JORGE: APPROXIMATE PRECONDITIONING FOR GPU-EFFICIENT SECOND-ORDER OPTIMIZATION

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ABSTRACT

Despite their better convergence properties compared to first-order optimizers, second-order optimizers for deep learning have been less popular due to their significant computational costs. The primary efficiency bottleneck in such optimizers is matrix inverse calculations in the preconditioning step, which are expensive to compute on GPUs. In this paper, we introduce Jorge, a second-order optimization technique maintains the statistical efficiency of second-order optimizers, while getting closer to first-order optimizers in terms of wall-clock time. We address the primary computational bottleneck of computing matrix inverses by completely eliminating them using an approximation of the preconditioner computation. This makes Jorge optimizers extremely efficient on GPUs in terms of wall-clock time. Our empirical evaluations demonstrate the distinct advantages of using Jorge, outperforming state-of-the-art optimizers such as SGD, AdamW, and Shampoo across multiple deep learning models, both in terms of sample efficiency and wall-clock time.

1 INTRODUCTION

Stochastic optimization methods such as stochastic gradient descent (SGD) (**?**) and *Adam* (**?**) are the de-facto standard for optimizing the objective function in the training of deep neural networks. These first-order optimization methods are relatively inexpensive in terms of their compute and memory requirements, and hence extremely popular. Second-order optimization methods typically have better convergence properties (fewer epochs to reach target validation metrics) than those of first-order methods. However, they are considerably slower in terms of per-iteration (per-batch) wall-clock times for training than first-order methods. This is because they often use a preconditioner, which multiplies the gradient by a matrix before taking a step. Computing these preconditioners requires performing matrix inversions, which are highly inefficient on GPU platforms due to the iterative nature of matrix inverse algorithms and their irregular memory access patterns.

If one could develop a second-order optimizer that has better convergence than first-order methods and is on par with them in terms of wall-clock time per iteration, we could achieve the best of both worlds. In this paper, we present Jorge[1], a new second-order optimizer method that uses an approximation for preconditioning by avoiding the calculation of the inverse of matrices in all steps. It has similar convergence properties to other second-order optimization methods but its wall-clock time per iteration, when applied to a second-order optimizer, is similar to that of inexpensive first-order methods. This is a win-win situation, which leads to much faster total training times for several different deep learning models when compared to other state-of-the-art optimizers.

A new optimization method is most useful and promising if users do not have to spend significant time in tuning its hyperparameters. We show in Section **??** that JorgeKFAC consistently outperforms SGD and AdamW at various common hyperparameter values, making hyperparameter tuning less of a hassle for practitioners.

1.1 CONTRIBUTIONS

This paper makes the following important contributions:

[1]Jorge is named after Dr. Jorge Nocedal, an applied mathematician & expert in nonlinear optimization.

- 2 new second-order optimizers (JorgeShampoo, JorgeKFAC) that avoid matrix inverse calculations when computing the preconditioner, making them extremely efficient on GPUs. This results in per-iteration wall-clock times within 5-10% of those of first-order optimizers such as SGD and AdamW, while matching the sample efficiency of Shampoo, a second-order optimizer. For training ResNet-50 on ImageNet, we demonstrate improvements of nearly 25% in the total training wall-clock time over SGD.
- Most second-order optimizers need to exploit complex parallelism requiring multiple GPUs to get their total training times to be faster than those of first-order optimizers. Since Jorge optimizers are highly efficient, they can be run locally on each GPU and still outperform highly optimized parallel implementations of second-order optimizers.

1.2 Related work

There have been several research efforts to develop computationally tractable second-order optimizers for deep learning. **?** proposes Hessian-free optimization, which exploits conjugate gradient (CG) to directly compute Hessian-vector products without explicitly computing the Hessian. Since CG requires multiple iterations, there has been subsequent work on reducing this cost (**?**). Several optimizers based on the L-BFGS method have also been proposed that approximate Hessian-vector products from the history of past gradients, again without explicitly computing the Hessian (**???**).

Most state-of-the-art second-order optimizers rely on block-diagonal approximations of the Hessian to reduce the computational and memory requirements. The "blocks" typically correspond to substructures in the neural network, like a layer or a parameter tensor. Some recent methods in this category include Shampoo (**?**), K-FAC (**??**), K-BFGS (**?**) and the GGT method (**?**). However, these methods need to compute the inverse of their approximate Hessian matrices, which can be expensive to compute even with the block-diagonal approximations. As we show later in Section 5, JorgeShampoo outperforms one such optimizer, Shampoo, by nearly 37% in terms of the total wall-clock time for training ResNet-50 on ImageNet. Closely related to Jorge is a line of work that exploits the Sherman-Morrison based Matrix identity to approximate the update steps in K-FAC without computing any matrix inverses (**???**).

To mitigate the large computational costs of matrix inverses, researchers have also proposed parallel implementations of second-order optimizers, which aim to distribute the work of the optimizer across multiple GPUs. Several efforts focus on developing efficient parallel implementations of the K-FAC optimizer (**??????**). On the other hand, **?** and **?** aim to accelerate the Shampoo (**?**) optimizer via parallelism. **?** present a heterogeneous solution that offloads the computation of the inverses to the CPU. Even though we implement Jorge without any multi-GPU parallelism, we demonstrate that its performance is better than one of the state-of-the art parallel optimizers – Distributed Shampoo (**?**).

2 Background

Second-order optimizers make use of both the gradients and curvature (second derivatives) of the loss function. By considering the curvature, second-order methods can approximate the loss function more accurately than first-order optimizers, and thus reduce the number of iterations required for convergence. Most second-order optimizers approximate the Newton step shown in Equation 1.

parameters at timestep t and t-1

$$\theta_t = \theta_{t-1} - H_t^{-1} G_t \tag{1}$$

Hessian at timestep t — gradients at timestep t

This equation can be derived by minimizing a second-order Taylor's approximation of the loss function at θ_t. This step of multiplying the gradients with H_t^{-1} is called preconditioning, and H_t^{-1} is often referred to as a preconditioner.

Instead of using the actual Hessian, optimizers typically use positive semi-definite approximations of the Hessian (**??**) to account for the non-convexity of the training objective (**?????**). One of our proposed optimizers, JorgeKFAC, is of this class. Our other proposed optimizer, JorgeShampoo,

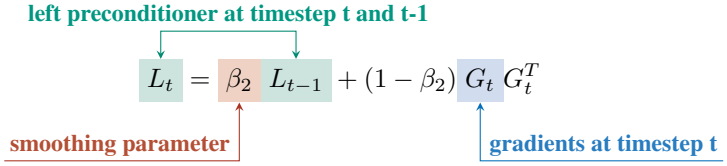
belongs to a class of methods called "adaptive optimizers", which use the inverse of the gradient covariance matrix (or the empirical Fisher matrix) to precondition gradients. Examples of adaptive second-order optimizers include the full matrix version of Adagrad (**?**) and Shampoo (**?**). Note that several first-order adaptive optimizers have also been proposed in literature, which only use the diagonal elements of the covariance matrix. Popular examples include Adam (**?**) and RMSProp. **???** provide justification for the usage of the gradient covariance matrix as an approximation of the Hessian.

