Tensor Programs V: Tuning Large Neural Networks via Zero-Shot Hyperparameter Transfer

Abstract

Hyperparameter (HP) tuning in deep learning is an expensive process, prohibitively so for neural networks (NNs) with billions of parameters. We show that, in the recently discovered Maximal Update Parametrization (μ P), many optimal HPs remain stable even as model size changes. This leads to a new HP tuning paradigm we call μ Transfer: parametrize the target model in μ P, tune the HP indirectly on a smaller model, and zero-shot transfer them to the full-sized model, i.e., without directly tuning the latter at all. We verify μ Transfer on Transformer and ResNet. For example, 1) by transferring pretraining HPs from a model of 13M parameters, we outperform published numbers of BERT-large (350M parameters), with a total tuning cost equivalent to pretraining BERT-large once; 2) by transferring from 40M parameters, we outperform published numbers of the 6.7B GPT-3 model, with tuning cost only 7% of total pretraining cost. A Pytorch implementation of our technique can be found at github.com/microsoft/mup.

1 Introduction

Hyperparameter (HP) tuning is critical to deep learning. Poorly chosen HPs result in subpar performance and training instability. Many published baselines are hard to compare to one another due to varying degrees of HP tuning. These issues are exacerbated when training extremely large deep learning models, since state-of-the-art networks with billions of parameters become prohibitively expensive to tune.

Recently, [45] showed that different neural network parametrizations induce different infinite-width limits and proposed the *Maximal Update Parametrization* (abbreviated μP) (summarized in Table 3) that enables "maximal" feature learning in the limit. Intuitively, it ensures that each layer is updated on the same order during training regardless of width.³ In contrast, while the

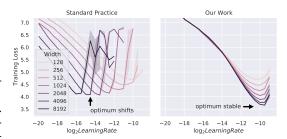


Figure 1: Training loss against learning rate on Transformers of varying d_{model} trained with Adam. Conventionally and in contrast with our technique, different widths do not share the same optimal hyperparameter; wider networks do not always perform better than narrower ones; in fact they underperform the same-width networks in our technique even after tuning learning rate. See Sections 3 and 4 for experimental setup.

standard parametrization (SP) ensures activations are of unit order at initialization, it actually causes

[†]Work done partly during Microsoft AI Residency Program.

^{*}Equal contribution. Order is random. Correspondence to {gregyang, edwardhu}@microsoft.com

²See arxiv.org for the full, up-to-date version of this work.

³i.e., the updates' effect on activations becomes roughly independent of width in the large width limit.

Algorithm 1 Tuning a Large Target Model via μ Transfer

- 1: Parametrize target model in Maximal Update Parametrization (μ P)
- 2: Tune a smaller version (in width and/or depth) of target model
- 3: Copy tuned hyperparameters to target model

Table 1: Hyperparameters That Can Be μ Transferred, Not μ Transferred, or μ Transferred Across, with a few caveats discussed in Section 5.1. * means *empirically validated only* on Transformers, while all others additionally have theoretical justification.

μ Transferable	Not μ Transferable	μ Transferred $Across$
optimization related, init, parameter multipliers, etc	regularization (dropout, weight decay, etc)	width, depth*, batch size*, training time*, seq length*

them to blow up in wide models during training [45] essentially due to an imbalance of per-layer learning rate (also see Fig. 8). We leverage μP to zero-shot transfer HPs from small models to large models in this work – that is, we obtain near optimal HPs on a large model without directly tuning it at all! While practitioners have always guessed HPs of large models from those of small models, the results are hit-or-miss at best because of incorrect parametrization. For example, as shown in Fig. 1, in a Transformer, the optimal learning rate is stable with width in μP (right) but far from so in standard parametrization (left). In addition to width, we empirically verify that, with a few caveats, HPs can also be transferred across depth (in Section 5.1) as well as batch size, language model sequence length, and training time (in Appendix I.2.1). This reduces the tuning problem of an (arbitrarily) large model to that of a (fixed-sized) small model. Our overall procedure, which we call $\mu Transfer$, is summarized in Algorithm 1 and Fig. 2, and the HPs we cover are summarized in Tables 1 and 2.

There are several benefits to our approach: 1. **Better Performance:** μ Transfer is not just about predicting how the optimal learning rate scales in SP. In general, we expect the μ Transferred model to outperform its SP counterpart with learning rate optimally tuned. For example, this is the case in Fig. 1 with the width-8192 Transformer. We discuss the reason for this in Appendices B and C. 2. **Speedup:** It provides massive speedup to the tuning of large models. For example, we are able to outperform published numbers of (350M) BERT-large [9] purely by zero-shot HP transfer, with tuning cost approximately equal to 1 BERT-large pretraining. Likewise, we outperform the published numbers of the 6.7B GPT-3 model [6] with tuning cost being only 7% of total pretraining cost. For models on this scale, HP tuning is not feasible at all without our approach. 3. **Tune**

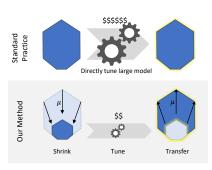


Figure 2: Illustration of μ Transfer

Once for Whole Family: For any fixed family of models with varying width and depth (such as the BERT family or the GPT-3 family), we only need to tune a single small model and can reuse its HPs for all models in the family. For example, we will use this technique to tune BERT-base (110M parameters) and BERT-large (350M parameters) simultaneously by transferring from a 13M model. 4. Better Compute Utilization: While large model training needs to be distributed across many GPUs, the small model tuning can happen on individual GPUs, greatly increasing the level of parallelism for tuning (and in the context of organizational compute clusters, better scheduling and utilization ratio). 5. Painless Transition from Exploration to Scaling Up: Often, researchers explore new ideas on small models but, when scaling up, find their HPs optimized during exploration work poorly on large models. μ Transfer would solve this problem.

Nevertheless, μ Transfer still has several limitations. For example, while it is very effective for pretraining, it cannot transfer regularization HPs,⁵ so it's generally not applicable to the finetuning of pretrained models. We discuss other limitations carefully in Section 5.1.

⁴but possibly *not* for different data and/or tasks.

⁵It can transfer regularization HPs to the extent they help *training* but it may not transfer their effect on *testing*.

Table 2: **Examples of** μ **Transferable Hyperparameters.** All of the below can also be specialized to per-layer hyperparameters.

Optimizer Related	Initialization	Parameter Multipliers
learning rate (LR), momentum, Adam beta, LR schedule, etc	per-layer init. variance	multiplicative constants after weight/biases, etc

Our Contributions

- We demonstrate it is possible to zero-shot transfer near optimal HPs to a large model from a small version via the Maximal Update Parametrization (μP) from [45].
- While [45] only covered SGD, here we derive μP for Adam as well (Table 3).
- We propose a new HP tuning technique, µTransfer, for large neural networks based on this
 observation that provides massive speedup over conventional methods and covers both SGD
 and Adam training;
- We thoroughly verify our method on machine translation and large language model pretraining (in Section 6.3) as well as image classification (in Appendix I.1);
- We release a PyTorch [27] package for implementing μTransfer painlessly. A sketch of this
 package is given in Appendix J.

Terminologies Sometimes, to be less ambiguous, we often refer to the "large model" as the *target model*, as it is the model we wish to ultimately tune, while we refer to the "small model" as the *proxy model*, as it proxies the HP tuning process. We follow standard notation d_{model} , $d_{head} = d_k$, d_v , n_{head} , d_{ffn} regarding dimensions in a Transformer; one can see Fig. 11 for a refresher.

Tensor Programs Series This paper is the 5th installment of the *Tensor Programs* series. While the target audience here are practitioners and empirical researchers, this paper presents the first major *practical* payoff of the *theoretical* foundation built in previous works [41–46].

2 Parametrization Matters: A Primer

In this section, we give a very basic primer on why the correct parametrization can allow HP transfer across width, but see Appendices L.1 to L.3 for more (mathematical) details.

The Central Limit Theorem (CLT) says that, if x_1,\ldots,x_n are iid samples from a zero-mean, unit-variance distribution, then $\frac{1}{\sqrt{n}}(x_1+\cdots+x_n)$ converges to a standard Gaussian $\mathcal{N}(0,1)$ as $n\to\infty$. Therefore, we can say that $\frac{1}{\sqrt{n}}$ is the right order of scaling factor c_n such that $c_n(x_1+\cdots+x_n)$ converges to something nontrivial. In contrast, if we set $c_n=1/n$, then $c_n(x_1+\cdots+x_n)\to 0$; or if $c_n=1$, then $c_n(x_1+\cdots+x_n)$ blows up in variance as $n\to\infty$.

Now suppose we would like to minimize the function

$$F_n(c) \stackrel{\text{def}}{=} \underset{x_1, \dots, x_n}{\mathbb{E}} f(c(x_1 + \dots + x_n)) \tag{1}$$

over $c \in \mathbb{R}$, for some bounded continuous function $f: \mathbb{R} \to \mathbb{R}$. If we reparametrize $c = \alpha/\sqrt{n}$ for $\alpha \in \mathbb{R}$, then by CLT, $G_n(\alpha) \stackrel{\mathrm{def}}{=} F_n(c) \to \mathbb{E} f(\mathcal{N}(0,\alpha^2))$ stabilizes into a function of α as $n \to \infty$. Then for sufficiently large n, the optimal $\alpha_n^* \stackrel{\mathrm{def}}{=} \arg\min_{\alpha} G_n(\alpha)$ should be close to α_n^* for any N > n, and indeed, for $N = \infty$ — this precisely means we can transfer the optimal c_n^* or α_n^* for a smaller problem (say F_n) to a larger problem (say F_n): G_n is approximately minimized by α_n^* and F_n is approximately minimized by σ_n^* and σ_n^* is approximately minimized by σ_n^* is the transfer algorithm is simply copying σ_n^* , we say the parametrization $c = \alpha/\sqrt{n}$ is the transfer algorithm for this problem.

In the scenario studied in this paper, x_1, \ldots, x_n are akin to randomly initialized parameters of a width-n neural network, c is akin to a HP such as learning rate, and f is the test-set performance of the network after training, so that F_n gives its expectation over random initializations. Just as in this example, if we parametrize the learning rate and other HPs correctly, then we can directly copy the optimal HPs for a narrower network into a wide network and expect approximately optimal

performance — this is the *hyperparameter transfer* we propose here. It turns out the Maximal Update Parametrization (μ P) introduced in [45] is correct (akin to the parametrization in α above), while the standard parametrization (SP) is incorrect (akin to the parametrization in c). We will review both parametrizations shortly. Theoretically, a μ P network has a well-defined infinite-width limit — akin to $(x_1 + \cdots + x_n)/\sqrt{n}$ having a $\mathcal{N}(0,1)$ limit by CLT — while a SP network does not (the limit will blow up) [45]. In fact, based on the theoretical foundation laid in [45], we argue in Appendix L.3 that μ P should also be the *unique* parametrization that allows HP transfer across width.

We emphasize that, to ensure transferability of any hyperparameter (such as learning rate), it's not sufficient to reparametrize *only* that hyperparameter, but rather, we need to identify and correctly reparametrize *all* hyperparameters in Table 2. For example, in Fig. 1, the wide models in SP still underperform their counterparts in μ P, even with learning rate tuned optimally. This is precisely because SP does not scale parameter multipliers and input/output layer learning rates correctly in contrast to μ P (see Table 3). See Appendix C for more intuition via a continuation of our example here. We shall also explain this more concretely in the context of neural networks in Appendix B.

3 Hyperparameters Don't Transfer Conventionally

In the community there seem to be conflicting assumptions about HP stability. *A priori*, models of different sizes don't have any reason to share the optimal HPs. Indeed, papers aiming for state-of-the-art results often tune them separately. On the other hand, a nontrivial fraction of papers in deep learning fixes all HPs when comparing against baselines, which reflects an assumption that the optimal HPs should be stable — not only among the same model of different sizes but also among models of different designs — therefore, such comparisons are fair. Here, we demonstrate HP *instability* across width explicitly in MLP and Transformers in the standard parametrization. We will only look at training loss to exclude the effect of regularization.

MLP with Standard Parametrization We start with a 2-hidden-layer MLP with activation function ϕ , using the standard parametrization⁷ with LeCun initialization⁸ akin to the default in PyTorch:

$$\begin{split} f(\xi) &= W^{3\top} \phi(W^{2\top} \phi(W^{1\top} \xi + b^1) + b^2) \\ \text{with init.} \quad W^1 &\sim \mathcal{N}(0, {}^1\!/a_{in}), \; W^{\{2,3\}} \sim \mathcal{N}(0, {}^1\!/n), \; b^{\{1,2\}} = 0, \end{split} \tag{2}$$

where $W^1 \in \mathbb{R}^{d_{in} \times n}, b^1 \in \mathbb{R}^n$, $W^2 \in \mathbb{R}^{n \times n}, b^2 \in \mathbb{R}^n$, $W^3 \in \mathbb{R}^{n \times d_{out}}$ and d_{in} , n, and d_{out} are the input, hidden, and output dimensions. The particular MLP we use has $\phi = ReLU$ and a cross-entropy (xent) loss function. We define the width of MLP as the hidden size n, which is varied from 256 to 8192. The models are trained on CIFAR-10 for 20 epochs, which is more than enough to ensure convergence.

As shown on the left in Fig. 3, the optimal learning rate shifts by roughly an order of magnitude as the width increases from 256 to 8192; using the optimal learning of the smallest model

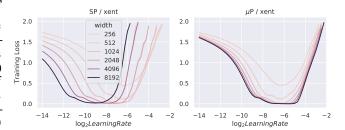


Figure 3: MLP width different hidden sizes trained for 20 epoch on CIFAR-10 using SGD. Left uses standard parametrization (SP); right uses maximal update parametrization (μ P). μ P networks exhibit better learning rate stability than their SP counterparts.

on the largest model gives very bad performance, if not divergence.

Transformer with Standard Parametrization This perhaps unsurprising observation holds for more complex architectures such as Transformer as well, as shown in Fig. 1 (left). We define width

 $^{^6}$ The more theoretically astute reader may observe that SP with a $\Theta(1/width)$ learning rate induces a well-defined infinite-width limit exists as well. Nevertheless, this does not allow HP transfer because this limit is in kernel regime as shown in [45]. See Appendix L.3 for more discussions.

⁷i.e. the default parametrization offered by common deep learning frameworks. See Table 3 for a review.

 $^{^8}$ The key here is that the init. variance $\propto 1/\mathrm{fan}$ _in, so the same insights here apply with e.g. He initialization.

Table 3: μ P[45] and SP for General Neural Networks, Basic Form. This basic form emphasizes the *scaling with width* (fan_in *or* fan_out); in practice, we may insert tunable multipliers in front of fan_in and fan_out as in Eq. (4). Notations: 1) η is the "master" learning rate. 2) The fan_out of a bias vector is its dimension (whereas fan_in is 1). 3) Purple text highlights key differences from standard parametrization (SP); Gray text recalls the corresponding SP. SGD (resp. Adam) here can be replaced by variants such as SGD with momentum (resp. Adagrad, Adadelta, etc). In general, the three columns here can be interpreted as linear layers that have {finite, infinite} input dimension and {infinite, finite, infinite} output dimension in an infinite-width network; this description generalizes more readily to other parameters such as those of layernorm. Transformer μ P requires one more modification (1/d attention instead of 1/ \sqrt{d}); see Definition 4.1. This version of μ P gets rid of parameter multipliers; for the version similar to that in [45], see Table 13. Also see Table 12 for a μ P formulation that is easier to implement (and compatible with input/output weight sharing).

