Inefficiency of K-FAC for Large Batch Size Training

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Abstract—In stochastic optimization, large batch training can leverage parallel resources to produce faster wall-clock training times per epoch. However, for both training loss and testing error, recent results analyzing large batch Stochastic Gradient Descent (SGD) have found sharp diminishing returns beyond a certain critical batch size. In the hopes of addressing this, the Kronecker-Factored Approximate Curvature (K-FAC) method has been hypothesized to allow for greater scalability to large batch sizes for non-convex machine learning problems, as well as greater robustness to variation in hyperparameters. Here, we perform a detailed empirical analysis of these two hypotheses, evaluating performance in terms of both wall-clock time and aggregate computational cost. Our main results are twofold: first, we find that K-FAC does not exhibit improved large-batch scalability behavior, as compared to SGD; and second, we find that K-FAC, in addition to requiring more hyperparameters to tune, suffers from the same hyperparameter sensitivity patterns as SGD. We discuss extensive results using residual networks on CIFAR-10, as well as more general implications of our findings.

I. INTRODUCTION

As the boundaries of parallelism are pushed by modern hardware and distributed systems, researchers are increasingly turning their attention toward leveraging these advances for faster training of deep neural networks (DNNs). Under the prevailing method of Stochastic Gradient Descent (SGD), a batch of training data is split across computational processing units, which together compute a stochastic gradient used to update the parameters of the DNN.

To allow for efficient parallel scalability to a large number of processors, we need a large batch of training data [4]. However, using large batch size changes the dynamics of the training. It has been demonstrated both theoretically [14, 16] and empirically [6, 12, 17, 20, 22] that in many cases, training with large-batch SGD comes with significant drawbacks. This includes degraded testing performance, worse implicit regularization, and diminishing returns in terms of training loss reduction. Among other things, there exists a critical batch size beyond which these effects are most acute. For practitioners operating on a data-driven computational budget, large batch size comes with the additional inconvenience of increased sensitivity to hyperparameters and thus increased tuning time or cost [20]. In attempts to mitigate these shortcomings, a number of solutions have been proposed and demonstrated to varying degrees of effectiveness [5, 7, 11, 18, 19, 21, 23, 24].

An important practical consideration in methods such as [5, 7, 11, 18, 19, 21] is the sensitivity to hyperparameters. Generally, this sensitivity is very strong, and thus the required tuning process is expensive in terms of both analyst time and in-cycle training time. If performing large batch training requires significant hyperparameter tuning for each batch-size, then one would not achieve any effective speed up in total training time (i.e., hyperparameter tuning time plus final training time). With the exception of the recent work of [23], these discussions are largely ignored in the proposed solutions.

Recently, it has been suggested [2, 17, 20] that the approximate second-order method known as Kronecker-Factored Approximate Curvature (K-FAC) [15] may help to alleviate the issues of large-batch data inefficiency and generalization degradation exhibited by the first-order SGD method. K-FAC takes the novel approach of treating parameter space as a manifold of distribution space, in which distance between parameter vectors is measured by a variant of the Kullback-Leibler divergence between their corresponding distributions. In certain circumstances, K-FAC has been demonstrated to attain comparable effectiveness with large batch size as SGD [2, 19], but the effects of batch size on training under K-FAC remain largely unstudied.

In this work, we investigate these issues, evaluating the conjecture that K-FAC is capable of alleviating the difficulties of large-batch SGD. In particular, we focus on the following two questions regarding K-FAC and large batch training:

- What is the scalability behavior of K-FAC when the batch size increases, and how does it compare with that of SGD?
- How does increasing batch size affect the hyperparameter sensitivity of K-FAC?

To answer these questions, we conduct a comprehensive investigation in the context of image classification on CIFAR-10 [13], using a Residual Network (ResNet20) classifier [9]. We investigate the problem of large-batch diminishing returns by measuring iteration speedup and comparing it to an ideal scaling scenario. Our key observations are as follows:

- **Performance.** Even with extensive hyperparameter tuning, K-FAC has comparable, but not superior, train/test performance to SGD (Fig. 2).
- **Speedup.** Increasing batch size for K-FAC yields lower, i.e., less prominent, speedup, as compared with SGD, when measured in terms of iterations (Fig. 3 and Fig. 4).

