ADAHESSIAN: An Adaptive Second Order Optimizer for Machine Learning

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Abstract—We introduce ADAHESSIAN, a second order stochastic optimization algorithm which dynamically incorporates the curvature of the loss function via ADaptive estimates of the HESSIAN. Second order algorithms are among the most powerful optimization algorithms with superior convergence properties as compared to first order methods such as SGD and Adam. The main disadvantage of traditional second order methods is their heavier per-iteration computation and poor accuracy as compared to first order methods. To address these, we incorporate several novel approaches in ADAHESSIAN, including: (i) a new variance reduction estimate of the Hessian diagonal with low computational overhead; (ii) a root-mean-square exponential moving average to smooth out variations of the Hessian diagonal across different iterations; and (iii) a block diagonal averaging to reduce the variance of Hessian diagonal elements. We show that ADAHESSIAN achieves new state-of-the-art results by a large margin as compared to other adaptive optimization methods, including variants of Adam. In particular, we perform extensive tests on CV, NLP, and recommendation system tasks and find that ADAHESSIAN: (i) achieves 1.80%/1.45% higher accuracy on ResNets20/32 on Cifar10, and 5.55% higher accuracy on ImageNet as compared to Adam; (ii) outperforms AdamW for transformers by 0.27/0.33 BLEU score on IWSLT14/WMT14 and 1.8/1.0 PPL on PTB/Wikitext-103; and (iii) achieves 0.032% better score than Adagrad for DLRM on the Criteo Ad Kaggle dataset. Importantly, one may not observe the above problems for certain popular learning tasks, such as ResNet50 training on ImageNet. The reason is that, for these tasks, years of industrial scale hyperparameter tuning has lead to ideal SGD behaviour. That is, for this problem, hyperparameters have been brute-force engineered to compensate for the deficiencies of first order methods. Such a brute force approach is computationally and financially not possible for many large scale learning problems—certainly it is not possible to do routinely—and this has made it challenging to train and apply NN models reliably.

I. INTRODUCTION

The high dimensional and non-convex nature of many machine learning tasks has rendered many classical optimization methods inefficient for training and/or evaluating Neural Network (NN) models. Despite decades of research, first order methods, and in particular variants of Stochastic Gradient Descent (SGD), have become the main workhorse for training NN models. However, they are by no means an ideal solution for training NN models. There are often a lot of ad-hoc rules that need to be followed very precisely to converge (hopefully) to a point with good generalization properties. Even the choice of the first order optimizer has become an ad-hoc rule which can significantly affect the performance. For example, SGD with momentum is typically used in Computer Vision (CV); Adam is used for training transformer models for Natural Language Processing (NLP); and Adagrad is used for Recommendation Systems (RecSys). Using the wrong SGD variant can lead to significant performance degradation. Another challenging ad-hoc rule is the choice of hyperparameters and hyperparameter tuning methods, even after an optimizer is chosen. Hyperparameters include learning rate, decay schedule, choice of momentum parameters, number of warmup iterations, etc. As a result of these and other issues, one has to babysit the optimizer to make sure that training converges to an acceptable training loss, without any guarantee that a given number of iterations is enough to reach a local minima.

Importantly, one may not observe the above problems for certain popular learning tasks, such as ResNet50 training on ImageNet. The reason is that, for these tasks, years of industrial scale hyperparameter tuning has lead to ideal SGD behaviour. That is, for this problem, hyperparameters have been brute-force engineered to compensate for the deficiencies of first order methods. Such a brute force approach is computationally and financially not possible for many large scale learning problems—certainly it is not possible to do routinely—and this has made it challenging to train and apply NN models reliably.

Many of these issues stem from the fact that first order methods only use gradient information and do not consider the curvature properties of the loss landscape, thereby leading to their suboptimal behaviour. Second order methods, on the other hand, are specifically designed