	Input weights & all biases	Output weights	Hidden weights
Init. Var. SGD LR	$\frac{1/_{\mathrm{fan_in}}}{\eta \cdot \mathrm{fan_out}} (\eta)$	$\frac{1}{fan_in^2}$ $\frac{1}{fan_in}$ $\frac{1}{fan_in}$	$\frac{1}{\mathrm{fan_in}}$
Adam LR	η	$\eta/\text{fan_in}$ (η)	$\eta/_{\text{fan_in}}$ (η)

as d_{model} , with $d_k = d_q = d_v = d_{model}/n_{head}$ and $d_{ffn} = 4d_{model}$. The models are trained on wikitext-2 for 5 epochs. In Fig. 18 in the appendix we also show the instability of initialization scale and other HPs.

4 Unlocking Zero-Shot Hyperparameter Transfer with μ P

We show that μP solves the problems we see in Section 3.

MLP with μ **P** For the MLP in Section 3, to switch to μ P, we just need to modify Eq. (2)'s initialization of the last layer and its learning rates of the first and last layer as well as of the biases. The *basic form* is⁹

initialize
$$W^1 \sim \mathcal{N}(0, 1/d_{in}), \ W^2 \sim \mathcal{N}(0, 1/n), \ W^3 \sim \mathcal{N}(0, 1/n^2), \ b^{\{1,2\}} = 0$$

with SGD learning rates $\eta_{W^1} = \eta_{b^1} = \eta_{b^2} = \eta n, \ \eta_{W^2} = \eta, \ \eta_{W^3} = \eta n^{-1}$. (3)

Here, η specifies the "master" learning rate, and we highlighted in purple the differences in the two parametrizations. This basic form makes clear the *scaling with width* n of the parametrization, but in practice we will often insert (possibly tune-able) multiplicative constants in front of each appearance of n. For example, this is useful when we would like to be consistent with a SP MLP at a *base width* n_0 . Then we may insert constants as follows: For $\tilde{n} \stackrel{\text{def}}{=} n/n_0$,

initialize
$$W^1 \sim \mathcal{N}(0, 1/d_{in}), \ W^2 \sim \mathcal{N}(0, 1/n), \ W^3 \sim \mathcal{N}(0, 1/n \cdot \tilde{n}), \ b^{\{1,2\}} = 0$$

with SGD learning rates $\eta_{W^1} = \eta_{b^1} = \eta_{b^2} = \eta \tilde{n}, \ \eta_{W^2} = \eta, \ \eta_{W^3} = \eta \tilde{n}^{-1}.$ (4)

Then at width $n=n_0$, all purple factors above are 1, and the parametrization is identical to SP (Eq. (2)) at width n_0 . Of course, as n increases from n_0 , then Eq. (4) quickly deviates from Eq. (2). In other words, for a particular n, μ P and SP can be identical up to the choice of some constants (in this case n_0), but μ P determines a different "set" of networks and optimization trajectory than SP as one varies n. As we will see empirically in the next section, this deviation is crucial for HP transfer.

Indeed, in Fig. 3(right), we plot the CIFAR10 performances, over various learning rates and widths, of μP MLPs with $n_0=128$. In contrast to SP, the optimal learning rate under μP is stable. This means that, the best learning rate for a width-128 network is also best for a width-8192 network in μP —i.e. HP transfer works—but not for SP. In addition, we observe performance for a fixed learning rate always weakly improves with width in μP , but not in SP.

This MLP μ P example can be generalized easily to general neural networks trained under SGD or Adam, as summarized in Table 3, which is derived in Appendix L.

⁹While superficially different, this parametrization is equivalent to the μP defined in [45].

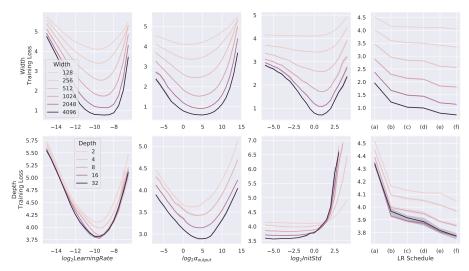


Figure 4: Empirical validation of the stability of four representative hyperparameters on pre-LN Transformers in μ P: learning rate, last layer weight multiplier α_{output} , weight initialization standard deviation, and learning rate schedule. We use the following learning rate schedules: (a) linear decay; (b) StepLR @ [5k, 8k] with a decay factor of 0.1; (c) StepLR @ [4k, 7k] with a decay factor of 0.3; (d) cosine annealing; (e) constant; (f) inverse square-root decay. All models are trained on wikitext-2 for 10k steps. When not specified in the legend, the width used is 256, depth 2, batch size 20, sequence length 256, and LR schedule constant. We sweep a particular HP, corresponding to each column, while fixing all others constant. See Section 5.1 for discussion of these results.

Transformers with μ **P** We repeat the experiments with base width $n_0 = 128$ for Transformers: **Definition 4.1.** The *Maximal Update Parametrization* (μ *P*) for a Transformer is given by Table 3 and 1/d attention instead of $1/\sqrt{d}$, i.e. the attention logit is calculated as $q^{\top}k/d$ instead of $q^{\top}k/\sqrt{d}$ where query q and key k have dimension d. We have d in the attention logit is calculated as d in the attention d in

The results are shown on the right in Fig. 1, where the optimal learning rate is stable, and the performance improves monotonically as width increases.

5 Which Hyperparameters Can Be μ Transferred?

In this section, we explore how common HPs fit into our framework. In general, they can be divided into three kinds, summarized in Table 1:

- 1. those that can transfer from the small to the large model, such as learning rate (Table 2);
- 2. those that primarily control regularization and don't work well with our technique; and
- 3. those that define training *scale*, such as width as discussed above as well as others like depth and batch size, across which we transfer other HPs.

Those in the first category transfer across width, as theoretically justified above in Section 2. To push the practicality and generality of our technique, we empirically explore the transfer across the other dimensions in the third category. Note that μ Transfer across width is quite general, e.g. it allows varying width ratio of different layers or number of attention heads in a Transformer; see Appendix G.2. This will be very useful in practice. For the second category, the amount of regularization (for the purpose of controlling overfitting) naturally depends on both the model size and data size, so we should not expect transfer to work if the parametrization only depends on model size. We discuss these HPs in more detail in Appendix G.1.

 $^{^{10}}$ This is roughly because during training, q and k will be correlated so $q^{\top}k$ actually scales like d due to Law of Large Numbers, in contrast to the original motivation that q, k are uncorrelated at initialization so Central Limit applies instead. See Appendix L.2.1 for a more in-depth discussion.

5.1 Empirical Validation and Limitations

Our empirical investigations focus on Transformers (here) and ResNet (in Appendix I.1.1), the most popular backbones of deep learning models today. We train a 2-layer pre-layernorm μ P¹¹ Transformer with 4 attention heads on Wikitext-2. We sweep one of four HPs (learning rate, output weight multiplier, initialization standard deviation, and learning rate schedule) while fixing the others and sweeping along width and depth (with additional results in Fig. 19 on transfer across batch size, sequence length, and training time). Fig. 4 shows the results averaged over 5 random seeds.

Empirically, we find that for language modeling on Transformers, HPs generally transfer across scale dimensions if some minimum width (e.g. 256), depth (e.g., 4), batch size (e.g., 32), sequence length (e.g., 128), and training steps (e.g., 5000) are met, with some caveats discussed below. While the exact optimum can shift slightly with increasing scale, this shift usually has very small impact on the loss, compared to SP (Figs. 1 and 3(left)). However, there are some caveats. For example, the best initialization standard deviation does not seem to transfer well across depth (2nd row, 3rd column), despite having a stabler optimum across width. In addition, while our results on width, batch size, sequence length, and training time still hold for post-layernorm (Fig. 17), ¹² the transfer across depth only works for pre-layernorm Transformer. Nevertheless, in practice (e.g. our results in Section 6.3) we find that fixing initialization standard deviation while tuning other HPs works well when transferring across depth.

6 Efficiency and Performance of μ Transfer

Now that the plausibility of μ Transfer has been established in toy settings, we turn to more realistic scenarios to see if one can achieve tangible gains. Specifically, we perform HP tuning only on a smaller proxy model, test the obtained HPs on the large target model directly, and compare against baselines tuned using the target model. We seek to answer the question: Can μ Transfer make HP tuning more efficient while achieving performance on par with traditional tuning? As we shall see by the end of the section, the answer is positive. We focus on Transformers here, while experiments on ResNets on CIFAR10 and Imagenet can be found as well in Appendix I.1. All of our experiments are run on V100 GPUs.

6.1 Transformer on IWSLT14 De-En

Setup IWSLT14 De-En is a well-known machine translation benchmark. We use the default IWSLT (post-layernorm) Transformer implemented in fairseq [25] with 40M parameters, which we denote as the $lx\ model.^{13}$ For μ Transfer, we tune on a $0.25x\ model$ with 1/4 of the width, amounting to 4M parameters. For this experiment, we tune via random search the learning rate η , the output layer parameter multiplier α_{output} , and the attention key-projection weight multiplier α_{attn} . See the grid and other experimental details in Appendix H.1.

We compare transferring from the 0.25x model with tuning the 1x model while controlling the total tuning budget in FLOPs. ¹⁴ To improve the reproducibility of our result: 1) we repeat the entire HP search process (a *trial*) 25 times for each setup, with number of samples as indicated in Table 4, and report the 25th, 50th, 75th, and 100th percentiles in BLEU score; 2) we evaluate each selected HP combination using 5 random initializations and report the mean performance. ¹⁵

We pick the HP combination that achieves the lowest validation loss ¹⁶ for each trial. The reported best outcome is chosen according to the validation loss during tuning. We compare against the default in fairseq, which is presumably heavily tuned. The result is shown in Table 4.

¹¹"2 layers" means the model has 2 self-attention blocks. To compare with SP Transformer, see Fig. 18.

¹²in fact, post-layernorm Transformers are much more sensitive to HPs than pre-layernorm, so our technique is more crucial for them, especially for transfer across width. Fig. 1 uses post-layernorm.

¹³ https://github.com/pytorch/fairseq/blob/master/examples/translation/README.md.

¹⁴Ideally we would like to measure the wall clock time used for tuning. However, smaller models such as the proxy Transformer used for IWSLT are not efficient on GPUs, so wall clock time would not reflect the speedup for larger models like GPT-3. Thus, we measure in FLOPs, which is less dependent on hardware optimization.

¹⁵We do not report the standard deviation over random initializations to avoid confusion.

¹⁶We find this provides more reliable result than selecting for the best BLEU score.

Table 4: **Transformer on IWSLT14 De-En.** 1x and 0.25x refers to scaling of width only. Compared to traditional tuning ("Tuning on 1x"), μ transfer from 0.25x provides better and more reliable outcome given fixed amount of compute. On the other hand, naive transfer (i.e. with SP instead of μ P) fails completely. The percentiles are over independent trials, with each trial involving the entire tuning process with a new HP random search.

			V	al. BLEU	Percenti	les
Setup	Total Compute	#Samples	25	50	75	100
fairseq[25] default	-	-	-	-	-	35.40
Tuning on 1x	1x	5	33.62	35.00	35.35	35.45
Naive transfer from 0.25x	1 x	64		training	diverged	
μ Transfer from 0.25x (Ours)	1x	64	35.27	35.33	35.45	35.53

Performance Pareto Frontier The result above only describes a particular compute budget. Is μ Transfer still preferable when we have a lot more (or less) compute? To answer this question, we produce the compute-performance Pareto frontier in Fig. 5(left), where we repeat the above experiment with different compute budgets. Evidently, our approach completely dominates conventional tuning.

Sample Quality of Proxy Model vs Target Model The Pareto frontier in Fig. 5(right) suggests that, given a fixed number of random *samples* from the HP space, 1) tuning the target model directly yields slightly better results than tuning the proxy model (while taking much more compute of course), but 2) this performance gap seems to vanish as more samples are taken. This can be explained by the intuition that the narrower proxy model is a "noisy estimator" of the wide target model [45]. With few samples, this noise can distort the random HP search, but with more samples, this noise is suppressed.

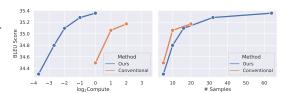


Figure 5: Efficiency-performance Pareto frontier of μ Transfer compared to conventional tuning, on IWSLT Transformer, using random HP search as the base method. We plot the median BLEU score over 25 trials (Left) against relative compute budget in log scale and (Right) against number of HP samples taken. While with the same number of samples, μ Transfer slightly underperforms conventional tuning, this gap vanishes with more samples, and in terms of compute, our Pareto frontier strongly and consistently dominates that of conventional tuning. Note that, in larger models (e.g. BERT or GPT-3, not shown here), we believe our efficiency advantage will only widen as our small proxy model can stay the same size while the target model grows.

6.2 Transformer on WMT14 En-De

We scale up to WMT14 En-De using the large (post-layernorm) Transformer from [37] with 211M parameters. We tune on a proxy model with 15M parameters by shrinking d_{model} , d_{ffn} , and n_{head} . For this experiment, we tune via random search the learning rate η , the output layer parameter multiplier α_{output} , and the attention key-projection weight multiplier α_{attn} following the grid in Appendix H.2. The result is shown in Table 5: While random search with 3 HP samples far underperforms the fairseq default, we are able to match it via transfer using the same tuning budget.

Table 5: **Transformers on WMT14 En-De.** 1x and 0.25x refers to scaling of width only. We report BLEU fluctuation over 3 independent trials, i.e., 3 independent random HP searches.

			Val. E	LEU Perce	entiles
Setup	Total Compute	#Samples	Worst	Median	Best
fairseq[25] default	-	-	-	-	26.40
Tuning on 1x	1x	3	training	diverged	25.69
Naive transfer from 0.25x	1x	64	trai	ning diverg	ged
μ Transfer from 0.25x (Ours)	1x	64	25.94	26.34	26.42

6.3 BERT

Finally, we consider large-scale language model pretraining where HP tuning is known to be challenging. Using Megatron (pre-layernorm) BERT [32] as a baseline, we hope to recover the performance of the published HPs by only tuning a proxy model that has roughly 13M parameters, which we call *BERT-prototype*. While previous experiments scaled only width, here we will also scale depth, as discussed in Section 5 and validated in Fig. 4. We use a batch size of 256 for all runs and follow the standard finetuning procedures. For more details on BERT-prototype, what HPs we tune, and how we finetune the trained models, see Appendix H.3.

During HP tuning, we sample 256 combinations from the search space and train each combination on BERT-prototype for 10^5 steps. The total tuning cost measured in FLOPs is roughly the same as training 1 BERT-large for the full 10^6 steps; the exact calculation is shown in Appendix H.3. The results are shown in Table 6. Notice that on BERT-large, we obtain sizeable improvement over the well-tuned Megatron BERT-large baseline.

Table 6: **BERT pretraining.** HP transfer outperforms published baselines without tuning the full model directly at all. We tune BERT-base and BERT-large simultaneously via a single proxy model, *BERT-prototype*. The total tuning cost = the cost of pretraining a single BERT-large. *Model speedup* refers to the training speedup of BERT-prototype over BERT-base or BERT-large. *Total speedup* in addition includes time saving from transferring across training steps. Both speedups can be interpreted either as real-time speedup on V100s or as FLOPs speedup (which turn out to be empirically very similar in this case).