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• Robustness. K-FAC hyperparameter sensitivity depends both on batch size and epochs/iterations. For fixed epochs, i.e., running for the same number of epochs, larger batch sizes result in greater hyperparameter sensitivity and smaller regions of hyperparameter space which result in "good convergence". For fixed iterations, i.e., running for the same number of iterations, larger batch sizes result in greater robustness and larger regions of hyperparameter space which result in "good convergence" (Fig. 5, Fig. 6).

We start with mathematical background and related work in Section II, followed by a description of our experimental setup in Section III. Our empirical results demonstrating the inefficiencies of K-FAC with large batch sizes appear in Section IV. Our conclusions are presented in Section V.

II. BACKGROUND AND RELATED WORK

For a supervised learning framework, the goal is to minimize a loss function \( L(\theta) \):
\[
L(\theta) = \frac{1}{N} \sum_{i=1}^{N} l(x_i, y_i, \theta),
\]
where \( \theta \in \mathbb{R}^d \) is the vector of model parameters, and \( l(x, y, \theta) \) is the loss for a datum \((x, y) \in (X, Y)\). Here, \( X \) is the input, \( Y \) is the corresponding label, and \( N = |X| \) is the cardinality of the training set. SGD is typically used to optimize Eqn. (1) by taking steps of the form:
\[
\theta_{t+1} = \theta_t - \eta_t \left( \frac{1}{B} \sum_{(x, y) \in B} \nabla l(x, y, \theta_t) \right),
\]
where \( B \) is a mini-batch of examples drawn randomly from \( X \times Y \), and \( \eta_t \) is the step size (learning rate) at iteration \( t \).

A. Kronecker-Factored Approximate Curvature

As opposed to SGD, which treats model parameter space as Euclidean, natural gradient descent methods [1] for DNN optimization operate in the space of distributions defined by the model, in which parameter distances between two vectors are defined using the KL-divergence between the two corresponding distributions. Denoting \( \tilde{D}_{KL} \) as our vector norm in this space, it can be shown that \( \tilde{D}_{KL}(\Delta \theta) \approx \frac{1}{2} \Delta \theta^\top F \Delta \theta \), where \( F \) is the Fisher Information Matrix (FIM) defined as:
\[
F = \text{E}[\nabla_\theta \log p(y|x, \theta) \nabla_\theta \log p(y|x, \theta)^\top],
\]
where the expectation is taken over both the model’s training data space and target variable space [15]. The update rule for natural gradient descent then becomes
\[
\theta_{t+1} = \theta_t - \eta_t F^{-1} \nabla_\theta \ell(\theta_t).
\]
As noted by [19] and others, the FIM is often poorly-conditioned for DNNs, leading to unstable training. To counter this effect, a damping term is often added (i.e. the FIM is preconditioned). Using the preconditioned FIM, the update rule then becomes:
\[
\theta_{t+1} = \theta_t - \eta_t (F + \lambda I)^{-1} \nabla_\theta \ell(\theta_t),
\]
with \( \lambda \) denoting a positive damping parameter.

Due to the computational intractability of the true Fisher matrix, natural gradient methods must necessarily rely on approximations to \( F \). [15] proposes an approximation, leveraging assumptions that, (i) \( F \) is largely block-diagonal\(^1\); and (ii) across the training distribution, the products of unit activations and products of unit output derivatives are statistically independent. While these assumptions are inexact, their accuracy is empirically verified by the authors in several cases. The approximation is written as:
\[
F_i = \text{E}[A_{i-1} A_{i-1}^\top \otimes G_i G_i^\top] \approx \text{E}[A_{i-1} A_{i-1}^\top] \otimes \text{E}[G_i G_i^\top],
\]
where \( F_i \) represents the Fisher matrix of \( i \)-th layer, \( G_i \) is the gradient of the loss with respect to the \( i \)-th layer output before non-linear activation function, and \( A_{i-1} \) is the activation output of the previous layer. Note that this is the approximation form we use in our implementation.

B. Difficulties of Large Batch Training

The problems of large batch training under SGD have been studied in detail through both analytical and empirical studies. [14] proves that for convex cases, increasing batch size by a factor \( f \) yields a no worse than a factor \( f \) speedup in the number of SGD iterations, so long as batch size is below a critical point. The batch sizes falling below this critical point that enjoy this property are referred to collectively as the linear scaling regime. [6] empirically investigates this in the context of non-convex training of DNNs for a variety of training workloads; and finds evidence of a similar critical batch size for the non-convex case, before which \( f \)-fold increases of batch size yield \( f \)-fold reductions in total iterations needed to converge, and after which diminishing returns are observed eventually leading to stagnation and no further benefit.