3 Approximate Preconditioning in JorgeShampoo

As described in Section 1.2, the primary efficiency bottleneck in state-of-the-art second-order optimizers such as K-FAC (**?**) and Shampoo (**?**) is the matrix inverse computations performed to calculate the preconditioners. To overcome this limitation, we introduce JorgeShampoo, an efficient, adaptive, second-order optimizer tailored for GPU execution. JorgeShampoo's formulation eliminates computing explicit matrix inversions, and is solely comprised of matrix multiplications and additions, which are highly optimized on GPUs. This results in JorgeShampoo's wall-clock time per iteration to be on par with those of first-order optimizers, while also having faster convergence properties typical of a second-order optimizer.

We propose JorgeShampoo as an enhancement of Shampoo (**?**), another adaptive second-order optimizer. We first describe Shampoo's optimizer algorithm at a high level before describing JorgeShampoo's optimizer algorithm. Note that, throughout this section, we discuss Shampoo and by extension JorgeShampoo, within the context of a single layer. Application to multiple layers simply involves repeating the same steps for their parameters.

Following **?**, let us assume that the parameters, θ, of a single layer are organized in a two-dimensional (2D) $m \times n$ matrix (N-dimensional parameter tensors, like those found in convolution layers are typically collapsed into 2D matrices, in practice). Shampoo maintains the second-order curvature information of the loss in two matrices – L_t (size $m \times m$) and R_t (size $n \times n$), which are called the left and right preconditioners, respectively. It iteratively updates the preconditioners from the current gradient information as shown in the equation below (for the left preconditioner):



(2)

Algorithm 1 shows how the preconditioners are used in Shampoo. Additional terms used in the algorithm are defined as follows. β_1 and β_2 are smoothing parameters for the exponential moving average (EMA) of the momentum and preconditioners. $\tilde{G}_t$ is the preconditioned gradients at timestep t. m_t is the EMA of the preconditioned gradients, and η_t is the learning rate at timestep t. Lines 5–8 of Algorithm 1 show how the Shampoo optimizer iteratively updates the left and right preconditioners from the current gradients' information. Line 11 illustrates the preconditioning step, wherein the gradients are multiplied by $L_t^{\frac{-1}{4}}$ and $R_t^{\frac{-1}{4}}$ on the left and right, respectively. The preconditioning step produces the preconditioned gradients, $\tilde{G}_t$, which minimize the loss faster than the raw gradients. Finally, we update the momentum estimate of the preconditioned gradients (line 14), and then use the momentum to update the weights (line 15). The matrix inverse computation in the preconditioning step (line 11) is the primary efficiency bottleneck in Shampoo, and is exactly what we want to optimize in JorgeShampoo. JorgeKFAC, discussed in Section **??**, follows a nearly identical process.

Algorithm 1 Shampoo

1: **Initialize** θ_0, $L_0 = \epsilon I_m$
2: $R_0 = \epsilon I_n$
3: **for** t=1 ,..., T **do**
4: **Update Preconditioners:**
5: $L_t = \beta_2 L_{t-1}$
6: $+(1-\beta_2) G_t G_t^T$
7: $R_t = \beta_2 R_{t-1}$
8: $+(1-\beta_2) G_t^T G_t$
9:
10: **Precondition Gradients:**
11: $\tilde{G}_t = L_t^{\frac{-1}{4}} G_t R_t^{\frac{-1}{4}}$
12:
13: **Update Weights:**
14: $m_t = \beta_1 m_{t-1} + (1-\beta_1)\tilde{G}_t$
15: $\theta_t = \theta_{t-1} - \eta_t m_t$
16: **end for**

Algorithm 2 JorgeShampoo compared to Shampoo

1: **Initialize** θ_0, $\hat{L}_0 = \epsilon^{-\frac{1}{4}} I_m$, $\hat{R}_0 = \epsilon^{-\frac{1}{4}} I_n$
2:
3: **for** t=1 ,..., T **do**
4: **Update Preconditioners:**
5: $X_L = \hat{L}_{t-1}^4 G_t G_t^T$
6: $\hat{L}_t = \beta_2^{\frac{-1}{4}} \hat{L}_{t-1} \left(I_m - \frac{(1-\beta_2)}{4\beta_2} X_L + \frac{5(1-\beta_2)^2}{32\beta_2^2} X_L^2 \right)$
7: $X_R = \hat{R}_{t-1}^4 G_t^T G_t$
8: $\hat{R}_t = (\beta_2')^{\frac{-1}{4}} \hat{R}_{t-1} \left(I_n - \frac{(1-\beta_2')}{4\beta_2'} X_R + \frac{5(1-\beta_2')^2}{32(\beta_2')^2} X_R^2 \right)$
9:
10: **Precondition Gradients:**
11: $\tilde{G}_t = \hat{L}_t G_t \hat{R}_t$
12:
13: **Update Weights:**
14: $m_t = \beta_1 m_{t-1} + (1-\beta_1)\tilde{G}_t$
15: $\theta_t = \theta_{t-1} - \eta_t m_t$
16: **end for**

In Algorithm 2, we show the functioning of JorgeShampoo side-by-side with Shampoo for the same 2D $m \times n$ parameter matrix of a single layer. The core idea behind Jorge is to approximate the computation of $L_t^{\frac{-1}{4}}$ and $R_t^{\frac{-1}{4}}$ in Shampoo (line 11 of Algorithm 1) in a GPU-efficient manner. In order to do this, we modify the computation in both lines 5–8 and line 11 of Algorithm 1. Just like Shampoo, JorgeShampoo also maintains two preconditioners, which we refer to as $\hat{L}_t$ and $\hat{R}_t$ in Algorithm 2. However, JorgeShampoo's preconditioners are an approximation of the inverse fourth root of Shampoo's preconditioners at every iteration, i.e. $\hat{L}_t \approx L_t^{\frac{-1}{4}}$ and $\hat{R}_t \approx R_t^{\frac{-1}{4}}$. We show the remaining steps for the left preconditioner approximation, and the right preconditioner approximation can be derived similarly.