Model	Method	Model Speedup	Total Speedup	Test loss	MNLI (m/mm)	QQP
$BERT_{base}$	Megatron Default	1x	1x	1.995	84.2/84.2	90.6
$BERT_{base}$	Naive Transfer	4x	40x	t	raining diverged	
BERT_{base}	μ Transfer (Ours)	4x	40x	1.970	84.3/84.8	90.8
$\overline{\text{BERT}_{large}}$	Megatron Default	1x	1x	1.731	86.3/86.2	90.9
$BERT_{large}$	Naive Transfer	22x	220x	t	raining diverged	
BERT_{large}	μ Transfer (Ours)	22x	220x	1.683	87.0/86.5	91.4

6.4 GPT-3

In order to further verify μ Transfer at scale, we applied it to GPT-3 6.7B [6]. This Transformer model (the *target model*) consists of 32 residual blocks with width 4096. We form the small *proxy model* by shrinking width to 256, resulting in roughly 40 million trainable parameters, 168 times smaller than the target model. HPs were then determined by a random search on the proxy model. The total tuning cost was only 7% of total pretraining cost. Details of the HP sweep can be found in Appendix H.4.

In order to exclude code difference as a possible confounder, we also re-trained GPT-3 6.7B from scratch using the original HPs from [6]. During training of the μ Transfer model we encountered numerical issues that lead to frequent divergences. In order to avoid them, the model was trained using FP32 precision, even though the original 6.7B model and our re-run were trained using FP16. The resulting μ Transfer model outperforms the 6.7B from [6], and is in fact comparable to the twice-as-large 13B model across our evaluation suite (see Table 9). Selected evaluation results can be found in Table 7 and further details are given in Table 8 and Appendix H.4.

7 Related Works

Hyperparameter Tuning Many have sought to speed up HP tuning beyond the simple grid or random search, such as via Bayesian optimization [34, 35] or multi-arm bandits [15, 18]. There are also dedicated tools such as Optuna [4] and Talos [3] which integrate with existing deep learning frameworks and provide an easy way to apply more advanced tuning techniques. Our work is complementary to the above, as they can be used to tune the proxy model. it is only for scientific reasons that we primarily did random search throughout this work.

¹⁷While we are mainly focused on the efficacy of μ Transfer regardless of precision, it would be interesting to ablate the effect of precision in our results, but we did not have enough resources to rerun the baseline in FP32

Table 7: **GPT-3 6.7B Pretraining.** Selected evaluation results for the GPT-3 6.7B model tuned with μ Transfer (transfered from a small proxy model of 40M parameters), compared to the results published in [6] and a re-run with original HPs. Note that the perplexities in this table are based on a custom tokenization and are not comparable to the literature. The validation loss refers to the loss achieved on a random held-out part of our dataset. *Zero-shot*, *One-Shot* and *Few-Shot* refer to the number of additional query and answer pairs passed in the context when performing the sampling-based evaluations. See Appendix H.4 for full evaluation results.

Task	Metric	$6.7\mathrm{B}$ + $\mu\mathrm{P}$	6.7B re-run	6.7B from [6]
Validation loss	cross-entropy	1.98	2.03	-
PTB	perplexity	11.4	13.0	-
WikiText-103	perplexity	8.56	9.13	-
One Billion Words	perplexity	20.5	21.7	-
LAMBADA Zero-Shot	accuracy	73.5	70.8	70.3
LAMBADA One-Shot	accuracy	69.9	64.8	65.4
LAMBADA Few-Shot	accuracy	74.7	77.1	79.1
HellaSwag Zero-Shot	accuracy	72.0	66.7	67.4
HellaSwag One-Shot	accuracy	71.1	65.9	66.5
HellaSwag Few-Shot	accuracy	72.4	66.4	67.3

Hyperparameter Transfer Many previous works explored transfer learning of HP tuning (e.g. [12, 28, 36, 49]). However, to the best of our knowledge, our work is the first to explore *zero-shot* HP transfer. In addition, we focus on transferring across model scale rather than between different tasks or datasets. Some algorithms like Hyperband [19] can leverage cheap estimates of HP evaluations (like using a small model to proxy a large model) but they are not zero-shot algorithms, so would still be very expensive to apply to large model training. Nevertheless, all of the above methods are complementary to ours as they can be applied to the tuning of our proxy model.

Previously Proposed Scaling Rules of Hyperparameters [11, 23, 31, 33] investigated the right way to scale learning rate with batch size, with sometimes conflicting proposals. which we summarize in Appendix F. [26] studied how learning rate (and batch size) should scale with width for MLPs and CNNs trained with SGD in NTK or standard parametrizations. We provide a detailed comparison of our work with theirs in Appendix F.

Many previous works proposed different initialization or parametrizations with favorable properties, such as better stability for training deep neural networks [5, 10, 13, 21, 30, 47, 48, 51]. Our work differs from these in that we focus on the transferability of optimal HPs from small models to large models in the same parametrization.

8 Conclusion

Leveraging the discovery of a feature learning neural network infinite-width limit, we hypothesized and verified that the HP landscape across NNs of different width is reasonably stable if parametrized according to Maximal Update Parametrization (μ P). We further empirically showed that it's possible to transfer across depth, batch size, sequence length, and training time, with a few caveats. This allowed us to indirectly tune a very large network by tuning its smaller counterparts and transferring the HPs to the full model.

Venues of Improvement Nevertheless, our method has plenty of room to improve. For example, initialization does not transfer well across depth, and depth transfer generally still does not work for post-layernorm Transformers. This begs the question whether a more principled parametrization in depth could solve these problems. Additionally, Fig. 4 shows that the optimal HP still shifts slightly for smaller models. Perhaps by considering finite-width corrections to μ P one can fix this shift. Finally, it will be interesting to consider if there's a way to transfer regularization HPs as a function of both the model size and data size.

Broader Impact Our work makes HP tuning of large models more efficient. This enables large models to be better tuned given the same compute budget, thereby increasing the performance per cost. Organizations large and small can focus their research on small models and scale up only once with reasonable confidence that the training would go well. We do not foresee any direct negative societal impact.

References

- [1] NVIDIA/DeepLearningExamples, apache v2 license. URL https://github.com/NVIDIA/DeepLearningExamples.
- [2] Davidnet, mit license, 2019. URL https://github.com/davidcpage/cifar10-fast.
- [3] Autonomio talos, mit license, 2019. URL http://github.com/autonomio/talos.
- [4] Takuya Akiba, Shotaro Sano, Toshihiko Yanase, Takeru Ohta, and Masanori Koyama. Optuna: A next-generation hyperparameter optimization framework, 2019.
- [5] Thomas Bachlechner, Bodhisattwa Prasad Majumder, Huanru Henry Mao, Garrison W. Cottrell, and Julian McAuley. ReZero is All You Need: Fast Convergence at Large Depth. arXiv:2003.04887 [cs, stat], June 2020. URL http://arxiv.org/abs/2003.04887. arXiv: 2003.04887.
- [6] Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot learners, 2020.
- [7] Ciprian Chelba, Tomas Mikolov, Mike Schuster, Qi Ge, Thorsten Brants, Phillipp Koehn, and Tony Robinson. One billion word benchmark for measuring progress in statistical language modeling, 2014.
- [8] Zihang Dai, Zhilin Yang, Yiming Yang, Jaime Carbonell, Quoc V. Le, and Ruslan Salakhutdinov. Transformer-xl: Attentive language models beyond a fixed-length context, 2019.
- [9] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *arXiv*:1810.04805 [cs], May 2019. URL http://arxiv.org/abs/1810.04805. arXiv: 1810.04805 version: 2.
- [10] Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In Yee Whye Teh and Mike Titterington, editors, *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, volume 9 of *Proceedings of Machine Learning Research*, pages 249–256, Chia Laguna Resort, Sardinia, Italy, May 2010. PMLR. URL http://proceedings.mlr.press/v9/glorot10a.html.
- [11] Elad Hoffer, Itay Hubara, and Daniel Soudry. Train longer, generalize better: closing the generalization gap in large batch training of neural networks. *arXiv:1705.08741 [cs, stat]*, May 2017. URL http://arxiv.org/abs/1705.08741. arXiv: 1705.08741.
- [12] Samuel Horváth, Aaron Klein, Peter Richtárik, and Cédric Archambeau. Hyperparameter transfer learning with adaptive complexity. *CoRR*, abs/2102.12810, 2021. URL https://arxiv.org/abs/2102.12810.
- [13] Xiao Shi Huang and Felipe Pérez. Improving Transformer Optimization Through Better Initialization. page 9.
- [14] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural Tangent Kernel: Convergence and Generalization in Neural Networks. *arXiv:1806.07572 [cs, math, stat]*, June 2018. URL http://arxiv.org/abs/1806.07572. 00000 arXiv: 1806.07572.
- [15] Kevin Jamieson and Ameet Talwalkar. Non-stochastic best arm identification and hyperparameter optimization, 2015.

- [16] Jared Kaplan, Sam McCandlish, Tom Henighan, Tom B. Brown, Benjamin Chess, Rewon Child, Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei. Scaling Laws for Neural Language Models. arXiv:2001.08361 [cs, stat], January 2020. URL http://arxiv.org/abs/2001. 08361. arXiv: 2001.08361.
- [17] Diederik Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
- [18] Liam Li, Kevin Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Moritz Hardt, Benjamin Recht, and Ameet Talwalkar. A system for massively parallel hyperparameter tuning, 2020.
- [19] Lisha Li, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. *JMLR 18*, page 52.
- [20] Liyuan Liu, Xiaodong Liu, Jianfeng Gao, Weizhu Chen, and Jiawei Han. Understanding the difficulty of training transformers. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 5747–5763, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.463. URL https://www.aclweb.org/anthology/2020.emnlp-main.463.
- [21] Liyuan Liu, Xiaodong Liu, Jianfeng Gao, Weizhu Chen, and Jiawei Han. Understanding the Difficulty of Training Transformers. *arXiv:2004.08249 [cs, stat]*, September 2020. URL http://arxiv.org/abs/2004.08249. arXiv: 2004.08249.
- [22] Xiaodong Liu, Pengcheng He, Weizhu Chen, and Jianfeng Gao. Multi-task deep neural networks for natural language understanding. In *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pages 4487–4496, Florence, Italy, July 2019. Association for Computational Linguistics. URL https://www.aclweb.org/anthology/P19-1441.
- [23] Sam McCandlish, Jared Kaplan, Dario Amodei, and OpenAI Dota Team. An Empirical Model of Large-Batch Training. arXiv:1812.06162 [cs, stat], December 2018. URL http://arxiv.org/abs/1812.06162. arXiv: 1812.06162.
- [24] Stephen Merity, Caiming Xiong, James Bradbury, and Richard Socher. Pointer sentinel mixture models, 2016.
- [25] Myle Ott, Sergey Edunov, Alexei Baevski, Angela Fan, Sam Gross, Nathan Ng, David Grangier, and Michael Auli. fairseq: A fast, extensible toolkit for sequence modeling, mit license. In *Proceedings of NAACL-HLT 2019: Demonstrations*, 2019.
- [26] Daniel S. Park, Jascha Sohl-Dickstein, Quoc V. Le, and Samuel L. Smith. The Effect of Network Width on Stochastic Gradient Descent and Generalization: an Empirical Study. May 2019. URL https://arxiv.org/abs/1905.03776v1.
- [27] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library, bsd-style license. In H. Wallach, H. Larochelle, A. Beygelzimer, F. dÁlché Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 8024–8035. Curran Associates, Inc., 2019. URL http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf.
- [28] Valerio Perrone, Rodolphe Jenatton, Matthias W Seeger, and Cedric Archambeau. Scalable Hyperparameter Transfer Learning. *NeurIPS 2018*, page 11.
- [29] Martin Popel and Ondřej Bojar. Training Tips for the Transformer Model. The Prague Bulletin of Mathematical Linguistics, 110(1):43-70, April 2018. ISSN 1804-0462. doi: 10.2478/ pralin-2018-0002. URL http://content.sciendo.com/view/journals/pralin/110/ 1/article-p43.xml.

- [30] Samuel S. Schoenholz, Justin Gilmer, Surya Ganguli, and Jascha Sohl-Dickstein. Deep Information Propagation. arXiv:1611.01232 [cs, stat], November 2016. URL http://arxiv.org/abs/1611.01232. arXiv: 1611.01232.
- [31] Christopher J. Shallue, Jaehoon Lee, Joseph Antognini, Jascha Sohl-Dickstein, Roy Frostig, and George E. Dahl. Measuring the Effects of Data Parallelism on Neural Network Training. arXiv:1811.03600 [cs, stat], November 2018. URL http://arxiv.org/abs/1811.03600. arXiv: 1811.03600.
- [32] Mohammad Shoeybi, Mostofa Patwary, Raul Puri, Patrick LeGresley, Jared Casper, and Bryan Catanzaro. Megatron-lm: Training multi-billion parameter language models using model parallelism. *CoRR*, abs/1909.08053, 2019. URL http://arxiv.org/abs/1909.08053.
- [33] Samuel L. Smith, Pieter-Jan Kindermans, and Quoc V. Le. Don't Decay the Learning Rate, Increase the Batch Size. *arXiv:1711.00489 [cs, stat]*, November 2017. URL http://arxiv.org/abs/1711.00489. arXiv: 1711.00489.
- [34] Jasper Snoek, Hugo Larochelle, and Ryan P. Adams. Practical bayesian optimization of machine learning algorithms, 2012.
- [35] Jasper Snoek, Oren Rippel, Kevin Swersky, Ryan Kiros, Nadathur Satish, Narayanan Sundaram, Md. Mostofa Ali Patwary, Prabhat, and Ryan P. Adams. Scalable bayesian optimization using deep neural networks, 2015.
- [36] Danny Stoll, Jörg K.H. Franke, Diane Wagner, Simon Selg, and Frank Hutter. Hyperparameter transfer across developer adjustments, 2021. URL https://openreview.net/forum?id=WPOOvDYLXem.
- [37] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. CoRR, abs/1706.03762, 2017. URL http://arxiv.org/abs/1706.03762.
- [38] Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R Bowman. Glue: A multi-task benchmark and analysis platform for natural language understanding. *EMNLP 2018*, page 353, 2018.
- [39] Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R. Bowman. Glue: A multi-task benchmark and analysis platform for natural language understanding, 2019.
- [40] Adina Williams, Nikita Nangia, and Samuel Bowman. A broad-coverage challenge corpus for sentence understanding through inference. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long Papers)*, pages 1112–1122. Association for Computational Linguistics, 2018. URL http://aclweb.org/anthology/N18-1101.
- [41] Greg Yang. Tensor Programs I: Wide Feedforward or Recurrent Neural Networks of Any Architecture are Gaussian Processes. *arXiv:1910.12478 [cond-mat, physics:math-ph]*, December 2019. URL http://arxiv.org/abs/1910.12478.
- [42] Greg Yang. Scaling Limits of Wide Neural Networks with Weight Sharing: Gaussian Process Behavior, Gradient Independence, and Neural Tangent Kernel Derivation. arXiv:1902.04760 [cond-mat, physics:math-ph, stat], February 2019. URL http://arxiv.org/abs/1902.04760.
- [43] Greg Yang. Tensor Programs II: Neural Tangent Kernel for Any Architecture. *arXiv:2006.14548* [cond-mat, stat], August 2020. URL http://arxiv.org/abs/2006.14548.
- [44] Greg Yang. Tensor Programs III: Neural Matrix Laws. arXiv:2009.10685 [cs, math], September 2020. URL http://arxiv.org/abs/2009.10685.
- [45] Greg Yang and Edward J. Hu. Feature learning in infinite-width neural networks. arXiv, 2020.
- [46] Greg Yang and Etai Littwin. Tensor Programs IIb: Architectural Universality of Neural Tangent Kernel Training Dynamics. arXiv:2105.03703 [cs, math], May 2021. URL http://arxiv.org/abs/2105.03703.