Subsequent to [6], [17, 20] obtain broadly similar conclusions with more detailed studies. In particular, [17] goes further to predict the critical batch size to the nearest order of magnitude, demonstrating that critical batch size can be predicted from the gradient noise scale representing the noise-to-signal ratio of the stochastic estimation of the gradient. The authors further find that gradient noise scale increases during the course of training. This principle motivates the success of techniques as in [3, 21, 23], in which batch size is adaptively increased during training.

Apart from increasing batch size during training, effort has been undertaken to increase critical batch size and linear scaling throughout the entire training process. [7] attempts to improve SGD scalability by tuning hyperparameters more carefully using a linear batch-size to learning-rate relationship. While this proves effective for the authors’ training setup, [6] demonstrates that for a wide variety of other training workloads a linear scaling rule is ineffective to counter inefficiencies of large batch.

[20] proposes that K-FAC may help to extend the linear scaling regime and critical batch size further than SGD, allowing for greater scalability with large batch. Recent work has shown K-FAC applied to large-batch training settings, as in [19] training ResNet50 on ImageNet within 35 epochs.

\(^1\)Although the K-FAC authors propose an alternative tridiagonal approximation that eases the strength of this assumption, we consider their block diagonal approximation of the Fisher due to its demonstrated performance.
along with the development of a large-batch parallelized K-FAC implementation [2]. Both provide discussion of this, and demonstrate “near-perfect” scaling behavior for large-batch K-FAC. [2] goes further in depth to suggest that K-FAC scalability is superior over SGD for high training losses and low batch sizes for a single training workload. Our work more formally investigates the scalability of K-FAC versus SGD, and finds evidence to the contrary; that is, for the workload and batch sizes we consider, K-FAC scalability is no better than that of SGD.

III. EXPERIMENTAL SETUP

We investigate the performances of both K-FAC and SGD on CIFAR-10 [13] with ResNet20 [9]. To be comparable with state-of-art results for K-FAC [25], we apply batch normalization to the ResNet model along with standard data augmentation during the training process. We further regularize with a weight decay parameter of $5 \times 10^{-4}$. We perform extensive hyperparameter tuning individually for each batch size ranging from 128 to 16,384.

A. Training Budget and Learning Rate Schedule

In many scenarios, training within a hyperparameter search is stopped at some fixed amount of time. When this time is specified in terms of number of epochs, we call this a (normal) epoch budget. For our training of K-FAC and SGD, we use a modified version of this stopping rule which we refer to as an adjusted epoch budget, in which the epoch limit of training is extended proportionally to the log of the batch size. Specifically, we use the rule: number of training epochs equals $(\log_2(\text{batch size}/128) + 1) \times 100$. This allows larger-batch training runs more of a chance to converge by affording them a greater number of iterations than would normally be allowed under a traditional epoch budget.

We decay the learning rate twice for each run over the course of training by a factor of ten. These two learning rate decays separate the training process into three stages. Because training extends to a greater number of epochs for large batches under the adjusted epoch budget, for large batch runs we allow a proportionally greater number of epochs to pass before learning rate decay. For each run we therefore decay the learning rate at 40% and 80% of the total epochs. We refer to this decay scheme as a scaled learning rate schedule. In Section IV-A, we empirically validate our reasoning that our scaled learning rate schedule (as opposed to a fixed learning rate schedule$^3$) helps large-batch performance.

B. Hyperparameter Tuning

K-FAC: For K-FAC, we use the various techniques discussed in [2, 19]. We precondition the Fisher matrix based on Eqn. (4) according to the methodology presented in [8, Appendix A.2]. Although [15] argues in favor of an alternative damping mechanism that approximates the damping of Eqn. (4), we observed comparable performance using the normal approach. The details of these two methods and our comparison between them are laid out in the Appendix.

For hyperparameter tuning, we conduct a log-space grid search over 64 configurations with learning rates ranging from $10^{-3}$ to 2.187, and damping ranging from $10^{-3}$ to 0.2187. The decay rate for second-order statistics is held constant at 0.9 throughout training. We use update clipping as in [2], with a constant parameter of 0.1.

SGD: To ensure a fair comparison between methods, we employ a similarly extensive hyperparameter tuning process for SGD. We conduct a similar log-space grid search over 64 hyperparameter configurations, with learning rate ranging from 0.05 to 9.62, and momentum ranging from 0.9 to 0.999.