Since $\hat{L}_t \approx L_t^{\frac{-1}{4}}$, we can say that $L_t \approx \hat{L}_t^{-4}$, and $L_{t-1} \approx \hat{L}_{t-1}^{-4}$. We substitute L_t and L_{t-1} on both sides of Equation 2, which gives us:

$$\hat{L}_t^{-4} = \beta_2 \hat{L}_{t-1}^{-4} + (1-\beta_2) G_t G_t^T \tag{3}$$
$$\implies \hat{L}_t = \left(\beta_2 \hat{L}_{t-1}^{-4} + (1-\beta_2) G_t G_t^T \right)^{\frac{-1}{4}}$$

$$\hat{L}_t = \beta_2^{\frac{-1}{4}} \hat{L}_{t-1} \left(I_m + \frac{(1-\beta_2)}{\beta_2} \hat{L}_{t-1}^4 G_t G_t^T \right)^{\frac{-1}{4}} \tag{4}$$
$$= \beta_2^{\frac{-1}{4}} \hat{L}_{t-1} \left(I_m + \frac{(1-\beta_2)}{\beta_2} X_L \right)^{\frac{-1}{4}} \tag{5}$$

$\hat{L}_{t-1}^4 G_t G_t^T$ **(line 5, Algorithm 2)**

Next, we get rid of the inverse computation in Equation 5 by employing the binomial series expansion on the expression in parenthesis. The binomial theorem for negative exponents suggests that for a square matrix $A \in \mathbb{R}^{m \times m}$, provided $\|A\| < 1$ and $p > 0$, where $\|.\|$ is a valid matrix norm, the

following is true:

$$(I_m + A)^{-p} = \sum_{r=0}^{\infty} (-1)^r \frac{p(p+1)(p+2)...(p+r-1)}{r!} A^r \tag{6}$$

Substituting $A = \frac{(1-\beta_2)}{\beta_2} X_L$, and $p = \frac{1}{4}$ in Equation 6 yields:

$$\left(I_m + \frac{(1-\beta_2)}{\beta_2} X_L\right)^{\frac{-1}{4}} = I_m - \frac{1}{4}\frac{(1-\beta_2)}{\beta_2} X_L + \frac{5}{32}\frac{(1-\beta_2)^2}{\beta_2^2} X_L^2 + ... \tag{7}$$

Now, replacing the expression in parenthesis in Equation 5 with its binomial series expansion in Equation 7, we remove the inverse calculation entirely as shown below:

$$\hat{L}_t = \beta_2^{\frac{-1}{4}} \hat{L}_{t-1} \left(I_m - \frac{1}{4}\frac{(1-\beta_2)}{\beta_2} X_L + \frac{5}{32}\frac{(1-\beta_2)^2}{\beta_2^2} X_L^2 + ...\right) \tag{8}$$

Note that the binomial expansion is an infinite series and thus intractable. In practice, we have found that ignoring the cubic and higher powers of this expansion does not degrade the sample efficiency of JorgeShampoo in comparison to Shampoo (See Section 5). Hence we drop the higher-order terms in Equation 8, which gives us line 6 of Algorithm 2. Notice how our preconditioner update step is composed entirely of matrix-matrix multiplications and additions, which are highly efficient to compute on GPUs, thereby making Jorge-based optimizers more compute-efficient than other second-order optimizers. After updating the preconditioners, we precondition the gradients by multiplying them with $\hat{L}_t$ and $\hat{R}_t$ on the left and right (line 11). Unlike Shampoo, we do not have to invert our preconditioners because, by definition, they are an approximation of the inverse fourth roots of Shampoo's preconditioners. Finally, the weight update step in lines 14 and 15 is identical to Shampoo.

Note that Equation 6 is only valid for $\|A\| < 1$, and therefore for $\|\frac{(1-\beta_2)}{\beta_2} X_L\| < 1$. To ensure this, JorgeShampoo dynamically adjusts β_2 (and β_2' for the right preconditioner) in each iteration such that the above constraint is met. We discuss this in detail in Appendix A.2.

To improve performance, most second-order optimizers, including K-FAC and Shampoo, typically compute their preconditioners at regular intervals, instead of every iteration. Following suit, we also allow infrequent preconditioner updates for Jorge, with the interval kept as a user-configurable hyperparameter. In the iterations where we do not update the preconditioners, we simply reuse the preconditioners from the previous iteration.

As empirical evidence of the efficacy of our approximation we provide the per-iteration times of SGD, JorgeShampoo and AdamW for training ResNet-50 (**?**) and DeepLabv3 (**?**) on the Imagenet and MS-COCO datasets respectively in Table 1. For the ResNet-50 benchmark, we observe that JorgeShampoo's iteration times are only 1% slower than SGD, whereas it is 26% faster than Shampoo! For the DeepLabv3 benchmark, JorgeShampoo is only 10% slower than SGD, but a significant 21% faster than Shampoo.

Table 1: Comparison of wall-clock times per iteration (in seconds) for SGD, JorgeShampoo and Shampoo. For JorgeShampoo and Shampoo, we compute the preconditioner inverses every 50 iterations, in line with **?**.

Neural Network	Batch Size	# GPUs	SGD	Jorge	Shampoo
ResNet-50	1024	16	0.09	0.09	0.12
DeepLabv3	64	4	0.33	0.37	0.47

4 APPROXIMATE PRECONDITIONING IN JORGEKFAC

The formulation for JorgeKFAC largely follows JorgeShampoo: there are left and right preconditioners (named S and A here) for each linear or convolutional layer that we maintain and use to

precondition the gradients. K-FAC specifically uses the Kronecker product of S and A (covariance matrices of gradients and activations of each layer, respectively) to estimate the Fisher information matrix. Part of K-FAC's formulation is the inverse Fisher matrix, which requires taking the inverse of S and A. This simplifies the math a bit compared to JorgeShampoo, as we now have to use -1 instead of $-1/4$ as our exponent.

Algorithm 3 K-FAC

1: **Initialize** θ_0, $A_0, S_0 = \epsilon I_m, \epsilon I_n$
2: for l in L
3:
4: **for** t=1 ,..., T **do**
5: **Update Preconditioners:**
6: $aa_t = (1-\beta) a_t^T a_t$
7: $aa_t = \beta aa_{t-1} + aa_t$
8: $A_t = aa_t$
9: $ss = (1-\beta) s_t^T s_t$
10: $ss_t = \beta ss_{t-1} + ss_t$
11: $S_t = ss_t$
12: **Precondition Gradients:**
13: $\tilde{G}_t = S_t^{-1} G_{t-1} A_t^{-1}$
14: **Update Weights:**
15: $m_t = \beta_1 m_{t-1} + (1-\beta_1)\tilde{G}_t$
16: $\theta_t = \theta_{t-1} - \eta_t m_t$
17: **end for**

Algorithm 4 JorgeKFAC compared to K-FAC

1: **Initialize** θ_0, $\hat{A}_0, \hat{S}_0 = I_m, I_n$
2: for l in L
3:
4: **for** t=1 ,..., T **do**
5: **Update Preconditioners:**
6: $aa_t = a_t^T a_t$
7: $X_A = \hat{A}_{t-1}(aa_t * \epsilon I_m)$
8: $\hat{A}_t = \left(I_m - \frac{(1-\beta_2)}{\beta_2} X_A + \frac{(1-\beta_2)^2}{\beta_2^2} X_A^2\right) \frac{\hat{A}_{t-1}}{\beta_2}$
9: $ss_t = s_t^T s_t$
10: $X_S = \hat{S}_{t-1}(ss_t * \epsilon I_n)$
11: $\hat{S}_t = \left(I_n - \frac{(1-\beta_2)}{\beta_2} X_S + \frac{(1-\beta_2)^2}{\beta_2^2} X_S^2\right) \frac{\hat{S}_{t-1}}{\beta_2}$
12: **Precondition Gradients:**
13: $\tilde{G}_t = \hat{S}_t G_{t-1} \hat{A}_t$
14: **Update Weights:**
15: $m_t = \beta_1 m_{t-1} + (1-\beta_1)\tilde{G}_t$
16: $\theta_t = \theta_{t-1} - \eta_t m_t$
17: **end for**