- [47] Greg Yang and Sam S. Schoenholz. Deep Mean Field Theory: Layerwise Variance and Width Variation as Methods to Control Gradient Explosion. February 2018. URL https://openreview.net/forum?id=rJGY8GbR-.
- [48] Greg Yang and Samuel S. Schoenholz. Mean Field Residual Networks: On the Edge of Chaos. arXiv:1712.08969 [cond-mat, physics:nlin], December 2017. URL http://arxiv.org/abs/1712.08969. 00000 arXiv: 1712.08969.
- [49] Dani Yogatama and Gideon Mann. Efficient Transfer Learning Method for Automatic Hyperparameter Tuning. In *Artificial Intelligence and Statistics*, pages 1077–1085. PMLR, April 2014. URL http://proceedings.mlr.press/v33/yogatama14.html. ISSN: 1938-7228.
- [50] Sergey Zagoruyko and Nikos Komodakis. Wide residual networks, 2017.
- [51] Hongyi Zhang, Yann N. Dauphin, and Tengyu Ma. Residual Learning Without Normalization via Better Initialization. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=H1gsz30cKX.

A Practical Considerations

In this section, we outline several useful tips and tricks that can improve the quality of hyperparameter transfer in practice.

A.1 Zero Initialization for Output Layers

We find that the optimal hyperparameters of small and large width models match more closely when we initialize output layers at 0 (i.e. with variance σ^2/fan _in where $\sigma=0$ instead of positive σ). This is because the neural network in μ P is approximately a Gaussian process (GP) at initialization with variance on the order $\Theta(\sigma^2/width)$ (contrast this with SP networks, which approximates a GP with $\Theta(\sigma^2)$ variance) [41, 45]. Of course, when width is large, this variance vanishes, but this can be far from so in the small proxy model. This discrepancy in the initial GP can cause the training trajectory of the proxy model to be very different from the trajectory of the large target model, causing a mismatch in the optimal hyperparameters. By initializing the output layer at 0, we remove this mismatch in the initial GP. Empirically we do not find this modification to be detrimental to performance.

A.2 Activation Functions

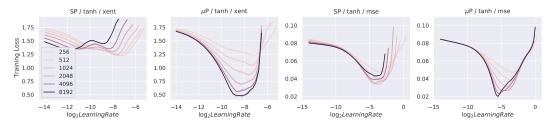


Figure 6: Squashing activation functions reduce transfer quality. MLP of different hidden sizes with tanh activation trained for 20 epoch on CIFAR-10 using SGD. Left uses cross-entropy as loss function; right uses mean square error; columns alternate between standard parametrization (SP) and maximal update parametrization (μ P). Compared to ReLU, tanh exhibits slower convergence for μ P, yet it still outperforms SP when width is increased

When the network is narrow, its approximation to the infinite-width behavior becomes crude, which is manifested as large fluctuations in preactivation coordinates. When using a squashing activation functions like softmax or tanh, this causes narrower networks to saturate the activation more than wider ones, which results in a systematic bias in the gradients and therefore the hyperparameter landscape. This can be seen in Fig. 6, where we use tanh as the network activation function.

Therefore, we recommend replacing non-essential squashing activation functions with ReLU, whose derivative depends only on the sign of the pre-activation. A similar reasoning can be applied to superlinear activation functions, where the distribution of activation values can have heavy tails, leading to slow convergence to the infinite-width limit. However, such activations are rarely used in practice.

A.3 Enlarge d_k

We find that small $d_{head} = d_k$ can lead to a highly noisy HP landscape, as shown in Fig. 7. This can significantly decrease the quality of random HP search on the small proxy model. To solve this, we find it useful to decouple d_k from d_{model} (so that $d_{model} \neq d_k \cdot n_{head}$) and maintain a relatively large d_k even as d_{model} is shrunk in the proxy model. For example, pegging $d_k = 32$ is generally effective. Training or inference speed are not usually affected much by the larger d_k because of CUDA optimizations. By Appendix G.2, this decoupling of d_k from d_{model} is theoretically justified, and as shown in Fig. 7, it significantly denoises the HP landscape.

A.4 Non-Gaussian vs Gaussian Initialization

We find non-Gaussian (e.g. uniform) initialization can sometimes cause wider models to perform worse than narrower models, whereas we do not find this behavior for Gaussian initialization. This is

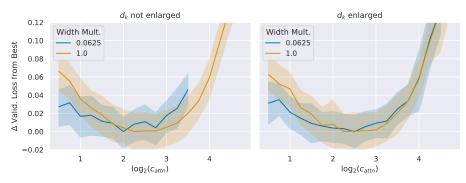


Figure 7: **Enlarging** d_k **makes** μ **Transfer more precise.** Here we plot all curves *after subtracting their minima* for easier visual comparison. Transformer on IWSLT 14 similar to the setup in Appendix H.1 where the $d_{model} = 512$ for a width multiplier of 1, $n_{head} = 4$, and $d_q = d_k$. (**Left**) We leave $d_q = d_k = \frac{d_{model}}{n_{head}}$, so $d_k = 8$ for width-multiplier 0.0625. The optimum for the attention logit multiplier c_{attn} is noisy and does not accurately transfer across width. (**Right**) We enlarge $d_q = d_k$ to a minimum of 128. The HP landscape is much smoother than in (Left), and the optima align between narrow and wide models.

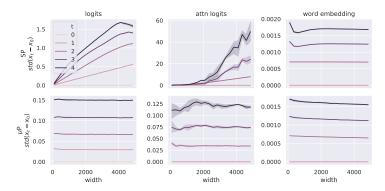


Figure 8: Logits and attention logits, but not word embeddings, of a Transformer blow up with width in SP after 1 step of training. In contrast, all three are well-behaved with width in μ P. Here we measure how much different values change coordinatewise from initialization over 4 steps of Adam updates, as a function of width. Specifically, we plot the standard deviation of the coordinates of $x_t - x_0$, for $t = 0, \ldots, 4$, and $x \in \{\text{logits, attention logits, word embeddings}\}$, where t = 0 indicates initialization.

consistent with theory, since in the large width limit, one should expect non-Gaussian initialization will behave like Gaussian initializations anyway (essentially due to Central Limit Theorem, or more precisely, universality), but the non-Gaussianity slows down the convergence to this limit.

A.5 Using a Larger Sequence Length

For Transformers, we empirically find that we can better transfer initialization standard deviation from a narrower model (to a wide model) if we use a larger sequence length. It is not clear why this is the case. We leave an explanation to future work.

B The Defects of SP and How μ P Fixes Them

The question of SP vs μ P has already been studied at length in [45]. Here we aim to recapitulate the key insights, with more explanations given in Appendix L.3.

An Instructive Example As shown in [45] and Appendix L.3, in SP, the network output will blow up with width after 1 step of SGD. It's instructive to consider a 1-hidden-layer linear perceptron $f(x) = V^{\top}Ux$ with scalar inputs and outputs, as well as weights $V, U \in \mathbb{R}^{n \times 1}$. In SP, $V_{\alpha} \sim$

 $\mathcal{N}(0,1/n)$ ad $U_{\alpha} \sim \mathcal{N}(0,1)$ for each $\alpha \in [n]$. This sampling ensures that $f(x) = \Theta(|x|)$ at initialization. After 1 step of SGD with learning rate 1, the new weights are $V' \leftarrow V + \theta U, U' \leftarrow U + \theta V$, where θ is some scalar of size $\Theta(1)$ depending on the inputs, labels, and loss function. But now

$$f(x) = V'^{\top}U'x = (V^{\top}U + \theta U^{\top}U + \theta V^{\top}V + \theta^2 U^{\top}V)x$$
 (5)

blows up with width n because $U^{T}U = \Theta(n)$ by Law of Large Numbers.

Now consider the same network in μ P. According to Table 3, we now have $V_{\alpha} \sim \mathcal{N}(0, 1/n^2)$ in contrast to SP, but $U_{\alpha} \sim \mathcal{N}(0, 1)$ as before, with learning rates $\eta_V = 1/n, \eta_U = n$. After 1 step of SGD, we now have

$$f(x) = (V^{\top}U + \theta n^{-1}U^{\top}U + \theta nV^{\top}V + \theta^2U^{\top}V)x,$$

and one can verify this is $\Theta(1)$ and thus does not blow up with width.¹⁸

Some Layers Update Too Fast, Others Too Slow One can observe the same behavior in more advanced architectures like Transformers and optimizers like Adam; in fact, in SP, other hidden quantities like attention logits will also blow up with width after 1 step, but in μ P still remain bounded, as shown in Fig. 8(middle).

One might think scaling down the learning rate with width can solve this problem in SP. However, other hidden activations like the word embedding (Fig. 8(right)) in a Transformer update by a width-independent amount for each step of training, so scaling down the learning rate will effectively mean the word embeddings are not learned in large width models. Similar conclusions apply to other models like ResNet (in fact, one can observe in the SP linear MLP example above, the input layer is updated much more slowly than the output layer). On the other hand, μ P is designed so that all hidden activations update with the same speed in terms of width (see Appendix L.2 for why).

Performance Advantage of μ **P** This is why a wide model tuned with μ Transfer should in general outperform its SP counterpart with (global) learning rate tuned. For example, this is the case for the width-8192 Transformer in Fig. 1, where, in SP, the optimal learning rate needs to mollify the blow-up in quantities like logits and attention logits, but this implies others like word embeddings do not learn appreciably. This performance advantage means μ Transfer does more than just predicting the optimal learning rate of wide SP models. Relatedly, we observe, for any fixed HP combination, training performance never decreases with width in μ P, in contrast to SP (e.g., the μ P curves in Figs. 1, 3 and 16 do not cross, but the SP curves do; see also Appendix D).

C Parametrization Matters: A Primer for Multiple Hyperparameters

Here we give more intuition why we need to reparametrize *all* hyperparameters. In practice, neural networks have multitudes of hyperparameters all interacting together. In our example of Section 2, hyperparameter optimization would be akin to minimizing the function ¹⁹

$$F_n(c^1,\ldots,c^k) \stackrel{\text{def}}{=} \underset{x_1,\ldots,x_n}{\mathbb{E}} f((c^1+\cdots+c^k)(x_1+\cdots+x_n)).$$

where x_1, \ldots, x_n are as in Eq. (1) and c^1, \ldots, c^k are analogous to k hyperparameters. For the same reasoning in Section 2, the *correct parametrization* is in $(\alpha^1, \ldots, \alpha^k)$ where $\alpha^i = c^i \sqrt{n}$.

While this is straightforward, in practice, researchers often fix some hyperparameters (e.g., they tune only learning rate but neglects to scale parameter multipliers or initialization correctly). For example, if we only partially reparametrize and optimize in α^1 while fixing c^2,\ldots,c^k , then the optimal α^1 is $(\alpha^1)^* = \alpha^* - (c^1+\ldots+c^k)\sqrt{n}$ where α^* is the optimal α for Eq. (1). Thus, as $n\to\infty$, $(\alpha^1)^*$ still blows up even though we parametrized α^1 correctly. More generally, the incorrect parametrization of some hyperparameters forces other hyperparameters to increasingly compensate for it as width grows, distorting their optima, even if the latter are correctly parametrized.

¹⁸Note in this example, Glorot initialization [10] (i.e. with variance $1/(\text{fan_in} + \text{fan_out}))$ would scale asymptotically the same as μP and thus is similarly well-behaved. However, if one adds layernorm or batchnorm, then Glorot will cause logit blowup like SP, but μP still will not.

¹⁹Here, for simplicity of the example, we model the interaction between "hyperparameters" c^1, \ldots, c^k as additive, but in real neural networks such interactions are usually much more complicated.

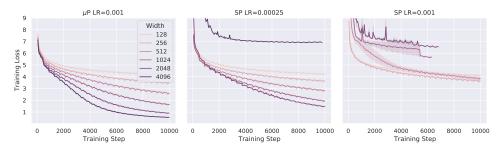


Figure 9: Wider is always better in training loss under μ P, but not in SP, given the same HP. Learning curves for μ P and SP with different learning rates, aggregated over 5 seeds. (Left) Wider μ P models always achieve better training loss at any time in training. (**Middle**) If using a small learning rate, SP models can appear to do so up to some large width, at which point the pattern fails (at width 2048 in our plot). (**Right**) If using a large learning rate, SP model can do worse with width; here the SP model is identical to the μ P model in (Left) at width 128.

Wider is Better in μ P Throughout Training

In earlier plots like Figs. 1 and 3, we saw that at the end of training, wider is always better in μ P but not in SP. In fact, we find this to be true throughout training, as seen in Fig. 9, modulo noise from random initialization and/or data ordering, and assuming the output layer is zero-initialized (which has no impact on performance as discussed in Appendix A.1). We then stress-tested this on a μ P GPT-3 Transformer (on the GPT-3 training data) by scaling width from 256 to 32,768 using a fixed set of HPs (Fig. 10). Wider models consistently match or outperform narrower models at each point in training (except a brief period around 1e8 training tokens, likely due to noise because we ran only 1 seed due to computational cost). Our observation suggests that wider models are strictly more data-efficient if scaled appropriately. By checking "wider-is-better" early in

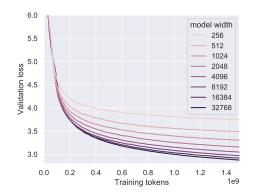


Figure 10: Stress-testing "wider-is-better" in μ P. Here we trained a GPT-3 transformer with 4 layers and widths from 256 to 32,768. Modulo a brief period around 1e8 training tokens, wider is better throughout training.

training, one can also cheaply debug a μP implementation.

Useful Hyperparameter Transfer: A Theoretical Puzzle

We want to tune HPs on a small model with width N such that its HP landscape looks like that of a large model with width $\gg N$. Our intuition in Section 2 and Appendices C and L leads us to μP . However, for this to be useful, we do not want the small model (as a function) after training to be close to that of the large model — otherwise there is no point in training the large model to begin with. So N 1) must be large enough so that the HP optimum converges, but 2) cannot be so large that the functional dynamics (and the loss) converges. The fact that such N exists, as demonstrated by our experiments, shows that: In some sense, the HP optimum is a "macroscopic" or "coarse" variable which converges quickly with width, while the neural network function (and its loss) is a very "microscopic" or "fine" detail that converges much more slowly with width. However, theoretically, it is unclear why this should happen, and where else we should expect such useful HP transfer. We leave an explanation to future work.

F Detailed Discussions on Related Works

F.1 Hyperparameter Tuning

Many have sought to speedup HP tuning beyond the simple grid or random search. Snoek et al. [34] treated HP tuning as an optimization process and used Bayesian optimization by treating the performance of each HP combination as a sample from a Gaussian process (GP). Snoek et al. [35] further improved the runtime by swapping the GP with a neural network. Another thread of work investigated how massively parallel infrasture can be used for efficient tuning under the multi-arm bandit problem [15, 18]. There are also dedicated tools such as Optuna [4] and Talos [3] which integrate with existing deep learning frameworks and provide an easy way to apply more advanced tuning techniques.

Our approach is distinct from all of the above in that it does not work on the HP optimization process itself. Instead, it decouples the size of the target model from the tuning cost, which was not feasible prior to this work. This means that **no matter how large the target model is, we can always use a fixed-sized proxy model to probe its HP landscape** Nevertheless, our method is complementary, as the above approaches can naturally be applied to the tuning of the proxy model; it is only for scientific reasons that we use either grid search or random search throughout this work.

F.2 Previously Proposed Scaling Rules of Hyperparameters

(Learning Rate, Batch Size) Scaling [33] proposed to scale learning rate with batch size while fixing the total epochs of training; [11] proposed to scale learning rate as $\sqrt{batchsize}$ while fixing the total number of steps of training. However, [31] showed that there's no consistent (learning rate, batch size) scaling law across a range of dataset and models. Later, [23] studied the trade-off of training steps vs computation as a result of changing batch size. They proposed an equation of a/(1+b/batchsize), where a and b are task- and model-specific constants, for the optimal learning rate (see their fig 3 and fig 5). This law suggests that for sufficiently large batch size, the optimal learning rate is roughly constant. This supports our results here as well as the empirical results in [31, fig 8].