C. Speedup Ratio

We use speedup ratio [6] to measure the efficiency of large batch training based on iterations. We define the convergence rate $k_c(m)$ as the fewest number of iterations to reach a certain criteria $c$ under the batch size $m$, where $c$ is defined as attaining a target accuracy or loss threshold. $k_c(m)$ is a minimum as it is picked across all configurations of hyperparameters. We then define the speedup ratio $s_c(m; m_0)$ as $k_c(m_0)/k_c(m)$, in which we rely on some small batch size $m_0$ as our reference for convergence rate when comparing to larger batch sizes $m > m_0$. In an ideal scenario, the batch size has no effect on the performance increase per training observation, so in such cases $s_c(m; m_0) = m/m_0$.

It should be noted that for K-FAC speedup we solely measure the number of iterations and ignore the cost of computing the inversion of the Fisher matrix. The latter can actually become very expensive, and multiple approaches such as stochastic low-rank approximation and/or inexact iterative solves can be used. However, as we will show, K-FAC speedup is far from ideal even when ignoring this cost.

IV. EXPERIMENTAL RESULTS

We perform extensive experiments using ResNet20 on the CIFAR-10 dataset with both K-FAC and SGD. Section IV-A compares training trajectories under fixed and scaled learning rate schedules to provide validation of our experimental setup. Section IV-B compares the training and test performances of K-FAC and SGD resulting from extensive hyperparameter tuning for each batch size. Section IV-C discusses the large-batch scaling behaviors of K-FAC and SGD and compares them to the ideal scaling scenario [6, 20]. Finally, Section IV-D investigates the hyperparameter robustness of the K-FAC method.

A. Scaled Learning Rate Decay Schedule

We first evaluate the scaled learning rate schedule discussed in Section III against a fixed learning rate schedule. Extensive grid search is applied for both schedules, giving rise to best-performing runs which are illustrated in Fig. 1.
In Fig. 1a and 1c, we plot the highest-accuracy and lowest-loss training runs (chosen across the all hyperparameter configurations) for fixed learning rate schedule versus scaled learning rate schedule for SGD. Across all batch sizes, scaled learning rate schedule training gives rise to a higher final test accuracy and lower final training loss. For large batch sizes (e.g. 16K), the difference is more pronounced, with fixed learning rate schedule SGD making much slower progress than the scaled learning rate schedule counterpart. In particular, for the 16K batch size with fixed learning rate schedule, after 80 epochs it can be observed that the early decay severely slows the previously-rapid progress since the learning rate becomes too small. As a result the fixed-scaling large batch SGD slows its climb in accuracy while the scaled learning rate schedule variant surges ahead.

In Fig. 1b and 1d, we plot the analogous runs for K-FAC with decays following a fixed versus scaled learning rate schedule. Similarly, scaled learning rate schedule K-FAC demonstrates higher end-of-training accuracy and lower loss across all batch sizes. Based on these observations, we argue that our experimental setup is geared towards boosting large-batch scalability through its use of a scaled schedule for learning rate decay.

B. Comparing Best Performance of K-FAC and SGD

We run K-FAC and SGD for multiple batch sizes, with stopping conditions according to the adjusted epoch budget and scaled learning rate schedule mentioned in the previous section. The highest test accuracy and the lowest training loss achieved for each batch size are plotted in Fig. 2. Note that a separate hyperparameter selection criteria was used for the two plots, either for maximizing accuracy or minimizing training loss.
loss. We include the detailed training trajectories over time for both SGD and K-FAC in Appendix A.

In this training context, K-FAC minimizes training loss most effectively for medium-sized batches (from $2^8$ to $2^{12}$). Inspecting the training trajectories, we found that both the smallest ($2^7$) and largest batch sizes ($2^{13}$ and $2^{14}$) needed more epochs/iterations to converge. For example, from Fig. 1, the scaled learning rate schedule curve of batch size $2^{14}$ (16K) is still on an upwards trajectory when the training is terminated.

For SGD however, training loss is minimized prominently at larger batch sizes. When comparing training trajectories with K-FAC, we found that SGD made much more progress per-iteration in reducing loss, allowing it to minimize the objective with a smaller number of updates, as shown in Fig. 2. A more detailed comparison of the per-iteration progress of SGD versus K-FAC can be found in the following section.