On line 13, we again see that we calculate $\tilde{G}_t$ without having to invert any matrices! For JorgeKFAC, we perform an ablation study for 3 optimizers: JorgeKFAC, SGD, and AdamW. We perform a grid search over hyperparameter values for each optimizer to (1) find the optimal set of hyperparameters for a given optimizer, (2) to ensure fairness between optimizers in future experiments by using that optimal set of hyperparameters, and (3) to show that JorgeKFAC consistently performs better than other SGD and AdamW on the task at hand. The task being training a ResNet-18 on the CIFAR-10 dataset to do image classification. The gridsearch was done by running the experiment over all combinations of the following learning rate and weight decay values: [0.1, 0.03, 0.01, 0.03, 0.001].

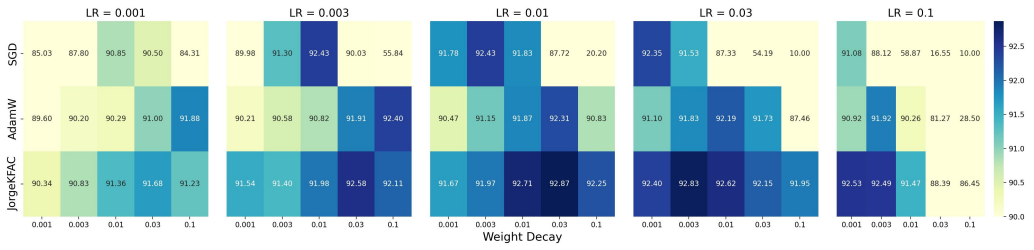


Figure 1: Accuracies of SGD, AdamW, and JorgeKFAC on the image classification task. Each heatmap has a fixed learning rate value, and each subcolumn is a fixed weight decay value.

We see in Figure 1 that across the tested hyperparameter values, JorgeKFAC not only has the highest overall accuracy, but tends to have a higher accuracy than SGD and AdamW at many of the given learning rate and weight decay combinations.

5 Experimental Results

In this section, we discuss the empirical experiments conducted to evaluate the efficacy of Jorge-Shampoo against other state-of-the-art optimizers used in deep learning.

5.1 Setup: Benchmarks and Metrics

Table 2 lists the training benchmarks used in our experiments, all of which are sourced from the torchvision repository (**?**). For each benchmark, we consider two types of training runs – one where we let a given optimizer train for the maximum number of epochs specified in the repository, and the other where we only train up to the validation metrics specified in Table 2. The former helps us measure the generalization of each optimizer, whereas the latter helps us measure the sample efficiencies and total wall-clock times for training. Mask-RCNN (**?**) and DeepLabv3 (**?**) use ResNet-50 as their backbone. We use SGD as our baseline and also compare with AdamW, Shampoo, and a recently proposed parallel implementation of Shampoo (**?**),

Table 2: List of benchmarks used to evaluate Jorge against other optimizers. The validation targets for the first two tasks are the same as those used in MLPerf. For the image segmentation task, it is the same as specified in the torchvision repository.

Training Task	Neural Network	Dataset	Batch Size(s)	Target Validation Metric
Image Classification	ResNet-50	ImageNet	256/1024	75.9% Accuracy
Object Detection	Mask-RCNN	MS-COCO 2017	32	37.7 Bbox mAP
Image Segmentation	DeepLabv3	MS-COCO 2017	64	66.4 IoU

Choice of Hyperparameters: For direct comparisons with SGD and AdamW, we use the default small batch sizes specified by torchvision, which are 256, 32 and 64 respectively for ResNet-50, Mask-RCNN, and DeepLabv3. To the best of our knowledge, most evaluations of second-order optimizers have been conducted at batch sizes much larger than these values. Thus, to facilitate a direct comparison with Shampoo, we also ran the ResNet-50 benchmark with a larger batch size of 1024. By doing this, we could directly borrow the hyperparameters from **?**, who evaluated Shampoo in a similar setting.

All the benchmarks from torchvision used in our experiments employ an SGD optimizer, pre-optimized with a well-calibrated set of hyperparameters. Accordingly, for our evaluations with SGD, we adhere to these pre-set values. For our proposed optimizer, Jorge, we adopt the single-shot hyperparameter configuration outlined in Section **??**, which is derived directly from SGD's parameters. We borrow AdamW hyperparameters for the ImageNet benchmarks from **?**. The complete list of all hyperparameters used in this study can be found in Appendix A.6.

Evaluation Metrics: In our evaluation of each benchmark, we record validation accuracy/IoU/mAP with respect to both number of epochs and wall-clock time. While the epoch-based measurements provide insights into the sample efficiencies of different optimizers, wall-clock time offers an understanding of their computational speed and efficiency on GPU platforms. Together, these metrics offer a comprehensive assessment of each optimizer's practical efficacy.

5.2 Comparative Evaluation

Rapid convergence toward a target validation accuracy is not the only goal of an optimizer. The balance between quick initial convergence and eventual generalization can dictate an optimizer's selection. For example, SGD remains the optimizer of choice in computer vision due to its better final validation accuracy, even though Adam converges faster initially. We evaluate JorgeShampoo's peak validation accuracy against SGD and AdamW across benchmarks, and detail the results in

Table 3. In these experiments, we let each optimizer train for the maximum number of epochs specified in the repository. Notably, for ResNet-50 benchmarks, JorgeShampoo exceeds SGD's best validation accuracy – 76.02% vs 76.70% (large batch size), and 75.97% – 76.85% (small batch size). For the Mask-RCNN benchmark, JorgeShampoo's IoU of 38.92% represents a notable improvement over SGD's 38.3%. It's worth highlighting that these results were achieved using the single-shot tuning strategy described in Section **??**. Though DeepLabv3's performance with JorgeShampoo is marginally worse than that with SGD, the difference is within SGD's standard deviation, suggesting that small hyperparameter tweaks could bridge the gap. Notably, AdamW falls short of SGD's generalization in three out of four benchmarks but JorgeShampoo does better than SGD in three out of four benchmarks. Note that this gap in AdamW's generalization compared to SGD has been a focal point in several prior studies (**????**).

Table 3: Maximum validation accuracy ($\mu_{\pm\sigma}$) for SGD, AdamW, and JorgeShampoo across benchmarks.