Learning Rate Scaling with Width Assuming that the optimal learning rate should scale with batch size following [33], [26] empirically investigated how the "noise ratio" LR/batchsize scales with width for MLP and CNNs in NTK parametrization (NTP) or standard parametrization (NTP) trained with SGD. They claimed that, in networks without batch normalization, the optimal noise ratio is constant in SP but scales like 1/width for NTP. However, they found this law breaks down for networks with normalization.

Here in our work, Fig. 3 contradicts their results on SP MLP by showing the optimal learning rate (fixing batch size) shifts with width. We believe this difference is 1) due to their erroneous assumption that optimal learning rate scales with batch size (as debunked by [23, 31]) and 2) because their SP experiments were done by fixing the learning rate and only sweeping batch size.

Furthermore, Fig. 1 clearly shows the optimal learning rate is *not* constant in SP for Transformers (trained with Adam). Other differences in our works include our applicability to 1) networks with normalization, 2) Adam and other adaptive optimizers, 3) our empirical validation of transfer across depth and sequence length, and 4) explicit validation of tuning via μ Transfer on large models like BERT-large.

Finally, as argued in [45] and Appendix L.3, SP and NTP lead to bad infinite-width limits in contrast to μ P and hence are suboptimal for wide neural networks. For example, sufficiently wide neural networks in SP and NTP would lose the ability to learn features, as concretely demonstrated on word2vec in [45].

Input Layer Parametrization While typically, the input layer is initialized with fanin initialization, in language models where the input and output layers are shared (corresponding to word embeddings), it can actually be more natural to use a fanout initialization (corresponding to fanin initialization of

²⁰while the optimal learning is roughly linear in batch size when the latter is small

the output layer). In fact, we found that fairseq [25] by default actually implements our proposed input layer parametrization (both the fanout initialization and the $\sqrt{\text{fan out}}$ multiplier).²¹

From the Theory of Infinite-Width to the Practice of Finite-Width Neural Networks and Back [45] introduced μ P as the unique parametrization that enables all layers of a neural network to learn features in the infinite-width limit, especially in contrast to the NTK parametrization [14] (which gives rise to the NTK limit) that does not learn features in the limit. Based on this theoretical insight, in Appendix L.3, we argue that μ P should also be the *unique* parametrization that allows HP transfer across width; in short this is because it both 1) preserves feature learning, so that performance on feature learning tasks (such as language model pretraining) does not become trivial in the limit, and 2) ensures each parameter tensor is not stuck at initialization in the large width limit, so that its learning rate does not become meaningless. At the same time, our results here suggest that μ P is indeed the *correct* parametrization for large neural networks and thus provide empirical motivation for the theoretical study of the infinite-width μ P limit.

G Which Hyperparameters Can Be Transferred? (Continued)

G.1 Further Discussions on Hyperparameter Categories

Below, we discuss the reasoning behind each kind, which are supported by our empirical evidence collected in Fig. 4 on Transformers as well as those in Appendix I.1 on ResNet.

Transferable Hyperparameters In Table 2, we summarize which HPs can be transferred across training scale. The transfer across *width*, as explained in Section 2, is theoretically justified, while we present the transfer across the other dimensions as empirical results.

These cover most of the well-known and important HPs when the need for regularization is not paramount, e.g., during large scale language model pretraining. Parameter Multipliers are not well-known HPs, yet we include them here as they serve a bridge between SP and μ P and can impact model performance in practice. Concretely, any SP and μ P neural networks of the same width can have their Parameter Multipliers tuned so that their training dynamics become identical.

Hyperparameters That Don't Transfer Well Not all HPs transfer well even if we use μ P. In particular, those whose primary function is to regularize training to mitigate "overfitting" tend not to transfer well. Indeed, intuitively, regularization needs to be applied more heavily in larger models, so naturally we do not expect the same regularization HPs to stay constant across model sizes.

To the best of our knowledge, there is no strict separation between HPs that regularize and those that don't. However, conventional wisdom tells us that there exists a spectrum of how much regularizing effect a HP has. For example, dropout probability and weight decay are among those whose primary function is to regularize, whereas batch size and learning rate might regularize training in some cases but affect the dynamics more so in other ways. Our empirical exploration tells us that the former do not transfer well, while the latter do. Our subsequent discussion will focus on the latter; we leave to future works the expansion to the former.

Hyperparameters Transfered *Across* We have left out a category of HPs that defines the training *scale*, or in practical terms, training cost. This includes 1) those that define how many operations a model's forward/backward pass takes, such as the model's width, depth, and in the case of language modeling, sequence length; and 2) those that define how many such passes are performed, such as batch size and number of training steps.

As recent works have shown [6, 16], improvements along any of these *scale* dimensions lead to apparently sustainable gain in performance; as a result, we are primarily interested in transferring other HPs *across* these dimensions that define scale, rather than finding the optimal scale.²² This category of HPs is particularly crucial as one can speedup training by downsizing in one or multiple

²¹But it certainly does not implement other parts of our parametrization, like Adam learning rate scaling or the output multiplier.

²²In particular, we are not fixing the total training FLOPs when we scale, which requires understanding the tradeoff of different scale HPs. For example, when we transfer across batch size, we *fix* the number of steps of training (*not* the number of epochs), so that the total FLOPs scales linearly.

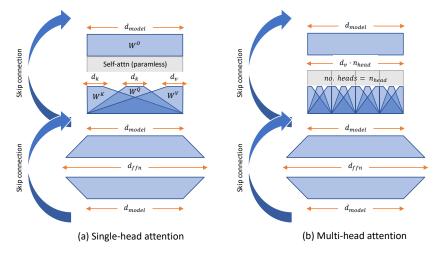


Figure 11: Schematics of each Transformer layer. Commonly, the key and value dimensions d_k and d_v are both set to d_{model}/n_{head} , and this is referred to as d_{head} .

such dimensions. Indeed, it's very common for practitioners to implicitly transfer HPs across the number of training samples by tuning on only a subset of the full training data.

Our insights from the infinite-width limit inspired us to explore HP transfer across *width*, which does not work under SP as we have shown earlier. Building upon our success with width, which is well explained theoretically, we hope to push the limit of compute-saving by investigating the other dimensions empirically. To the best of our knowledge, the transferability of optimal HPs across depth, batch size, sequence length, and training time has not been rigorously investigated previously, with the main exception of the literature on (learning rate, batch size) scaling [31, 33] where our transferability result of learning rate across batch size recapitulates [23].²³ See Appendix F.2 on how our results relate to prior works. We will primarily focus on the Transformer architecture in the main text with evidence for ResNet in Appendix I.1.

G.2 On the Definitions of Width

Our theory allows more general notions of width. This is especially relevant in Transformers, where $d_{model}, d_{head} = d_k, d_v, n_{head}, d_{ffn}$ (see Fig. 11) can all be construed as measures of width. We briefly discuss these here, with more theoretical justification in Appendix L.2.1 and empirical validation below.

Varying Width Ratio So far we have assumed that every hidden layer is widened by the same factor. But in fact we can widen different hidden layers differently. This is useful, for example, in a Transformer where we may want to use a smaller d_{ffn} during tuning. If we are using Adam, as long as the width of every layer still tends to infinity, we still obtain approximately the same limit²⁴, so the μ Transfer remains theoretically justified.

See Fig. 12 for an empirical validation on IWSLT-14 using a Transformer.

Number of Attention Heads In attention-based models, one typically splits hidden size into multiple attention heads following $d_{model} = d_{head} \times n_{head}$. So far we have assumed d_{head} and d_{model} to be width, but it's possible and potentially advantageous to fix d_{head} and treat n_{head} as the width, or increasing both simultaneously. This allows our technique to handle many popular models, including GPT-3 [6], which scale up by fixing d_{head} and increasing n_{head} . See Fig. 13 for an empirical validation on Wikitext-2.

²³There's also a literature on the proper initialization for training deep networks effectively (e.g. [5, 13, 21, 30, 47, 48, 51]), but they do not study the *transferability* per se. See Appendix F.2

²⁴This also applies for SGD, but we need more involved scaling to keep the limit approximately the same.

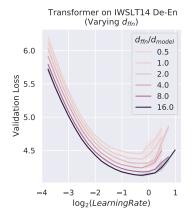


Figure 12: Learning rate landscape in μP is stable even if we vary d_{ffn} by a factor of 32, fixing d_{model} .

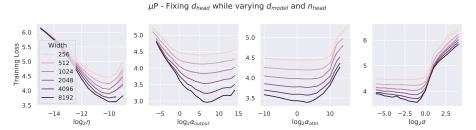


Figure 13: μ Transfer across width when we fix d_{head} and vary d_{model} and n_{head} . α_{output} , α_{attn} are multipliers for output and key weights, and σ is initialization standard deviation.

Varying Just the Width of Attention Heads A specific useful instance of varying width ratio is decoupling the key and value dimensions d_k and d_v and scaling d_k differently from (typically larger than) d_{model}/n_{head} . This works as long as we use 1/d scaled-attention as in Definition 4.1 (instead of $1/\sqrt{d}$ as is done commonly). When tuning on the small proxy model, if d_k is too small, the HP landscape can be quite noisy. Keeping d_k relatively large while shrinking all other dimensions solves this problem, while still obtaining significant speedup.

H Experimental Details

H.1 IWSLT

IWSLT14 De-En is a well-known machine translation benchmark. We use a Transformer implemented in fairseq [25] with a default $d_{model} = ^1/4d_{ffn} = 512$ and $d_k = d_q = d_v = ^{d_{model}}/n_{head} = 128$ (amounting to 40M parameters), which we denote as the lx model. For transfer, we tune on a proxy model with the same n_{head} but with d_{model} and other dimensions 4 times smaller; we will call this the 0.25x model (but it has 4M parameters). All models are trained with Adam for 100 epochs and validated at the end of every epoch. We tune via random search the learning rate η , the output layer parameter multiplier α_{output} , and the attention key-projection weight multiplier α_{attn} following the grid

- η : $5 \times 10^{-4} \times 2^z$, where $z \in \{-1.5, -1.25, -1, ..., 1.25\}$
- α_{output} : 2^z , where $z \in \{-8, -7, -6, ..., 7\}$
- α_{attn} : 2^z , where $z \in \{-3, -2, -1, ..., 8\}$

H.2 WMT

We scale up to WMT14 En-De using the large Transformer from [37], with a $d_{model}=1/4d_{ffn}=1024$ and $d_q=d_k=d_v=\frac{d_{model}}{n_{head}}=64$. We use the exact same setup and reproduce their result as our baseline. Then, we build the proxy model by shrinking the target model's d_{model} from

the original 1024 to 256, d_{ffn} from 4096 to 256 and n_{head} from 16 to 4. This reduces the total parameter count from 211M to 15M. We then perform the HP search on the proxy model and take the best according to validation loss, before testing on the target model. We tune via random search the learning rate η , the output layer parameter multiplier α_{output} , and the attention key-projection weight multiplier α_{attn} following the grid

```
• \eta: 6 \times 10^{-4} \times 2^z, where z \in \{-1.5, -1.25, -1, ..., 1.25\}
```

- α_{output} : 2^z , where $z \in \{-8, -7, -6, ..., 7\}$
- α_{attn} : 2^z , where $z \in \{-3, -2, -1, ..., 8\}$

H.3 BERT

Details of BERT Prototype Our proxy model has 10 Transformer layers with $d_{model} = d_{ffn} = 256$. We also reduce the number of attention heads to 8 with a d_{head} of 32. We call it BERT Prototype since we can increase its width and depth according to our definitions to recover both BERT Base and BERT Large, which enables us to sweep HPs once and use for both models. Overall, BERT Prototype has 13M trainable parameters, a fraction of the 110M in BERT Base and the 350M in BERT Large.

Hyperparameters Tuned for Pretraining We tune the following HPs for pretraining: Adam learning rate η , embedding learning rate η_{emb} , output weight multiplier α_{output} , attention logits multiplier α_{attn} , layernorm gain multiplier $\alpha_{LN_{gain}}$, and bias multiplier α_{bias} .

We sample 256 combinations from the follow grid:

```
• \eta: 1 \times 10^{-4} \times 2^z, where z \in \{1.5, 2, 2.5, 3, 3.5\}
```

- η_{emb} : $1 \times 10^{-4} \times 2^z$, where $z \in \{-1, -0.5, 0, 0.5, 1\}$
- α_{output} : 2^z , where $z \in \{2, 4, 6\}$
- α_{attn} : 2^z , where $z \in \{3, 3.5, 4, ..., 7\}$
- $\alpha_{LN_{qain}}$: 2^z , where $z \in \{8.5, 9, 9.5, 10, 10.5\}$
- α_{bias} : 2^z , where $z \in \{8.5, 9, 9.5, 10, 10.5\}$

The ranges are chosen to include the implicit choices of these HPs in SP BERT Large.

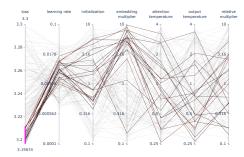
Finetuning Procedure and Hyperparameters We hand-pick the finetuning HPs after training the full-sized model. As regularization is an essential ingredient in successful finetuning, we do not transfer such HPs (at least via the suite of techniques presented in this work) (see Table 1). We focus on MNLI [40] and QQP, which are two representative tasks from GLUE [38]. Following [22], we used Adam [17] with a learning rate of 5×10^{-5} and a batch size of 64. The maximum number of epochs was set to 5. A linear learning rate decay schedule with warm-up of 0.1 was used. All the texts were tokenized using wordpieces and were chopped to spans no longer than 128 tokens.

H.4 GPT-3

Baseline 6.7B GPT-3 Transformer As the GPT-3 codebase has evolved since the publication of [6], we re-trained the 6.7B model from scratch to remove changes in our codebase as a possible confounder. The main differences to [6] are the use of relative positional encoding [8] instead of absolute position embeddings, and a modified learning rate decay schedule, where the learning rate is decayed to zero at the end of training rather than being decayed to 0.1 of the initial value. Ultimately, as shown in Table 8, the difference between our rerun and the published results of [6] is negligible compared to the μ P model.

Random Search using reduced width model In order to find a good set of hyperparameters for the μ Transfer version of the 6.7B model, we performed a hyperparameter search over a reduced version of the model, where the width is set to 256 hidden units. The search space consists of the following hyperparameters:

- learning rate: Sampled from $10^{\text{Uniform}(-4,-1)}$
- ullet initialization scale: All the parameters are multiplied sampled from $10^{\mathrm{Uniform}(-1,1)}$



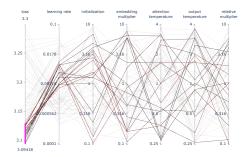


Figure 14: Results of the random search over reduced width models trained on 4 (left) and 16 (right) billion tokens. Only the best performing runs are highlighted.

- attention temperature: Reciprocal of the multiplier applied to the input to attention softmax. Sampled from 4^{Uniform(-1,1)}.
- output temperature: Reciprocal of the multiplier applied to the input to softmax that produces the distribution over output tokens. Sampled from $4^{\text{Uniform}(-1,1)}$.
- embedding multiplier: Scalar by which we multiply the output of the embedding layer. Sampled from $10^{\text{Uniform}(-1,1)}$.
- relative position embedding multiplier: Scalar by which we multiply vectors representing relative position. Sampled from $10^{\text{Uniform}(-1,1)}$.

In order to make the search more efficient we reduced the total number of training tokens. We hypothesized that tuning hyperparameters on a reduced total number of tokens does not significantly affect optimal hyperparameters. To verify, we trained two different horizons and compared the results. While the target model was to be trained on 300 billion tokens, we tuned the proxy model on only subsets consisting of 4 billion and 16 billion tokens. This impacts both the total training time and and the length of the linear learning rate decay schedule. Other than hyperparameters explicitly listed above and the training horizon, the rest was the same as what we intended to use for the full width 6.7B training run.