The gap between SGD and K-FAC in large-batch training loss is also present in their generalization performance. Whereas large-batch K-FAC is terminated by the adjusted epoch budget before reaching a high accuracy, SGD’s greater efficiency in maximizing per-iteration accuracy allows it to attain a higher level of test performance with the same number of training epochs.

C. Large-Batch Scalability of K-FAC and SGD

Training efficiency was measured for each batch size in terms of iterations to a target training loss or test accuracy ($k_c(m)$). The results are displayed in Fig. 3. Dotted lines denote the ideal scaling relationship between batch size and iterations.

To ensure a fair comparison between batch sizes, similar to what is done in [6], we select target loss values as follows:

- We wish to analyze how fast different batch sizes reach a threshold, but not all thresholds are feasible, since large batch sizes may never reach a low training loss, whereas small batches may reach it easily (see Fig. 1). For speed up comparison purposes, we set a threshold such that all the batch sizes can reach it. We choose a selected run that belongs to the worst-performing batch size and method. This selection is made after loss-based hyperparameter tuning is finished for each batch size.
- Now, for each of the three training stages of the selected run$, we generate a training loss target, using the value that is linearly interpolated at 80% between the loss value directly before and directly after the training stage.

An analogous process is used to select target accuracy values. We use the resulting target values in Fig. 3 and 4.

For both K-FAC and SGD, diminishing return effects are present. In all examined cases, K-FAC deviates from ideal scaling (dotted lines) to a greater extent than SGD as batch

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The per-iteration training trajectories supporting Fig. 3 gives evidence contrary to the conjectures of [20], which posits that K-FAC may exhibit a larger regime of perfect scaling than SGD. The speedup of SGD is closer to the ideal line than that of K-FAC, suggesting that K-FAC has no better scalability than SGD. This gives evidence contrary to the conjectures of [20], which posits that K-FAC may exhibit a larger regime of perfect scaling than SGD. The per-iteration training trajectories supporting Fig. 3 and 4 can be observed in Appendix A.

For all three target losses and accuracies, note that the two methods across target losses and target test accuracies, where m is a given batch size.

The relationship demonstrates that the linear scaling regime is largely nonexistent, particularly for the high-performance targets noted in green; diminishing returns begin immediately from the smallest batch size.

Notice that the large-batch scalability behavior is captured in the slope of each line in Fig. 3. To better visualize scaling behavior across methods and target values for training loss, we normalize each method-target line independently, dividing by the iterations at the smallest batch size k(2^7) so that each of the dotted ideal lines is aligned in the plots, and take the reciprocal to obtain the speedup function s(m; 2^7) = k(2^7)/k(m), where m is a given batch size.

Figure 4 displays the resulting speedup curves for the two methods across target losses and target test accuracies, allowing us to compare speedup behavior with the same ideal scaling. For all three target losses and accuracies, note that the speedup of SGD is closer to ideal line than that of K-FAC, suggesting that K-FAC has no better scalability than SGD. This gives evidence contrary to the conjectures of [20], which posits that K-FAC may exhibit a larger regime of perfect scaling than SGD. The per-iteration training trajectories supporting Fig. 3 and 4 can be observed in Appendix A.

D. Hyperparameter Robustness of K-FAC

The hyperparameter tuning space for K-FAC is laid out in Fig. 5, which relates the selected hyperparameters for damping and learning rate with test accuracy achieved under the adjusted epoch budget. All heatmaps we observe (including those not plotted) demonstrate a consistent trend in terms of:

• A positive correlation between damping and learning rate.
• A shrinking of the high-accuracy region with increasing batch size.

The second point suggests a relationship between batch size and hyperparameter sensitivity for K-FAC, which can be measured in terms of the volume of hyperparameter space corresponding to successful training. In evaluating hyperparameter sensitivity (or inversely robustness), we take the approach of [20], distinguishing between two types of robustness, each corresponding to a different definition of “successful training”:

• Epoch-based robustness, in which success is defined by training to a desired accuracy or loss within a fixed number of epochs.
• Iteration-based robustness, in which success is defined by training to a desired accuracy or loss within a fixed number of iterations.

It is important to note that a set of hyperparameters considered to be acceptable to a practitioner under an iteration budget may at the same time be considered unacceptable to a practitioner operating under an epoch budget. It is for this reason that we make this distinction.

