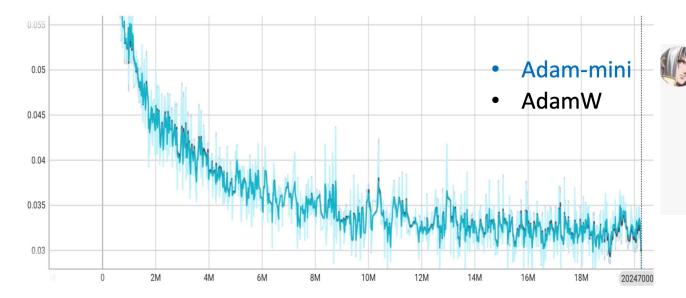


Table 3: Averaged GPT-4 evaluation score (\uparrow) of SFT and RLHF on the MT-Bench.

	SFT (LoRA)		(SFT		RLHF	
	AdamW	Adam-mini	AdamW	Adam-mini	AdamW	Adam-mini	
MT-Bench	4.23	4.41	5.37	5.40	5.54	5.68	

Adam-mini performs slightly better than AdamW, with 50% less memory

Diffusion models



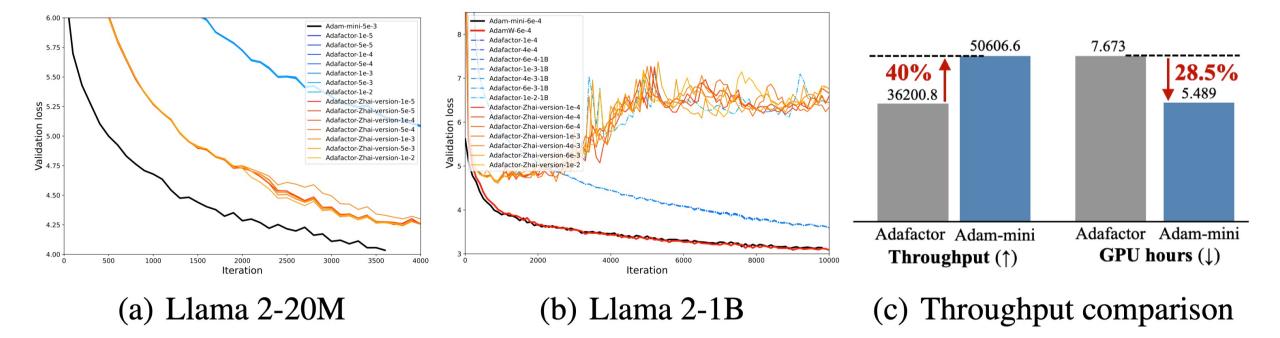
Diffusion model training: Loss vs. iteration 青龍聖者 ♀ @bdsqlsz · 4小时 ···· Just tests with Adam-mini on the diffusion model SDXL and it works great and really saves VRAM. Batch size 8 only requires about 16G of VRAM.



Independent verifier on twitter: SDXL: Stable Diffusion XL (sized 2.6B) One of the SOTA Diffusion model

Adam-mini performs slightly better than AdamW, with 50% less memory

Comparison to Adafactor (variants)



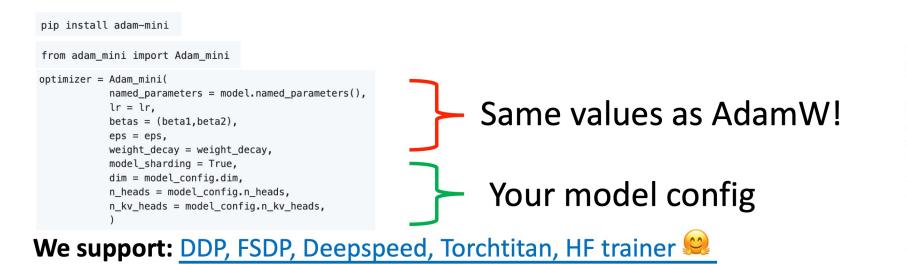
We did NOT find the good hyperparams for Adafactor to work (9 hyperparams! Hard to find the correct combination) Further, Adafactor has higher latency (due to more matrix produts)

Summary

- Part I: We provide an explanation why Transformer needs Adam, not SGD
 - Hetereogeneity of block-Hessian-spectra is one reason

- Part II: We propose a 50%-memory-saving variant of Adam: Adam-mini
 - **Two features**: Principled block partition; block-mean of v

How to Use? Just 1-line code change



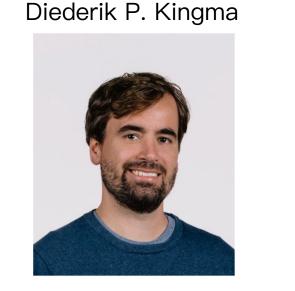


Code for Adam-mini
 Currently:
 -- 300+ stars

If you like Adam, Adam-mini is a no-brainer switch!

Mainly based on:

- Zhang, Chen, Ding, Li, Sun, & Luo, Why Transformers Need Adam: A Hessian Perspective, NeurIPS 24
- Zhang*, Chen*, Li, Ding, Chen, Kingma, Ye, Luo & Sun, Adam-mini: Use Fewer Learning Rate To Gain More, preprint.









Zhi-Quan Luo



Thanks to all the collaborators!