Analyzing the results of the random search We performed 467 reduced-size training runs, out of which 350 were for 4 billion tokens (286 completed without diverging) and 117 for 16b tokens (80 completed without diverging). See Fig. 14 for summary of the results.

As suspected, we observed that the results are well-aligned for both 4 and 16 billion tokens versions. We observe learning rate and initialization scale impact the results the most. Based on the results we chose 0.006 for the former and 2.5 for the latter. Since most other hyperparameters appear to have negligible effect on performance, they were kept at their default values of 1, the only exception being the embedding scale, where higher values seem to perform better and it was therefore set to 10.

Training the μ Transfer model We encountered frequent divergences in our initial attempt to train the μ Transfer model. We traced the issue back to underflow of FP16 tensors in the backwards pass and therefore switched to training the model in FP32. This allowed us to finish the training run without divergences. We hypothesize that the divergence issue is related to μ Transfer picking more aggressive hyperparameters, for example a higher learning rate on linear weight tensors compared to the original model. In order to exclude code differences as a possible confounder, we re-trained GPT-3 6.7B from scratch using the original hyperparameters. The only difference compared to the version published in [6] is that the learning rate was decayed fully, whereas the learning rate of the model from [6] was only decayed to 10% of its starting value. The retrained model performs slightly worse than the original published in [6]. We suspect that this is because it made less progress during the last phase of training where the learning rate is close to zero. The training curves of the μ Transfer model and the re-run of the original 6.7B can be seen in Fig. 15. Detailed evaluation results can be found in Table 8 and Table 9.

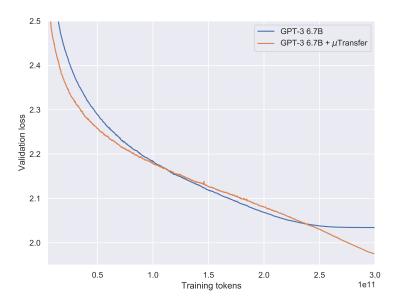


Figure 15: The training curves of the GPT-3 6.7B model with μ Transfer (orange) and a re-run with the original settings from [6] (blue). The μ Transfer model was trained using FP32 activations and weights after initially encountering stability issues with the hyperparameters computed using μ P, while the re-run used the original FP16 training. The μ Transfer model seems to underperform in the middle of training, but achieves a much better final validation loss once the learning rate is fully decayed. The μ Transfer model uses a linear learning rate decay schedule while the original model uses a cosine schedule.

Ratio of tuning cost to pretraining cost in FLOPs can be approximated as

$$\frac{s(t_1N_1 + t_2N_2)}{ST} \approx 0.07$$

where

- s=40 Million is number of parameters of the proxy model
- S=6.7 Billion is number of parameters of the target model
- $t_1=4$ Billion is the number of training tokens for the short horizon HP search, and $N_1=350$ is the corresponding number of random HP search trials.
- $t_2 = 16$ Billion is the number of training tokens for the longer horizon HP search, and $N_1 = 117$ is the corresponding number of random HP search trials.
- T = 300 Billion is the number of training tokens for the 6.7B target model.

Here we are using the fact that the training FLOPs of a Transformer per token is roughly proportional to its number of parameters.

I Additional Experiments

I.1 Experiments on ResNets

I.1.1 ResNet on CIFAR-10

Setup For this case we use Davidnet [2], a ResNet variant that trains quickly on CIFAR-10, so as to efficiently investigate its HP landscape. We train with SGD on CIFAR-10 for 10 epochs; all results are averaged over 15 random seeds. We use a width multiplier to identify models of different width, and a multiplier of 1 corresponds to the original model in [2]. We look at validation accuracy here as the model barely overfits, and our observations will hold for the training accuracy as well. We first

Table 8: **Full evaluation results of our GPT-3 6.7B models**: The new model tuned with μ Transfer (marked μ P), the original model from [6], and a re-training of this model from scratch with the original hyperparameter settings (marked re-run). The sampling-based evaluations shown here are a subset of the ones from [6]. Since the sampling-based evaluations are subject to high variance, Wikitext 103 and the LM1B benchmark have been added to help distinguish the relative performance of the μ P and non- μ P model. Note that Wikitext-103 [24] and the LM1B [7] benchmarks overlap with the training dataset. Accuracies and F1 scores have been multiplied by 100. The perplexities reported in this table are based on a custom BPE encoding and are not comparable to other results in the literature. The number k of examples in the context for each task is identical to [6].

Note: Zero-shot, One-Shot and Few-Shot refer to the number of additional query and answer pairs passed in the context when performing the sampling-based evaluations, not the "shots" involved in hyperparameter transfer.

			2	Zero-sho	ot	(One-sho	t		Few-sh	ot
Task	Split	Metric	μ P	[6]	re-run	μ P	[6]	re-run	μ P	[6]	re-run
Validation dataset PTB Wikitext 103 LM1B	valid test test test	ce ppl ppl ppl	1.98 11.4 8.56 20.5		2.03 13.0 9.13 21.7						
HellaSwag LAMBADA StoryCloze NaturalQS TriviaQA	dev test test test dev	acc acc acc acc	72.0 73.5 79.4 5.73 33.0	67.4 70.3 77.7 5.79 38.7	66.7 70.8 77.3 7.76 39.0	71.1 69.9 80.6 9.17 40.9	66.5 65.4 78.7 9.78 44.4	65.9 64.8 78.3 10.2 42.1	72.4 74.7 84.2 15.8 54.0	67.3 79.1 81.2 17.0 51.6	66.4 77.1 81.1 16.0 49.8
WebQS Winograd Winogrande PIQA	test test dev dev	acc acc acc acc	8.27 85.3 66.8 79.1	7.73 85.7 64.5 78.0	10.3 86.8 62.5 78.0	13.3 84.6 67.6 77.3	15.1 84.6 65.8 76.3	15.4 84.2 64.5 76.9	23.7 86.4 71.0 79.2	27.7 85.4 67.4 77.8	27.5 83.9 67.2 77.7
ARC (Challenge) ARC (Easy) OpenBookQA Quac	test test test dev	acc acc acc f1	42.1 64.3 54.4 22.8	41.4 60.2 50.4 36.1	42.5 61.9 52.6 37.1	44.0 65.3 56.4 29.2	41.5 62.6 53.0 39.0	42.4 63.4 52.8 38.9	43.8 67.3 58.4 44.0	43.7 65.8 55.2 39.9	42.7 65.3 54.4 39.8
RACE-h RACE-m SQuADv2 CoQA	test test dev dev	acc acc f1 f1	45.0 58.4 42.0 53.8	44.1 54.4 52.7 72.8	43.2 54.0 51.1 72.8	44.9 57.9 48.2 61.3	44.3 54.7 57.1 75.1	42.9 53.8 55.4 73.7	45.2 58.6 68.9 81.3	44.7 55.4 62.1 77.3	43.4 55.4 58.4 75.3
DROP BoolQ CB Copa	dev dev dev dev	f1 acc acc acc	17.1 69.4 21.4 82.0	17.0 65.4 28.6 80.0	17.4 60.9 37.5 77.0	23.3 74.1 60.7 81.0	27.3 68.7 33.9 82.0	25.7 65.0 32.1 81.0	33.9 73.9 62.5 88.0	29.7 70.0 60.7 83.0	28.7 69.7 66.1 82.0
RTE WiC ANLI R1 ANLI R2 ANLI R3	dev dev test test test	acc acc acc acc	55.2 0. 33.7 33.8 32.7	55.2 0. 32.3 33.5 34.8	46.2 0. 33.4 33.0 33.4	61.0 50.0 32.4 34.8 34.8	54.9 50.3 31.6 33.9 33.1	58.8 50.3 31.7 33.7 33.3	52.7 50.5 30.9 35.0 36.9	49.5 53.1 33.1 33.3 33.9	59.9 51.3 30.7 32.2 32.3

Table 9: Evaluation results comparing the GPT-3 6.7B model trained with μ Transfer against the twice as large GPT-3 13B model from [6]. The two models have similar performance on most of the evaluation tasks.

			Zero-shot		One-shot		Few-shot	
Task	Split	Metric	$6.7B+\mu P$	13B[6]	$6.7B+\mu P$	13B[6]	$6.7B+\mu P$	13B[6]
HellaSwag	dev	acc	72.0	70.9	71.1	70.0	72.4	71.3
LAMBADA	test	acc	73.5	72.5	69.9	69.0	74.7	81.3
StoryCloze	test	acc	79.4	79.5	80.6	79.7	84.2	83.0
NaturalQS	test	acc	5.73	7.84	9.17	13.7	15.8	21.0
TriviaQA	dev	acc	33.0	41.8	40.9	51.3	54.0	57.5
WebQS	test	acc	8.27	8.22	13.3	19.0	23.7	33.5
Winograd	test	acc	85.3	87.9	84.6	86.1	86.4	82.4
Winogrande	dev	acc	66.8	67.9	67.6	66.9	71.0	70.0
PIQA	dev	acc	79.1	78.5	77.3	77.8	79.2	79.9
ARC (Challenge)	test	acc	42.1	43.7	44.0	43.1	43.8	44.8
ARC (Easy)	test	acc	64.3	63.8	65.3	66.8	67.3	69.1
OpenBookQA	test	acc	54.4	55.6	56.4	55.8	58.4	60.8
Quac	dev	f1	22.8	38.4	29.2	40.6	44.0	40.9
RACE-h	test	acc	45.0	44.6	44.9	44.6	45.2	45.1
RACE-m	test	acc	58.4	56.7	57.9	56.9	58.6	58.1
SQuADv2	dev	f1	42.0	56.3	48.2	61.8	68.9	67.7
CoQA	dev	f1	53.8	76.3	61.3	77.9	81.3	79.9
DROP	dev	f1	17.1	24.0	23.3	29.2	33.9	32.3
BoolQ	dev	acc	69.4	66.2	74.1	69.0	73.9	70.2
CB	dev	acc	21.4	19.6	60.7	55.4	62.5	66.1
Copa	dev	acc	82.0	84.0	81.0	86.0	88.0	86.0
RTE	dev	acc	55.2	62.8	61.0	56.3	52.7	60.6
WiC	dev	acc	0.	0.	50.0	50.0	50.5	51.1
ANLI R1	test	acc	33.7	33.2	32.4	32.7	30.9	33.3
ANLI R2	test	acc	33.8	33.5	34.8	33.9	35.0	32.6
ANLI R3	test	acc	32.7	34.4	34.8	32.5	36.9	34.5

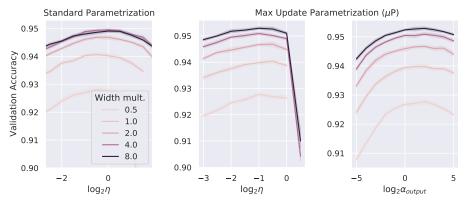


Figure 16: ResNet on CIFAR-10 for different widths (compared to a base network). On the **left**, the widest network SP underperforms; on the **right**, the μ P network has a more consistent HP landscape and performs better. Both networks are tuned at the smallest width for the HP (η or α_{output}) not in the x-axis.

conduct a learning rate sweep for models of different widths using SP; the result is shown in Fig. 16, on the left.

Hyperparameter Stability Note that the best model with a width multiplier of 8 under-performs that with a multiplier of 4. We run the same sweep with μ P, along with a sweep of the output multiplier (α_{output}); the result is shown in Fig. 16, on the right. We notice that wider models always perform better under μ P and that the optimal learning rate η and α_{output} are stable across width.

Hyperparameter Transfer Next, we perform a grid search for learning rate (η) and α_{output} on the 0.5x model for both SP and μ P.²⁵ Then, we take the best combination and test on the 8x model, simulating how a practitioner might use μ Transfer. The result is shown in Table 10, where μ P outperforms SP by $0.43\% \pm .001\%$.

Table 10: CIFAR10: Transferring the best learning rate (η) and α_{output} from widening factor 0.5 to 8; μ P significantly outperforms SP given the same search grid. The best HPs are different as the models are parametrized to be identical at 1x width.²⁵

Transfer Setup	Best η	Best α_{output}	Valid. Acc. (0.5x)	Valid. Acc. (8x)
SP	0.707	4	92.82%	94.86%
$\mu\mathrm{P}$	0.5	4	92.78%	95.29%

I.1.2 Wide ResNet on ImageNet

Setup For this case we use Wide-Resnet, or WRN [50], a ResNet variant with more channels per layer, to further showcase μ Transfer across width, i.e., number of channels. We train with SGD on ImageNet for 50 epochs following standard data augmentation procedures. We use a width multiplier to identify models of different width, and a multiplier of 1 corresponds to the original WRN-50-2-bottleneck in [50].

Hyperparameter Transfer We start with a proxy model with a width multiplier of 0.125 and tune several HPs using the following grid:

- η : $1 \times 2.048 \times 2^z$, where $z \in \{-5, -4, -3, ..., 4\}$
- α_{output} : 10×2^z , where $z \in \{-5, -4, -3, ..., 4\}$
- weight decay co-efficient γ : $3.05 \times 10^{-5} \times 2^{z}$, where $z \in \{-2, -1.5, -1, ..., 1.5\}$
- SGD momentum $\beta \colon 0.875 \times 2^z, \text{where } z \in \{-2, -1.5, -1, ..., 1.5\}$

The grid is centered around the default HPs used by [1] for ResNet-50; while not expected to be competitive for WRN, they represent a reasonable starting point for our experiment.

We randomly sample 64 HP combinations from the grid and train for 50 epochs, before selecting the one with the highest top-1 validation accuracy. Then, we scale up the model following both μP and SP and run with the same HPs we just selected. The result is shown in Table 11, where μP outperforms SP by 0.41% in terms of top-1 validation accuracy.

Table 11: Imagenet: Transferring the best learning rate (η) , α_{output} , γ , and β from widening factor 0.125 to 1; μ P significantly outperforms SP given the same search grid.

Transfer Setup	Best η	Best α_{output}	Best γ	Best β	Valid. Acc. (0.125x)	Valid. Acc. (1x)
SP	32.768	.625	.000015	.4375	58.12%	76.75%
μP	32.768	.625	.000015	.4375	58.12%	77.16%

I.2 Experiments on Transformers

I.2.1 Verifying Transfer across Batch Size, Sequence Length, and Training Time on Wikitext-2

See Fig. 19.

I.3 Post-Layernorm Transformers

Fig. 17 shows the transferability of learning rate, α_{output} , initialization standard deviation, and Adam β_2 across width, batch size, sequence length, and training steps for post-layernorm Transformers. However, in general, we find transfer across depth to be fragile.

²⁵Here we tune the 0.5x model instead of the 1x model to simulate the situation that one does "exploratory work" on the 1x model but, when scaling up, would like to tune faster by using a smaller proxy model.

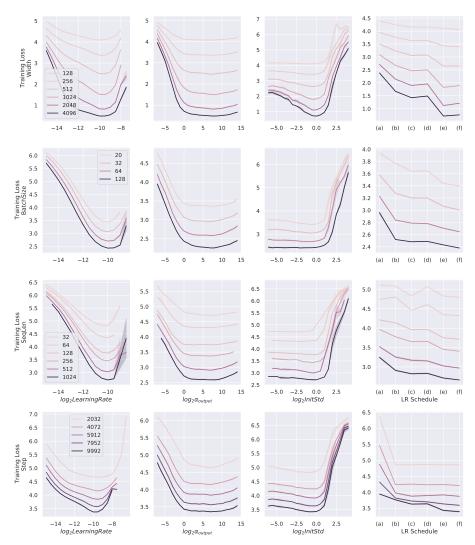


Figure 17: Empirical validation of μ Transfer for Post-LN Transformers. Same setting as Fig. 4.