Through this lens, the robustness behavior of K-FAC is exhibited in Fig. 6. Distributions of training accuracy across hyperparameters are represented by box plots composed from the 64 hyperparameter configurations (8 damping parameters, 8 learning rate parameters). In Fig. 6a and 6d, we show the distributions of test accuracies and training losses for each batch size at the end of training under the adjusted epoch budget. The greater spread of accuracies observed for larger batch sizes indicates that given this budget we should consider batch sizes from 2^{12} to 2^{14} as more sensitive to hyperparameter tuning than batch sizes from 2^8 to 2^{11}. Intuitively, if we draw a horizontal line at a desired test accuracy of e.g. 0.8, the batch sizes with box plots containing the majority of their hyperparameter distribution above the 0.8 line should be favored as more robust.

We can simulate stopping of training in terms of epochs and iterations to extract insight about robustness for other types of budgets than our own. Regardless of the stopping criteria, we expect that longer training will yield greater robustness (although at the cost of significantly higher computational/budget overhead).

Figure 6b and 6e show how the hyperparameter robustness of different batch sizes changes as a function of stopping epoch. Each group along the X-axis corresponds to a hypothetical epoch budget. The relationship demonstrates that for K-FAC, robustness increases with amount of training, but more interestingly decreases with batch size. This can be observed by noting that for any fixed epoch, the distributions
of accuracies corresponding to larger batch sizes fall lower than their smaller-batch counterparts, meaning fewer hyperparameter configurations will fall above a desired accuracy threshold. A similar robustness trend is observed with the distributions of training losses.

We perform a similar analysis for iteration budgets in Fig. 6c and 6f, and find as expected that robustness increases with training. Unlike the case of an epoch budget however, we find that for iteration budgets robustness increases with larger batch size. This is observed by noting that the distributions corresponding to large batch are more concentrated towards higher accuracy and lower loss, although the effect is not as pronounced as in the fixed epoch case.

Together, the results show that (i): epoch-based robustness is inversely related to batch size, and (ii): iteration-based robustness is directly related to batch size, analogous to the findings of [20] for SGD. Further work may seek to compare the nature of iteration-based or epoch-based robustness between the two methods in more detail.

V. CONCLUSIONS

Through extensive experimentation and training of ResNet20 on the CIFAR-10 dataset, we find that K-FAC exhibits similar diminishing returns with large batch training as SGD. In our results, K-FAC has comparable but not better training or testing performance than SGD given the same level of training and tuning. Comparing the scalability behaviors of the two methods, we find that K-FAC exhibits a smaller regime of ideal scaling than SGD, suggesting that K-FAC’s scalability to large batch training is no better than SGD’s. Finally, we find that K-FAC exhibits a similar relationship between budget and robustness as SGD, in which K-FAC is less robust to tuning under epoch budgets, but more robust to tuning under iteration budgets, mirroring the findings of similar work in literature for SGD [20]. Taken as a whole, our results suggest that, although K-FAC has been applied to large batch training scenarios, it encounters the same large-batch issues to an equal or greater extent as SGD.

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Fig. 6: (a)(d): Accuracy / training loss distribution vs. batch size for K-FAC at the end of training under an adjusted epoch budget. Larger batch sizes result in lower accuracies and higher training losses that are more sensitive to hyperparameter choice. (b)(e): Comparison of accuracy / training loss distributions over various epochs. Smaller batch sizes provide better solutions that are less sensitive to choice of hyperparameters. (c)(f): Comparison of accuracy / training loss distributions over various iteration numbers. Large batch sizes exhibit a trend of providing better solutions that are less sensitive to choice of hyperparameters.

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A. Detailed Training Curves and Heatmaps

In this section we show the detailed Training Curves for K-FAC and SGD, and the detailed accuracy heatmaps for K-FAC. We plot the training loss and test accuracy over time for the optimal runs of each batch size for both SGD and K-FAC to support Fig. 2, 3 and 4 in the main text. Time is measured in terms of both epochs (Fig. 7) and iterations (Fig. 8).

The best performance of each curve in Fig. 7 helps to explain the shape of Fig. 2, in which we plot the best test accuracy and training loss for each batch size for SGD and K-FAC. Best achieved accuracy can be seen to drop for both K-FAC and SGD beyond a certain batch size. Lowest loss is achieved at higher batch sizes for SGD than for K-FAC.