Neural Network	Batch Size	# Trials	# Epochs	SGD	AdamW	JorgeShampoo
ResNet-50	1024	3	90	$76.02_{\pm 0.05}$	$71.85_{\pm 0.11}$	$\mathbf{76.70}_{\pm 0.07}$
ResNet-50	256	3	90	$75.97_{\pm 0.11}$	$76.56_{\pm 0.09}$	$\mathbf{76.85}_{\pm 0.12}$
DeepLabv3	64	5	30	$\mathbf{67.19}_{\pm 0.16}$	$66.26_{\pm 0.20}$	$67.12_{\pm 0.12}$
Mask-RCNN	32	5	26	$38.30_{\pm 0.13}$	$36.58_{\pm 0.11}$	$\mathbf{38.92}_{\pm 0.10}$

Next, we compare the sample efficiency of JorgeShampoo to other optimizers. In this case, we only train up to the target validation metrics specified in Table 2. Figure 2 (left) showcases the progression of validation accuracy over training epochs for ResNet-50 on ImageNet with the larger batch size of 1024. For other benchmarks, we depict this progression in Figure 3. It is evident that in the context of sample efficiency, JorgeShampoo outperforms the first-order optimizers we compare with – SGD and AdamW. Across both the small (256) and large (1024) batch size training scenarios for ResNet-50, JorgeShampoo outperforms SGD by requiring around 27% fewer iterations to reach the target validation accuracy of 75.9%. The improvements in sample efficiency over SGD across other benchmarks are markedly higher – 40% for DeepLabv3, and 41% for Mask-RCNN. Again, we achieve these results by simply bootstrapping JorgeShampoo's hyperparameters from SGD, only making the changes outlined in Section **??**. The improvements in sample efficiency over AdamW are similar to those over SGD. Also, AdamW falls short of achieving the target validation metric in two out of four experiments.

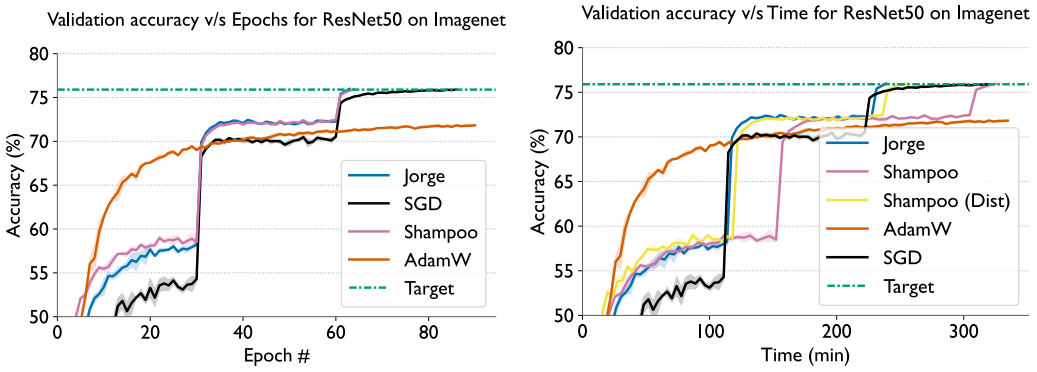


Figure 2: Validation accuracy $[\mu \pm \sigma]$ v/s epochs (left) and time (right) for the large batch size training (1024) of ResNet-50 on the ImageNet dataset (experiments run on 16 A100 GPUs).

As discussed in Section 3, we have designed JorgeShampoo to approximate Shampoo with a focus on GPU efficiency. Figure 2 (left) demonstrates that JorgeShampoo achieves the target validation accuracy in almost the same number of epochs as Shampoo (62 vs. 63). This observation strongly validates our approach and confirms that JorgeShampoo's approximations do not degrade its statistical efficiency.

Let us now turn our attention to an equally crucial metric: wall-clock time required for training. Figure 2 (right) demonstrates the progression of validation accuracy over time for the large batch size training of ResNet-50. We observe that JorgeShampoo achieves the target validation accuracy in 25% less time compared to SGD, which is a significant improvement. If we consider the serial implementation of Shampoo (pink line), it takes more total time to converge than SGD despite requiring 27% fewer epochs. This observation demonstrates the prowess of JorgeShampoo as a GPU-efficient adaptation of Shampoo: it's significantly faster than Shampoo's wall-clock time for convergence (239 minutes vs. 325 minutes), despite requiring a similar number of epochs. As noted in Section 1.2, the prevailing approach for mitigating the large overhead of preconditioning has been to develop distributed implementations of these optimizers. Within this context, Figure 2 (right) also presents the wall-clock time of a state-of-the-art parallel implementation of Shampoo (yellow line) (**?**). Notably, even though JorgeShampoo executes locally on each GPU, it still manages to yield a 4% speedup over the parallel version of Shampoo.

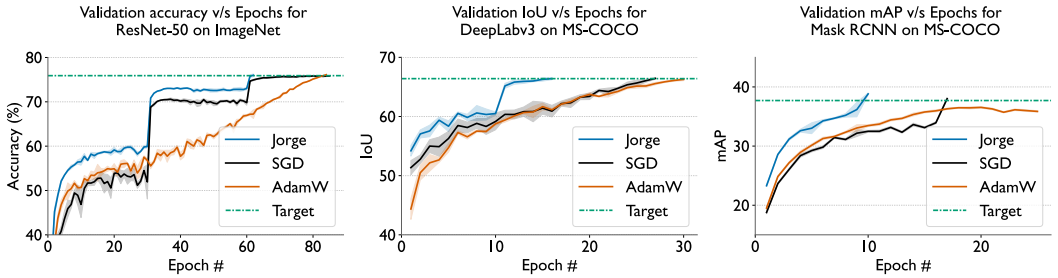


Figure 3: Validation accuracy, IoU, and mAP $[\mu \pm \sigma]$ v/s epochs for ResNet-50 on ImageNet (left) (batch size of 256), DeepLabv3 on MS-COCO (center), and Mask-RCNN on MS-COCO (right).

While a 4% improvement might seem modest, its implications are more far-reaching. Often times, AI practitioners do not have access to large numbers of GPU resources. In such resource-constrained settings, JorgeShampoo might be an ideal optimizer when parallelizing across GPUs is not an option. This also applies to environments with limited interconnect bandwidth.

Finally, we focus on the small batch size benchmarks to evaluate how JorgeShampoo's training wall-clock times compare with other first-order optimizers. We present these results in Table 4. Once again, JorgeShampoo makes significant improvements in the total training wall-clock times. Compared to SGD, JorgeShampoo improves the time to convergence by 23%, 34%, and 45% for ResNet-50, DeepLabv3, and Mask-RCNN respectively. The corresponding improvements over AdamW are even higher – 26%, 41%, and 58% (the last number is much higher since AdamW did not converge on that run). The wall-clock time improvements in these experiments highlight JorgeShampoo's applicability to small batch size training scenarios, where the overheads of a second-order optimizer cannot be masked behind network computation, making it more challenging for JorgeShampoo to beat first-order optimizers.

Table 4: Comparison of the total training time (in minutes) of JorgeShampoo with SGD and AdamW for the small batch size benchmarks (experiments run on four A100 GPUs).