I.3.1 Hyperparameter Instability of SP Transformers

Fig. 18 and Fig. 20 show the HP instability inherent in SP Transformers.

J Implementing μ Transfer in a Jiffy

As we have shown, one can enable μ Transfer by just reparametrizing the desired model in Maximal Update Parametrization (μ P). While conceptually simple, switching from Standard Parametrization (SP) to μ P can be error-prone, as popular deep learning frameworks are built around SP. We strive to build a tool that fulfills two goals:

- 1. Minimize code changes when switching to μP ;
- 2. Keep model behavior invariant, under this switch, at a given base model shape.

By *model shape*, we mean the collection of dimensions of all parameters of the model. The latter goal, which we call *parametrization backward compatibility*, ensures that any code base works exactly as before at the base model shape, similar to Eq. (4), e.g. the loss at any time step remains exactly the same before and after the switch to μ P. Of course, when widths start to differ from the base model shape, the model behavior necessarily changes so that HPs can be transferred.

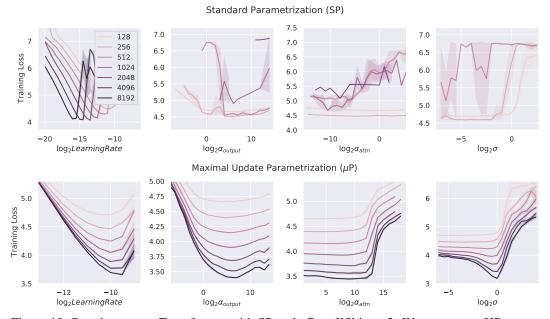


Figure 18: Post-layernorm Transformer with SP and μ P on Wikitext-2. We sweep one HP across width (d_{model}) at a time while keeping the rest fixed; we also scale d_{head} linearly with d_{model} and fixing n_{head} . α_{output} , α_{attn} are multipliers for output and key weights, and σ is initialization standard deviation. This yields unstable result for SP, as expected, where missing points/curves represent divergence; in μ P, the optimal HP choices stabilize as width increases.

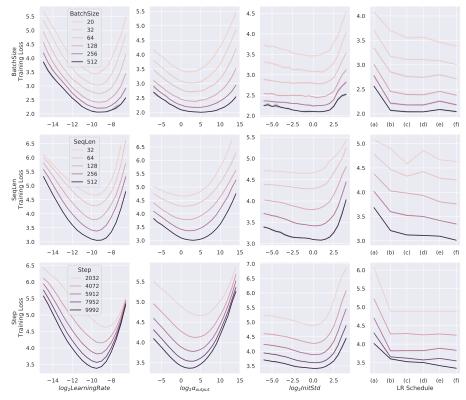


Figure 19: Empirical validation of Hyperparameter Transfer across Batch Size, Sequence Length, and Training Time on pre-LN Transformers. Same setting as Fig. 4. Despite some shift, the optimal HPs are roughly stable when transferring from batch size 32, sequence length 128, and 5000 training steps.

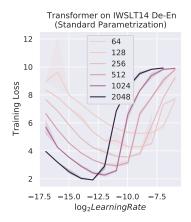


Figure 20: Learning rate landscape is highly unstable under standard parametrization in IWSLT.

Table 12: Alternative (Equivalent) μ P Formulation for Easier Implementation. Same format as in Table 3. In contrast to the formulation in Table 3, here all "vector-like" parameters (i.e. those that have only one dimension tending to infinity), including input and output weights and biases, have the same width scaling for initialization variance and SGD/Adam LR (note the $1/\text{fan_in}$ for input weight/bias init. var. is $\Theta(1)$ in width). This has two benefits in practice: 1) implementation is unified and simplified for all "vector-like" parameters; 2) input and output weights can now be tied, in contrast to Table 3, which is a common design feature of Transformer models. Note that in this table, for biases, the fan_in is 1 (compare to PyTorch nn.Linear default initialization of biases, where fan_in refers to fan_in of the layer.)

	Input weights & all biases	Output weights	Hidden weights
Init. Var.	$1/\mathrm{fan}_{\mathrm{in}}$	$1 \qquad \qquad (1/_{\mathrm{fan_in}})$	$1/fan_in$
Multiplier	1	$\frac{1}{\text{fan}_{\text{in}}}$ (1)	1
SGD LR	$\eta \cdot \text{fan_out} (\eta)$	$\eta \cdot \text{fan_in} (\eta)$	η
Adam LR	η	η	$\eta/_{\text{fan_in}}$ (η)

There are two common approaches to setting the base model shape: 1) If one intends to tune a large target model, then the user can set the base model shape to be the shape of the target model (e.g. BERT-large or T5-large), so that the target model itself is in standard parametrization. Then one can tune a proxy model with e.g. width = 124 to obtain the optimal HPs for the target model. In addition, if one wishes to scale up further e.g. width = 1024, then these HPs remain optimal. 2) If one has done exploration on a new idea with a small model and now wishes to scale up, reusing the HP found during this exploration, then one can set the base model shape to be the shape of the exploratory small model. Of course, in both scenarios, depth, batch size, and sequence lengths can be scaled up and down as well according to Fig. 19 (though note that currently we require users to recreate the base model shape at new depths, since the number of parameters now change with depth).

The mup **Package** We provide our tool as a Python package called mup designed to work with PyTorch. The following example illustrates the usage of our package.

Table 13: μ **P Formulation in the Style of [45].**

	,		
	Input weights & all biases	Output weights	Hidden weights
Init. Var.	$\frac{1}{\text{fan_out}}$ $\left(\frac{1}{\text{fan_in}}\right)$	$1/\mathrm{fan}_\mathrm{in}$	$1/_{\rm fan_in}$
Multiplier	$\sqrt{\text{fan_out}}$ (1)	$1/\sqrt{\text{fan}_{in}}$ (1)	1
SGD LR	η	η	η
Adam LR	$\eta/\sqrt{\text{fan_out}}$ (η)	$\eta/\sqrt{\text{fan}_{in}}$ (η)	$\eta/_{\text{fan_in}}$ (η)

What Happens in the mup Package Under the hood, mup implements the μP formulation in Table 12. By invoking set_base_shape(model, base_model), each parameter tensor p of model gets a p.infshape attribute that stores, for each of its dimensions, the corresponding base dimension and whether that dimension should be considered "infinite" (i.e. will be scaled up/down, e.g., d_{model} of a Transformer) or "finite" (i.e. will be fixed, e.g., vocabulary size). This information is used in the initializers and optimizers to automatically scale the parameters or learning rates to be compliant with μP . For example, by Table 12, the Adam learning rate of hidden weights p is calculated as η/p . infshape.width_mult(), where p.infshape.width_mult() essentially calculates $\frac{fan_i in}{base_f fan_i in}$.

K Width-Related Training Issues are Hyperparameter Issues

Large Transformers are famously fickle to train [20, 29]. This is especially true in low-precision floating point formats such as float16 that is required to train enormous models today. Throughout our investigations, we find that, with the HPs transferred from the proxy model (which should be close to optimal), we do not observe such instability. This suggests that the training instability problems

could in fact be HP problems, not necessarily structural issues associated with the architecture or optimizer (which work just fine when tuned properly).²⁶ We hypothesize that

The common manifestations of training instability are caused by practitioners naively transferring learning rate and other HPs tuned on a small Transformer.

This is certainly consistent with Fig. 1, which shows that the optimal learning rate for small Transformers can lead to trivial performance in large Transformers. We support this hypothesis further by reverse-transferring the instability-inducing HPs from a large Transformer to a small one and replicating the training instability. This is shown in Fig. 21.

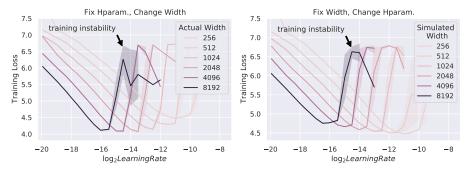


Figure 21: Replicating training instability on a small Transformer by reverse-transferring hyperparameters. These experiments concern 2-layer Transformers in Standard Parametrization (SP) on Wikitext-2, trained with Adam, where width is defined as $d_{model} = d_{ffn}$. (Left) LR-vs-loss for wider and wider Transformers. (Right) Likewise for simulated width: Here each point ($\log_2 \eta, loss$) for simulated width n indicates the loss from training a width-256 μ P Transformer with base width n and LR η (i.e. loosely speaking, it's using LR transferred from η in a width-n SP Transformer). Takeaway: The overall shapes of the curves are identical between the left and right plots²⁷; in particular, a learning rate leads to instability in a wide model iff it does so when transferred back to a narrow model.

L An Intuitive Introduction to the Theory of Maximal Update Parametrization

In what follows, we seek to describe useful intuitions and rule of thumbs that would be helpful to practitioners and empirical researchers alike in figuring out what is the right neural network parametrization. The intuitions we shall describe regarding SGD can be made rigorous as in [44, 45]; those regarding Adam are new, and their formalization will be done in an upcoming paper.

L.1 Behaviors of Gaussian Matrices vs Tensor Product Matrices

Central to the derivation of μP for any architecture are key insights on the behaviors of two kinds of random matrices: 1) iid Gaussian random matrix and 2) tensor product matrix (by which we mean a sum of outer products) and more generally what we call *nonlinear* tensor product matrix (see Eq. (7)). For example, a neural network, randomly initialized in the typical way, will have each weight matrix look like the former. However, every step of training by gradient descent adds a sum of outer products to this initial matrix, so that the *change in weights* constitute a tensor product matrix. For Adam, the change in weights is not a tensor product but a more general *nonlinear tensor product matrix* (see Eq. (7)). In this section, we will particularly focus on the *right scaling* for the entries of such matrices, leading to a discussion of *the right neural network parametrization* in the next section. We concentrate on the key heuristics but eschew burdensome rigor.

²⁶Of course, it is still worthwhile to research layers or architectures that are more insensitive to poor HP choices. But with our results, good HPs are obtained much more easily, so this issue is now much less urgent.

²⁷ Note that the curves on the left are "lower" than curves on the right. This just reflects the increasing capacity of wider models able to fit the training data better, so is orthogonal to our point.

Table 14: Expected entry size of Av for different matrices A and vector v correlated with each other, both having entries of size $\Theta(1)$.

	Standard Gaussian $A \in \mathbb{R}^{n \times n}$	(Nonlinear) Tensor Product $A \in \mathbb{R}^{n \times n}$	
Entry size of Av	$\Theta(\sqrt{n})$	$\Theta(n)$	$\Theta(n)$

Key Insights Consider a random vector $v \in \mathbb{R}^n$ with approximately iid entries and a random matrix A of either size $n \times n$ or $1 \times n$, both having entries of size $\Theta(1)$.²⁸ In the context of deep learning, v for example can be an activation vector in an MLP, a Gaussian A the hidden weights at initialization, a (nonlinear) tensor product A the change in hidden weights due to training, and a vector A the readout layer weights. Then Av corresponds to a part of the next layer preactivation or the network output. To make sure the preactivations and the output don't blow up, we thus need to understand the scale of Av, especially in the general case where A is correlated with v.²⁹ This is summarized in Table 14, with the derivations below. Intuitively, a (nonlinear) tensor product or vector A will interact with a correlated v via Law of Large Numbers, hence the v-scaling, while a Gaussian v-scaling.

In the derivations below, we answer a slightly different but equivalent question of "how to scale A such that Av has entry size $\Theta(1)$?"

L.1.1 Preparation for the Derivations

By the results of [45], each (pre-)activation vector and its gradient vector in a multi-layer perceptron have approximately iid coordinates in the large width limit, 30 and something similar can be said for more advanced networks such as ResNet and Transformers 31 . In particular, to each such vector v, we can associate a random variable Z^v that represents the coordinate distribution of v. If vector u is correlated with v, then Z^u will also be correlated with Z^v , and $\lim_{n\to\infty} v^\top u/n = \mathbb{E} Z^u Z^v$.

L.1.2 Linear Tensor Product Matrix (e.g. SGD Updates)

The case of (linear) tensor product matrix can be reduced to the outer product case by linearity. Given $u, v, x \in \mathbb{R}^n$ having approximately iid coordinates (of size $\Theta(1)$) like so, we can form the outer product

$$A \stackrel{\text{def}}{=} u \otimes v/n = uv^{\top}/n, \tag{6}$$

which is the form of a single (batch size 1) gradient update to a weight matrix. Then, by Law of Large Numbers,

$$Ax = u \frac{v^{\top}x}{n} \approx cu$$
, where $c = \mathbb{E} Z^v Z^x$.

So Ax also has approximately iid coordinates, distributed like $Z^{Ax} \stackrel{\mathrm{def}}{=} Z^u \mathbb{E} Z^v Z^x$. Likewise, if A is a sum of outer products $A = \sum_{i=1}^k u^i \otimes v^i/n$, then

$$Ax = \sum_{i=1}^k u^i \frac{v^{i\top}x}{n}, \quad \text{with coordinates distributed as} \quad Z^{Ax} = \sum_{i=1}^k Z^{u^i} \mathbb{E} \, Z^{v^i} Z^x.$$

Notice that each coordinate of A has size $\Theta(1/n)$. The above reasoning shows that, in order for Ax to have coordinate size $\Theta(1)$ (assuming x does), then $\Theta(1/n)$ is the right coordinate size for A, in

²⁸ in the sense that the the variance of the entries are $\Theta(1)$

²⁹Here "correlated" formally means v depends on W^{\top} in a Tensor Program. This essentially captures all scenarios of "v correlated with W" that occurs in deep learning.

³⁰Our intuition here is derived from the assumption that width is much larger than training time; of course, as illustrated by our myriad experiments, these intuition are very useful even when this is not the case, such as when training to convergence.

³¹E.g. in a convnet, the (pre-)activations are iid across channels, but correlated across pixels

the general case that v^i and x are correlated (as is generically the case during gradient descent, with $A = \Delta W$ for some weights W and x being the previous activations).³²

L.1.3 Nonlinear Tensor Product Matrix (e.g. Adam Updates)

When using Adam or another adaptive optimizer that normalizes the gradient coordinatewise before applying them, we need to modify our argument slightly to obtain the right coordinate size scaling of the matrix. The gradient update A, after such normalization, will take the form of

$$A_{\alpha\beta} = \psi(u_{\alpha}^1, \dots, u_{\alpha}^k, v_{\beta}^1, \dots, v_{\beta}^k), \quad \text{for some } \psi : \mathbb{R}^{2k} \to \mathbb{R} \text{ and vectors } u^i, v^j \in \mathbb{R}^n. \tag{7}$$

We say a matrix of this form is a nonlinear tensor product matrix.

First, note the tensor product matrices (e.g. the form of SGD update) discussed previously (Eq. (6)) already takes this form, with $\psi(u_{\alpha}^1,\ldots,u_{\alpha}^k,v_{\beta}^1,\ldots,v_{\beta}^k)=n^{-1}(u_{\alpha}^1v_{\beta}^1+\cdots+u_{\alpha}^kv_{\beta}^k)$, so Eq. (7) is a strict generalization of linear tensor products. Next, for the example of Adam, each gradient update is μ/σ where μ (resp. σ^2) is the moving average of previous (unnormalized) gradients (resp. the coordinatewise square of the same).³³ If these unnormalized gradients are the outer products $u^1\otimes v^1,\ldots,u^k\otimes v^k$, then the update has coordinates

$$(\mu/\sigma)_{\alpha\beta} = \psi(u_{\alpha}^{1}, \dots, u_{\alpha}^{k}, v_{\beta}^{1}, \dots, v_{\beta}^{k}) \stackrel{\text{def}}{=} \sum_{i} \gamma_{i} u_{\alpha}^{i} v_{\beta}^{i} / \sqrt{\sum_{i} \omega_{i} (u_{\alpha}^{i} v_{\beta}^{i})^{2}}, \tag{8}$$

where γ_i and ω_i are the weights involved in the moving averages.