Figure 8 gives clues regarding the large-batch training speedup of both K-FAC and SGD. We can see from the figure that as batch size grows, fewer iterations are necessary to reach specific performance targets, represented by horizontal dotted lines. In the ideal scaling case, the intersections of training loss curves for each batch size would fall along the dotted target lines in the pattern of a geometric sequence with common ratio $1/2$. Iterations-to-target for each batch size are plotted directly in Fig. 3, and speedup ratios are plotted in Fig. 4.

Figure 9 displays the complete accuracy heatmaps over hyperparameter space. For each hyperparameter configuration, training was run until terminated according to the adjusted epoch budget.

Fig. 7: (a)(c): Test accuracy vs. epoch for the accuracy-maximizing runs of each batch-size, with K-FAC above and SGD below. (b)(d): Training loss vs. epoch for the loss-minimizing runs of each batch-size, with K-FAC above and SGD below. For each plot, the star denotes the best (maximal accuracy or minimal loss) performance achieved. Horizontal dotted lines show the target values for accuracy and loss used in Fig. 3 and 4.
Fig. 8: (a)(c): Test accuracy vs. iteration for the accuracy-maximizing runs of each batch-size, with K-FAC above and SGD below. (b)(d): Training loss vs. iteration for the accuracy-maximizing runs of each batch-size, with K-FAC above and SGD below. For each plot, the star denotes the best performance achieved. Horizontal dotted lines show the target values for accuracy and loss used in Fig. 3 and 4.
Fig. 9: Best accuracy achieved under adjusted epoch budget vs. damping and learning rate for batch sizes from 128 to 16,384 with normal damping. A positive correlation between damping and learning rate is exhibited. When the batch size exceeds 4,096, we observe a shrinking of the high-accuracy region for large batch sizes.
B. Normal vs. Approximated Damping

In this section we explain the differences between two preconditioning mechanisms for K-FAC: normal damping as written in Eqn. (4), and approximated damping as recommended by [15]. We also provide an empirical evaluation of the two methods, and observe that approximate damping exhibits hyperparameter sensitivity that is comparable to normal damping. First we briefly discuss how to directly calculate the inverse of the preconditioned Fisher Information Matrix (preconditioned FIM), denoted \((F + \lambda I)^{-1}\). The preconditioned FIM block can be calculated as

\[
(F_i + \lambda I)^{-1} = \left[ (Q_A D_A Q_A^\top) \otimes (Q_G D_G Q_G^\top) + \lambda I \right]^{-1}
\]

\[
= \left[ (Q_A \otimes Q_G)(D_A \otimes D_G + \lambda I)(Q_A \otimes Q_G)^{-1} \right]
\]

\[
= (Q_A^\top \otimes Q_G^\top)(D_A \otimes D_G + \lambda I)^{-1}(Q_A \otimes Q_G),
\]

where \(Q_A D_A Q_A^\top\) is the eigendecomposition of \(E[A_i^{-1} A_i^{-1\top}]\) and \(Q_G D_G Q_G^\top\) is the eigendecomposition for \(E[G_i G_i^\top]\). A similar derivation can be found in Appendix A.2 in [8]. In our paper we call the use of this damping normal damping.

For efficiency reasons, [15] proposes an alternative calculation to alleviate the burden of eigendecomposition by preconditioning on the Kronecker-factored Fisher blocks first:

\[
(F_i + \lambda I)^{-1} \approx \left[ (E[A_i^{-1}] + \sqrt{\lambda} I) \otimes (E[G_i^2] + \sqrt{\lambda} I) \right]^{-1},
\]

where \(\lambda\) is a compound term that allows for complicated maneuvers of adaptive regularization (detailed in Section 6.2 [15]). We call this damping formulation approximated damping.

We compare normal damping and approximated damping for K-FAC, examining their effects for batch sizes 128 and 8,192. In Fig. 10 we compare the accuracy and training loss distributions of normal damping and approximated damping for batch sizes 128 and 8,192. For both damping methods, training appears to be more sensitive to hyperparameter tuning under large batch (batch size 8,192). More interestingly, we observe that the distributions generated with normal damping tend to be more robust. We can see, for instance, that for batch size 8,192, approximated damping has a high concentration of hyperparameter configurations yielding favorable values of loss and accuracy.

![Fig. 10: (a): Accuracy distribution vs. batch size for both normal damping and approximated damping. (b): Training loss distribution vs. batch size for both normal damping and approximated damping. All distributions are formed over the 64 runs of the hyperparameter grid search over damping and learning rate.](image-url)