Neural Network	Batch Size	# Trials	SGD	AdamW	JorgeShampoo
ResNet-50	256	3	$1005_{\pm 40}$	$1052_{\pm 36}$	$\mathbf{781}_{\pm 44}$
DeepLabv3	64	5	$217_{\pm 12}$	$244_{\pm 01}$	$\mathbf{144}_{\pm 30}$
Mask-RCNN	32	5	$332_{\pm 47}$	$438_{\pm 14}$	$\mathbf{182}_{\pm 11}$

Now we look at results for JorgeKFAC. In Figure 4, we show the accuracy curves for each optimizer's best performing run in our grid search in Figure 1. Note that in Figure 4, JorgeKFAC tends to have a higher training and testing accuracy than SGD and AdamW for at least half, if not most, of the standard 100 epochs of training. Importantly too, JorgeKFAC maintains KFAC's statistical advantages over first-order optimizers like SDG and AdamW by having the better final train and test accuracies. One explanation for why JorgeKFAC's training accuracy is closer to SGD's in the earlier epochs of training vs. AdamW's is because JorgeKFAC is essentially SGD with an exponential

moving average (EMA) of second-order information applied to its gradients. That EMA is stored as a variable in our code, and begins as the identity matrix, effectively doing very little to the gradients in the earlier epochs, thus JorgeKFAC acting as mostly SGD. Once the second-order information has saturated that variable, we see training accuracy increasingly diverge from that of SGD.

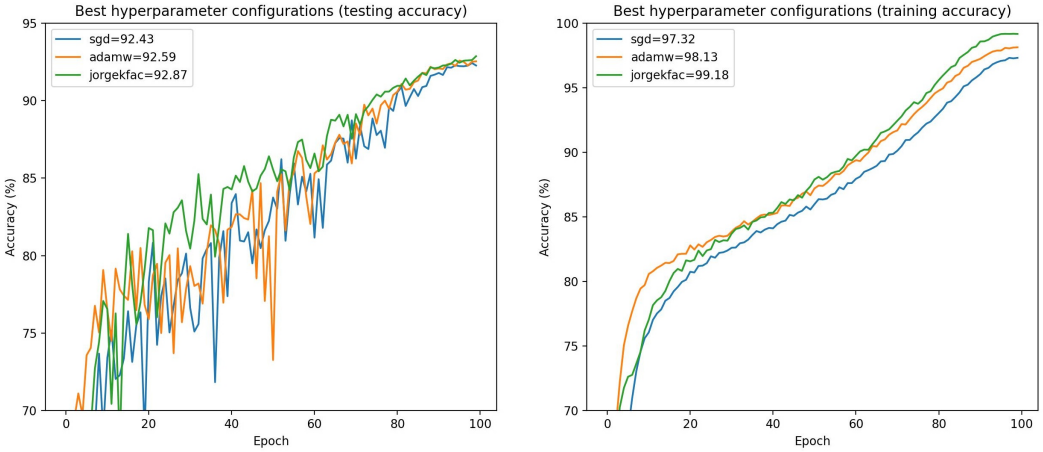


Figure 4: Test and train accuracy curves of the best hyperparameter combination for each optimizer.

6 Conclusion and Future Work

In this work, we introduced Jorge, a method to make efficient, adaptive, second-order optimizers tailored to GPU platforms - as well as two optimizers that use Jorge, JorgeKFAC and JorgeShampoo. We eliminated the primary computational bottleneck of computing matrix inverses in second-order optimizers by proposing a novel approximation of the preconditioner computation in Shampoo, which sidesteps the need to explicitly compute matrix inverses. We evaluated our optimizers against state-of-the-art first-order optimizers – SGD and AdamW, as well as Shampoo, and we demonstrated improvements in generalization, sample efficiencies, and training wall-clock times. As future work, we plan to develop a distributed implementation of Jorge to reduce its per-GPU memory consumption, which currently stands at 1.5–2$\times$ that of Adam (see Appendix A.7).

Reproducibility Statement: We are committed to enabling reproducibility of our work, as it ensures correct and transparent results. We plan to open source the code for JorgeShampoo and JorgeKFAC, as well as the benchmarks evaluated in this paper. Additionally, we provide a comprehensive list of all hyperparameters used in this study for each optimizer and each benchmark in Appendix A.6. The hyperparameters can be directly substituted as the arguments of SGD and AdamW shipped with PyTorch 2.0 in the "torch.optim" package. Similarly, the hyperparameters listed for Jorge will be compatible with our open source codebase.

References

A APPENDIX

A.1 BOOTSTRAPPING JORGE'S HYPERPARAMETERS FROM SGD

A new optimizer such as Jorge would be useful in practice only if it does not require rigorous hyperparameter tuning to achieve a desired level of generalization on a given training task. Arguably, an important reason behind the popularity of SGD is the existence of various heuristics for deciding hyperparameters configurations quickly that can achieve decent generalization. In this section, we demonstrate Jorge's ability to be an effective drop-in for SGD. We propose rules to deterministically bootstrap Jorge's hyperparameters from those of a well-tuned SGD baseline. We call this process "single-shot tuning". There are two implications of being able to single-shot tune Jorge's hyperparameters from a well-tuned SGD. First, it eliminates the need to explore the expensive, combinatorial search space of Jorge's hyperparameters. Second, the heuristics used to tune SGD's hyperparameters can also be transferred to Jorge.

Note that we focus on SGD over other adaptive optimizers such as Adam because prior research has demonstrated that SGD often outperforms adaptive methods in terms of generalization (**????**). Below, we propose some rules for transferring SGD's hyperparameters to Jorge.

Learning Rate: ? propose grafting, a technique for bootstrapping the learning rate and schedule of a new optimizer from another well-tuned optimizer. Grafting calculates the magnitude of the weight update by running a step of the well-tuned optimizer, and the direction of the weight update by running a step of the new optimizer. Using this approach, we employ grafting to directly use the learning rate of a well-tuned SGD baseline in Jorge. Integrating grafting in Jorge involves a small tweak to the weight update step in Algorithm 2 (lines 13-15), which we show in Appendix A.3. However, note that unlike **?**, we exploit grafting to adopt only the learning rate from SGD, but not the learning rate schedule (more details below).

Weight Decay Penalty: For regularization, in Jorge, we implement the decoupled weight decay scheme proposed by **?**, as it has been shown to generalize better than L2 regularization for adaptive optimizers. We now explain how the weight decay penalty for Jorge, λ_{Jorge}, can be bootstrapped from SGD. Let β_{SGD} and λ_{SGD} be the momentum factor and the weight decay penalty, respectively, of a well-tuned SGD optimizer. We propose deterministically setting λ_{Jorge} as follows:

$$\lambda_{\text{Jorge}} = \frac{1}{1 - \beta_{\text{SGD}}} \lambda_{\text{SGD}} \tag{9}$$

Using the almost universal value of 0.9 for β_{SGD}, we set Jorge's weight decay to $10\times$ that of SGD for our experiments. While surprisingly simple, we have found this heuristic to work well across several benchmarks. In Appendix A.4, we describe the intuition behind Equation 9 in more detail.