Now suppose we have some $A \in \mathbb{R}^{n \times n}$ of the form Eq. (7), where $u^i, v^i \in \mathbb{R}^n$ have approximately iid coordinates (of size $\Theta(1)$), and $\psi = n^{-1}\bar{\psi}$ where $\bar{\psi}$ doesn't depend on n (in terms of Adam where $\bar{\psi}$ corresponds to the ψ of Eq. (8), this corresponds to using a learning rate of 1/n). Then for $x \in \mathbb{R}^n$ having approximately iid coordinates of size $\Theta(1)$, by Law of Large Numbers,

$$(Ax)_{\alpha} = \frac{1}{n} \sum_{\beta=1}^{n} \bar{\psi}(u_{\alpha}^{1}, \dots, u_{\alpha}^{k}, v_{\beta}^{1}, \dots, v_{\beta}^{k}) x_{\beta} \approx \mathbb{E} \bar{\psi}(u_{\alpha}^{1}, \dots, u_{\alpha}^{k}, Z^{v^{1}}, \dots, Z^{v^{k}}) Z^{x} \stackrel{\text{def}}{=} \Psi(u_{\alpha}^{1}, \dots, u_{\alpha}^{k}).$$

Here we made the obvious definition

$$\Psi: \mathbb{R}^k \to \mathbb{R}, \qquad \Psi(r_1, \dots, r_k) \stackrel{\text{def}}{=} \mathbb{E} \bar{\psi}(r_1, \dots, r_k, Z^{v^1}, \dots, Z^{v^k}) Z^x.$$

Thus Ax also has approximately iid coordinates (of size $\Theta(1)$),

$$Z^{Ax} \stackrel{\text{def}}{=} \Psi(Z^{u^1}, \dots, Z^{u^k}).$$

For example, in the SGD example with $A = u \otimes v/n$ and $\bar{\psi}(u_{\alpha}, v_{\beta}) = u_{\alpha}v_{\beta}$, this formula gives $Z^{Ax} = \Psi(Z^u)$ where $\Psi(z) = z \mathbb{E} Z^v Z^x$, recovering the earlier derivation.

In any case, the point here is that A has coordinate size $\Theta(1/n)$, and this is the unique scaling that leads to Ax having coordinate size $\Theta(1)$.

L.1.4 Vector Case (e.g. Readout Layer)

The vector A case is similar to the tensor product cases above.

L.1.5 Gaussian Matrix (e.g. Hidden Weights Initialization)

Now consider the case where $A \in \mathbb{R}^{n \times n}$ is random Gaussian matrix with $A_{\alpha\beta} \sim \mathcal{N}(0,1/n)$ and $x \in \mathbb{R}^n$ has approximately iid coordinates distributed like Z^x . In the context of neural network training, A should be thought of as a randomly initialized weight matrix, and x for example can be taken to be an activation vector in the first forward pass.

 $[\]overline{}^{32}$ In some corner cases when x is uncorrelated with v, then $v^{\top}x = \Theta(\sqrt{n})$ by Central Limit, so actually Ax has $\Theta(1/\sqrt{n})$ coordinates. However, this case does not come up much in the context of training neural networks

³³Adam also has bias correction for the moving averages which can be accommodated easily, but for simplicity we omit them here.

A Quick Intuition By standard random matrix theory, A has $\Theta(1)$ operator norm with high probability. Thus, with high probability, for any vector x, we have $\|Ax\| \approx \|x\|$, even if x is correlated with A. If Ax's coordinates are "evenly distributed", then this would imply Ax has $\Theta(1)$ coordinates if x does. However, this is not so clear. Below we provide intuitions for why this would be the case.

Intuition for Evenness of Coordinate Distribution If x is independent from A (or sufficiently uncorrelated), then each coordinate $(Ax)_{\alpha}$ has variance $\mathbb{E}(Z^x)^2 = \Theta(1)$ (so by definition has size $\Theta(1)$). Thus, here A having $\Theta(1/\sqrt{n})$ coordinates leads to Ax having $\Theta(1)$ coordinates, in contrast to the tensor product case above.

When x is correlated with A, it turns out the same scaling applies $(\Theta(1/\sqrt{n}))$ is the unique scaling for A's entries such so that Ax has $\Theta(1)$ entries), but the reasoning is much more subtle: In the context of neural network training, it turns out all scenario where x is correlated with A can be reduced to the case where $x = \phi(A^{\top}y, \ldots)$ for some coordinatewise nonlinearity ϕ and some other vector \mathbb{R}^n . Yet's consider a very simple example with $x = A^{\top}\mathbf{1}$ for the all 1s vector $\mathbf{1} \in \mathbb{R}^n$ (which has coordinate size $\Theta(1)$ as can be checked easily). Then, for each index $\alpha \in [n]$, we can calculate

$$(AA^{\top}\mathbf{1})_{\alpha} = \sum_{\beta,\gamma} A_{\alpha\beta} A_{\gamma\beta} = \sum_{\beta} A_{\alpha\beta}^2 + \sum_{\beta} \sum_{\gamma \neq \alpha} A_{\alpha\beta} A_{\gamma\beta}.$$

Since $\mathbb{E}\,A_{\alpha\beta}^2=1/n$, by the Law of Large Number, the first sum $\sum_{\beta}A_{\alpha\beta}^2\approx 1$. On the other hand, there are n summands of the form $\sum_{\gamma\neq\alpha}A_{\alpha\beta}A_{\gamma\beta}$, all iid with variance $\frac{n-1}{n^2}=\Theta(1/n)$. Thus by the Central Limit Theorem, we expect $\sum_{\beta}\sum_{\gamma\neq\alpha}A_{\alpha\beta}A_{\gamma\beta}\approx\mathcal{N}(0,1)$. Therefore, each coordinate of $(AA^{\top}\mathbf{1})_{\alpha}$ looks like $1+\mathcal{N}(0,1)=\mathcal{N}(1,1)$ and thus has size $\Theta(1)$; again this is caused by A having $\Theta(1/\sqrt{n})$ coordinates.

This example can be generalized to more general x that is correlated with A, but the mathematics is quite involved. See [44] for more details.

L.2 Deriving μ P for Any Architecture

Armed with the insight from the last section, we now outline the key steps to derive μP in Table 3 for any architecture. In practice, μP implies the following desiderata

Desiderata L.1. At any time during training

- 1. Every (pre)activation vector in a network should have $\Theta(1)$ -sized coordinates³⁵
- 2. Neural network output should be O(1).
- 3. All parameters should be updated as much as possible (in terms of scaling in width) without leading to divergence.

Let's briefly justify these desiderata. For the desideratum 1, if the coordinates are $\omega(1)$ or o(1), then for sufficiently wide networks their values will go out of floating point range. This problem is particularly acute for low-precision formats that are essential for training large models such as BERT or GPT. Moreover, a general nonlinearity is only well-behaved if its input is in a fixed range (although this is not a problem for homogeneous nonlinearities like relu). For example, for tanh nonlinearity, if the preactivation is vanishing o(1), then tanh is essentially linear; if the preactivation is exploding $\omega(1)$, then the tanh gradient vanishes.

For the desideratum 2, a similar justification applies to the numerical fidelity of the loss function and loss derivative. Note that, with desideratum 3, this means the network output should be $\Theta(1)$ after training (but it can go to zero at initialization).

Finally, desideratum 3 means that 1) we are doing "maximal feature learning" [45] and 2) every parameter contribute meaningfully in the infinite-width limit. This ensures that learning rate "plays the same role" in the finite-width case as in the infinite-width limit. For example, it prevents the scenario where a weight matrix gets stuck at initialization in the limit for any learning rate (so

³⁴This is because every "reasonable" deep learning computation can be expressed in a Tensor Program.

³⁵In a convnet, a (pre-)activation vector corresponds to a single pixel across all channels; in general, we expect (pre-)activations are iid across channels, but correlated across pixels

learning rate does not matter) but evolves nontrivially in any finite-width network (so learning rate does matter).

These desiderata will essentially uniquely single out μ P. More formally, μ P is the unique parametrization that admits feature learning in all parameters of the neural network [45], and this property theoretically guarantees HP transfer across width (for sufficiently large width). However, for the sake of reaching a broader audience, we will focus more on the intuitive derivations from the desiderata rather than on this formal aspect.

Below, we first assume for simplicity that the width of every layer is n, and we focus only on dense weights. Later, we will discuss convolutions and varying the widths between layers.

L.2.1 μ P Derivation From the Desiderata

Output Weights Suppose $W \in \mathbb{R}^{1 \times n}$ is an output weight. By desideratum 1, the input x to W has $\Theta(1)$ -sized coordinates. Thus W should have $\Theta(1/n)$ coordinates so that Wx = O(1). We can initialize W with $\Theta(1/n)$ coordinates and scale its (per-layer) LR so that ΔW has $\Theta(1/n)$ coordinates as well. This means initializing $W_{\alpha\beta} \sim \mathcal{N}(0,\Theta(1/n^2))$ and use $\Theta(1/n)$ learning rate for both SGD and Adam.

Hidden Weights Consider a square weight matrix $W \in \mathbb{R}^{n \times n}$. Desiderata 1 guarantees that the input x to W has $\Theta(1)$ -sized coordinates. Generally, x will be correlated with W. By Table 14, we can immediately derive

Initialization W should be randomly initialized with coordinate size $\Theta(1/\sqrt{n})$

LR The learning rate should be scaled so that ΔW has coordinate size $\Theta(1/n)$

so that $(W_0 + \Delta W)x$ is $\Theta(1)$ if x is, inductively satisfying desideratum 1. With Adam, this just means the per-layer LR is $\Theta(1/n)$. With SGD and the scaling of output layers above, we can calculate that the gradient of W has $\Theta(1/n)$ coordinates, so the $\Theta(1)$ SGD LR derived above suffices as well.

Input Weights Suppose $W \in \mathbb{R}^{n \times d}$ is an input weight. To satisfy desideratum 1 (i.e. for any input $\xi, W\xi$ should have $\Theta(1)$ coordinates), we want W to have $\Theta(1)$ coordinates. We can initialize W with $\Theta(1)$ coordinates and scale its (per-layer) LR so that ΔW has $\Theta(1)$ coordinates as well. This implies initialization variance of $\Theta(1)$ (or $\Theta(1/\mathrm{fan_in})$ since $\mathrm{fan_in} = \Theta(1)$ here) and Adam learning rate $\Theta(n)$. As above, we can calculate that the gradient of W has $\Theta(1/n)$ coordinates, so we want SGD learning rate $\Theta(n)$.

Biases Biases follow the same reasoning as input weights (just think of it as an input weight with input 1).

Attention Suppose the key dimension d_k is tending to infinity with width with number of heads n_{head} fixed. Then the key-query contraction $q^{\top}k \in \mathbb{R}$ scales like $\Theta(d_k)$ by Law of Large Numbers (instead of Central Limit Theorem because q and k are generally correlated) and desideratum 1, hence the $1/d_k$ we propose rather than $1/\sqrt{d_k}$.

Now suppose instead that n_{head} tends to infinity with width with d_k fixed. Let $K,Q \in \mathbb{R}^{N \times d_k \times n_{head}}$, $V \in \mathbb{R}^{N \times d_v \times n_{head}}$ be keys, queries, and values across all heads and tokens. Thinking of $N \times d_k$ as constants, we may view attention as a nonlinearity coordinatewise in the n_{head} dimension. Then it's clear that our parametrization described above already works.

Finally, we may freely let d_k and n_{head} both tend to infinity, and the above reasoning shows that our parametrization still works.

Changing Width Ratios As noted above, at any time in training, every (pre-)activation vector will have approximately iid coordinates (of order $\Theta(1)$ by desideratum 1). Another desideratum for μP is to ensure that this coordinate distribution (at any particular time) stays roughly invariant as widths increases. When all layer widths are tied, this is automatic if the other desiderata are satisfied, hence why we did not list this above.

When width ratios vary, this is not automatic. In this case, we need to choose whether to replace each n with fan-in or fan-out (or some function of them). Making the wrong choices will let the coordinate distributions vary with width ratios.

Obviously, we should replace n with fan-in for the output layers and with fan-out for the input layers since they are the only dimension scaling with n. For the hidden weights, we replace n with fan-in so that the forward pass is preserved. When using Adam (and assuming the initialization of W is quickly dominated by the change in W), this ensures that the (pre-)activation coordinate distributions are preserved at any time during training even if we vary widths in different layers differently. (For SGD this doesn't quite work in general because the varying width ratios change the gradient sizes of different layers differently, whereas Adam always normalizes the gradient coordinatewise).

Convolution A convolution weight tensor $W \in \mathbb{R}^{\text{fan_out} \times \text{fan_in} \times s_1 \times s_2}$ with kernel size $s_1 \times s_2$ can be thought of just as a $s_1 s_2 = \Theta(1)$ -sized collection of fan_out \times fan_in dense weights. Then all of our discussions above apply accordingly.

L.3 Why Other Parametrizations Cannot Admit Hyperparameter Transfer

Standard Parametrization (SP) SP doesn't work essentially because it leads to blow-up in the infinite-width limit.

- 1. For Adam with LR $\Theta(1)$, ΔW would have $\Theta(1)$ coordinates, causing preactivations to blow up like $\Theta(n)$ by Desideratum 1 and Table 14. We can avoid this blowup with LR $\Theta(1/n)$, but this induces a non-maximal feature learning limit, which, as we argue below, cannot transfer hyperparameters in all situations.
- 2. For SGD, the gradient of $\mathbb{R}^{n\times n}$ weight has $\Theta(1/\sqrt{n})$ coordinates, so $\Theta(1)$ learning rate would make preactivation scale like $\Theta(\sqrt{n})$ and hence blow up. If we use $\Theta(1/width)$ learning rate, then blow-up does not occur. However, this infinite-width limit is in the kernel regime [45] and thus does not allow HP transfer for the same reason that NTP below does not.

Neural Tangent Parametrization (NTP) We have concrete examples, e.g. Word2Vec in [45], where the NTK limit has trivial performance — so HPs have no effect at all — vastly outperformed by finite-width networks — where HPs matter. More importantly, wider does not always do better in NTP, especially in tasks where feature learning is crucial [45]. So in the context of modern deep learning e.g. large language model pretraining, NTP (or SP with $\Theta(1/width)$ LR) does not make sense for wide neural networks.

Other Parametrizations Recall the *Dynamical Dichotomy Theorem* proven in [45], which says that any nontrivial stable "natural parametrization" (formally, "abc-parametrization," [45]) either admits a feature learning limit or a kernel limit, but not both.

Our argument above against SP and NTP will also work against any parametrization inducing a kernel limit. Therefore, it remains to ask, can other *feature learning* parametrizations transfer HPs?

We argue no. As shown in [45], any other feature learning parametrization differs from μP essentially only in that some parameters are not updated maximally. By [45, Sec 6.4], in the infinite-width limit, such parameters can be thought of as being fixed at initialization. Therefore, in such infinite-width limits, the learning rate of such parameters becomes useless. Therefore, we cannot hope for the HP landscape of the limit to reflect the HP landscape of finite-width neural networks.

 μP is the unique feature learning parametrization that updates all parameters maximally, so that the learning rate of each parameter plays approximately the same role in finite-width neural networks as in the infinite-width limit. Consequently, the HP landscape of the μP limit should reflect the HP landscape of finite-width neural networks.