Learning Rate Schedule As per **?**, grafting should allow us to borrow not only the learning rate, but also the learning rate schedule of a well-tuned SGD baseline. However, we find that certain learning rate schedules are not suitable for Jorge. In Figure 5, we plot the progression of validation metrics for training ResNet-18 (**?**) on CIFAR-10 (**?**) (left plot) and DeepLabv3 (**?**) on MS COCO (**?**) (right plot). Note that using the default learning rate schedules of SGD, which are the cosine (**?**) and polynomial rate schedules, respectively, leads to barely any improvements in sample efficiency over SGD. Interestingly, simply switching to the step decay schedule with 2 decay steps (reducing the learning rate by $10\times$ at each step) at one-third and two-thirds of the total training epochs (total epochs same as that of the tuned SGD baseline) resolves this issue. We observe sample efficiency gains of nearly 1.4–1.8$\times$ over SGD. Therefore, across all training tasks, we opt for the step decay learning rate schedule with the aforementioned configuration. Interestingly, in certain scenarios using the default learning rate schedule of a given well-tuned SGD baseline also leads to overfitting with Jorge. We discuss this in Appendix A.5.

Preconditioner Update Frequency: As mentioned in Section 3, Jorge has a user-configurable hyperparameter to control the frequency at which the preconditioners are updated. We suggest using a value for this hyperparameter that brings the iteration wall-clock times within 10% of SGD.

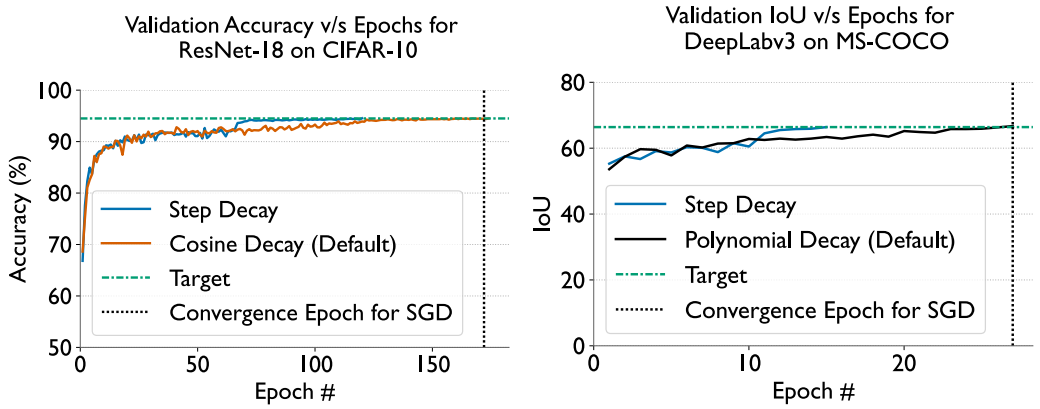


Figure 5: Comparing various learning rate schedules for Jorge. The left and right plots demonstrate the progression of validation accuracy for ResNet-18 on CIFAR-10, and validation IoU for DeepLabv3 on MS-COCO respectively.

A.2 Ensuring validity of the binomial expansion by dynamically adjusting β_2

In Section 3, we mentioned that for the binomial expansion in Equation 8 to be valid, we must also ensure that $\left\| \frac{(1-\beta_2)}{\beta_2} X_L \right\| < 1$. To ensure this condition is met at every iteration, Jorge dynamically updates the EMA update parameters β_2 and β_2' (for the right preconditioner) at each iteration. We start with the condition we want to ensure and derive a lower bound on β_2.

$$\left\| \frac{(1-\beta_2)}{\beta_2} X_L \right\| < 1 \implies \beta_2 > \frac{\|X_L\|}{\|X_L\|+1} \tag{10}$$

Therefore, we need to set β_2 to a value higher than $\frac{\|X_L\|}{\|X_L\|+1}$ to ensure the validity of the binomial expansion. In practice, we have seen that setting β_2 equal to this quantity works well, provided we are using the Frobenius norm as our matrix norm function of choice.

Substituting the value of β_2 from Equation 10 in Equation 8 and ignoring the cubic and higher powers, gives us the complete left preconditioner update step:

$$\hat{L}_t = \left(\frac{\|X_L\|+1}{\|X_L\|} \right)^{\frac{1}{4}} \hat{L}_{t-1} \left(I_m - \frac{1}{4} \frac{X_L}{\|X_L\|} + \frac{5}{32} \frac{X_L^2}{\|X_L\|^2} \right) \tag{11}$$

The corresponding formulation of β_2' for the right preconditioners can be derived in a similar manner.

A.3 Jorge with grafting

In Section **??**, we mentioned adding grafting to Jorge, which adds a step in the weight update step of Algorithm 2. Grafting maintains the direction of the current step ($\frac{m_t}{\|m_t\|}$), but uses the magnitude of the step of a well-tuned optimizer ($\|m_{\text{SGD},t}\|$ in this case). In Algorithm 5 below, we see m_t becomes $\|m_{\text{SGD},t}\| \frac{m_t}{\|m_t\|}$.

Algorithm 5 Jorge's modified weight update rule with SGD grafting

Update Weights:
$m_t = \beta_1 m_{t-1} + (1-\beta_1)\hat{G}_t$ ▷ Jorge weight update
$m_{\text{SGD},t} = \beta_1 m_{\text{SGD},t-1} + G_t$ ▷ SGD (with heavy ball momentum) weight update

$\theta_t = \theta_t - \eta_t \|m_{\text{SGD},t}\| \frac{m_t}{\|m_t\|}$ ▷ Grafted weight update

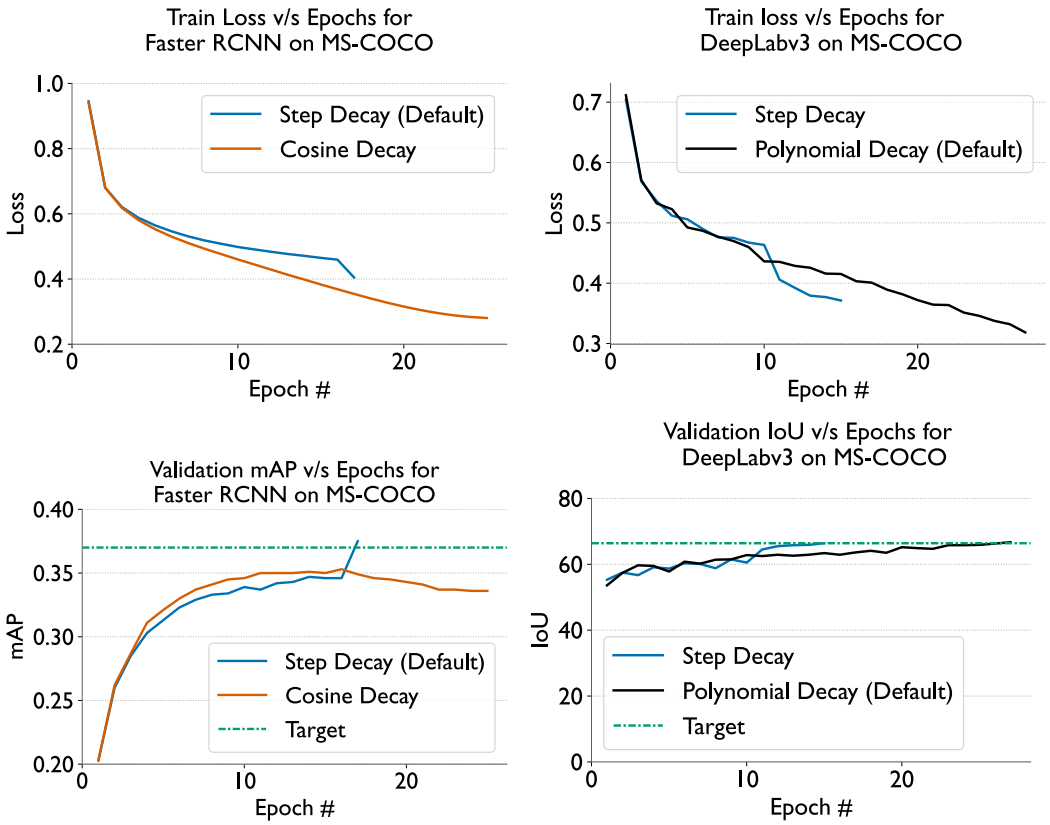


Figure 6: Comparison of different learning rate schedules with Jorge on two training tasks - Object Detection with Faster RCNN (**?**), and Image Segmentation with DeepLabv3 (**?**), both on the MS-COCO dataset (**?**). Both training tasks use a batch size of 64.

A.4 Intuition behind Jorge's weight decay heuristic

As mentioned in Section **??**, we created a simple heuristic for setting Jorge's weight decay. Let the parameters at time step t be θ_t. SGD will first calculate the weight decay update as $\lambda_{\text{SGD}}\theta_t$ and then update its running estimate of the momentum using the gradients from the loss and $\lambda_{\text{SGD}}\theta_t$. Since the weight decay is a part of the running momentum estimates, the weight decay calculated at time step t will influence the parameter updates at time step $t+\tau$, albeit attenuated by $\beta_{\text{SGD}}^{\tau}$. Therefore, the *effective* contribution of a weight decay update calculated at time step t is:

$$\sum_{\tau=0}^{T-t} \beta_{\text{SGD}}^{\tau} \lambda_{\text{SGD}} \theta_t \approx \frac{1}{1-\beta_{\text{SGD}}} \lambda_{\text{SGD}} \theta_t \tag{12}$$

Since we use a decoupled weight decay scheme for Jorge, the weight decay calculated at time step t does not contribute to future weight updates. Therefore, to match the effective contribution of the weight decay updates in SGD, we set the weight decay penalty for Jorge to $\frac{1}{1-\beta_{\text{SGD}}}\times$ that of SGD, as shown in Equation 9.

A.5 Experiments with learning rate schedules

Here we discuss the phenomenon of certain learning rate schedules leading to overfitting with Jorge, that we briefly alluded to in Section **??**. Figure 6 (left) demonstrates the training loss and validation mAP curves for Faster-RCNN on MS-COCO. Notice that while the cosine schedule never reaches the target validation mAP, this is not because it sufficiently fails to minimize the training loss. In-fact, it leads to a training loss significantly lower than the step decay schedule, thereby indicating overfitting.

Similarly, Figure 6 (right) demonstrates the training loss and validation IoUs for the image segmentation task with DeepLabv3. Here, the polynomial-scheduled Jorge must reach a lower training loss (loss of 0.32) than the stepwise-scheduled Jorge (0.37) to reach the same validation accuracy, once again symbolizing overfitting.

Our hypothesis for the phenomenon is that Jorge requires a high learning rate in the initial phases of training to escape sharp local minima. Due to its more accurate updates it is more prone towards falling into sharp minima compared to SGD, which might escape these because of its noisy updates. We plan to explore this phenomenon in more detail in future work.

A.6 List of Hyperparameters for Section 5

We list the hyperparameters used in this study for SGD, Jorge, and AdamW in Tables 5, 6, and 7 respectively. For Shampoo, we have used the same learning rate, weight decay and learning rate schedule as SGD, as per the recommendation of **?** and enabled SGD grafting.

Table 5: Hyperparameters used in this study for SGD. These are the defaults in torchvision.

Hyperparameter	Resnet-50 (batch size 1024)	ResNet-50 (batch size 256)	DeepLab-v3	Mask RCNN
Learning Rate	0.4	0.1	0.02	0.02
Weight Decay	$1e{-4}$	$1e{-4}$	$1e{-4}$	$1e{-4}$
Learning Rate Schedule	Linear warmup over 5 epochs. Then step decay at epochs 30 and 60	Step decay at epochs 30 and 60	Polynomial decay with 0.9 power	Step decay at epochs 16 and 22
Momentum	0.9	0.9	0.9	0.9
Nesterov	False	False	False	False

Table 6: Hyperparameters used in this study for Jorge.

Hyperparameter	Resnet-50 (batch size 1024)	ResNet-50 (batch size 256)	DeepLab-v3	Mask RCNN
Learning Rate	0.4	0.1	0.02	0.02
Weight Decay	$1e{-3}$	$1e{-3}$	$1e{-3}$	$1e{-3}$
Learning Rate Schedule	Linear warmup over 5 epochs. Then step decay at epochs 30 and 60	Step decay at epochs 30 and 60	Step decay at epochs 10 and 20	Step decay at epochs 8 and 16
Momentum	0.9	0.9	0.9	0.9
Preconditioner Update Freq.	50	2	4	8

A.7 Analysis of memory consumption

We mentioned in Section 6 that Jorge consumes $1.5 - 2\times$ the memory of Adam. This is because Adam uses 2 32-bit floating point optimizer states per parameter. In contrast, Jorge uses 3 (hence $1.5\times$), one each for the left preconditioner, right preconditioner, and momentum (see Algorithm 2). It becomes 4 once grafting is introduced (hence $2\times$), due to the fact that we now need to maintain the momentum for SGD as well. This is a major limitation of our method, and one which we plan to fix with a distributed implementation.

Table 7: Hyperparameters used in this study for AdamW.

Hyperparameter	Resnet-50 (batch size 1024)	ResNet-50 (batch size 256)	DeepLab-v3	Mask RCNN
Learning Rate	0.004	0.001	0.0002	0.0002
Weight Decay	0.1	0.1	$1e{-2}$	$1e{-2}$
Learning Rate Schedule	Cosine	Cosine	Cosine	Cosine
Momentum	0.9	0.9	0.9	0.9
βs	(0.9, 0.999)	(0.9, 0.999)	(0.9, 0.999)	(0.9, 0.999)
ϵ	$1e{-8}$	$1e{-8}$	$1e{-8}$	$1e{-8}$
amsgrad	False	False	False	False