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to capture and exploit the curvature of the loss landscape and to incorporate both gradient and Hessian information. They are among the most powerful optimization algorithms, and they have many favorable properties such as resiliency to ill-conditioned loss landscapes, invariance to parameter scaling, and robustness to hyperparameter tuning. The main idea underlying second order methods involves preconditioning the gradient vector before using it for weight update. This has a very intuitive motivation related to the curvature of the loss landscape. For a general problem, different parameter dimensions exhibit different curvature properties. For example, the loss could be very flat in one dimension and very sharp in another. As a result, the step size taken by the optimizer should be different for these dimensions, and we would prefer to take bigger steps for the flatter directions and relatively smaller steps for the sharper directions. This can be illustrated with a simple 2D quadratic function as shown in Figure 1, where we show the trajectories of different optimizers. As can be seen, first order methods need a large number of steps for convergence and/or are hard to converge at all without hyperparameter tuning. However, second order methods capture this curvature difference, by normalizing different dimensions through rotation and scaling of the gradient vector before the weight update. Nonetheless, this comes at a cost. Despite the theoretically faster convergence rate of second order methods, they are rarely used for training NN models. This is due in part to their high computational cost.

In this paper, however, we will show that it is possible to approximately compute an exponential moving average of the Hessian and use it to precondition the gradient adaptively. The result is ADAHESSIAN, an adaptive optimizer that exceeds the state-of-the-art performance for a wide range of learning problems, including ResNets [22] for CV, transformers [37] for NLP problems, and DLRM [34] models for RecSys tasks. In more detail, the main contributions of our work are the following.

1) To reduce the overhead of second order methods, we approximate the Hessian as a diagonal operator. This is achieved by applying Hutchinson’s method to approximate the diagonal of the Hessian. Importantly, this approximation allows us to efficiently apply a root-mean-square exponential moving average to smooth out “rugged” loss surfaces. The advantage of this approach is that it has $O(d)$ memory complexity.

2) We incorporate a block diagonal averaging to reduce the variance of Hessian diagonal elements. In particular, this has no additional computational overhead in the Hutchinson’s method, but it favorably affects the performance of the optimizer.

3) To reduce ADAHESSIAN overhead, we measure the sensitivity of ADAHESSIAN to different hyperparameters such as learning rate, block diagonal averaging size, and delayed Hessian computation. Interestingly, our results show that ADAHESSIAN is robust to those hyperparameters. See Section V-A and V-B.

4) We extensively test ADAHESSIAN on a wide range of learning tasks. In all tests, ADAHESSIAN significantly outperforms other adaptive optimization methods. Importantly note that these results are achieved even though we use the same learning rate schedule, weight decay, warmup schedule, dropout, as well as first/second order moment coefficients. In particular, we consider the following tasks.

a) **Computer Vision:** ADAHESSIAN achieves significantly higher accuracy, as compared to Adam. For instance, for ResNet32 on Cifar10, ADAHESSIAN achieves 93.08% as opposed to 91.63% achieved by Adam. Furthermore, for ResNet18 on ImageNet, ADAHESSIAN achieves 70.08% accuracy as opposed to 64.53% of Adam. For all tests, ADAHESSIAN achieves similar performance to the ideal SGD behavior, which is a result of hyperparameters having been tuned for many years at the industrial scale. Comparison with other optimizers and other models is discussed in Section IV-B.

b) **Natural Language Processing:** ADAHESSIAN improves the performances of transformers for machine translation and language modeling tasks as compared to AdamW. In particular, ADAHESSIAN significantly outperforms AdamW by 0.27/0.33 BLEU on IWSLT14/WMT14, and by 1.8/1.0 PPL on PTB/WikiText-103. See Section IV-C and IV-D for more details.

c) **Recommendation Systems:** ADAHESSIAN improves the performance of DLRM on the Criteo Ad Kaggle dataset by 0.032% as compared to AdamGrad, which is commonly used. See Section IV-E for more details.

II. PROBLEM FORMULATION AND RELATED WORK

We focus on supervised learning tasks where the goal is to solve a non-convex stochastic optimization problem of the form:

$$
\min_{\theta} \mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} l_i(x_i, y_i; \theta),
$$

(1)
where \( \theta \in \mathbb{R}^d \) denotes the model parameters, \( l_i(x_i, y_i; \theta) \) is the loss function, \((x_i, y_i)\) is the paired input data and its corresponding ground truth label, and \( N \) is the total number of data points in the training dataset. Furthermore, we denote the gradient of the loss w.r.t. model parameters as \( \mathbf{g} = \frac{1}{N_B} \sum_{i=1}^{N_B} \frac{\partial l_i}{\partial \theta} \), and the corresponding second derivative (i.e., Hessian) as \( \mathbf{H} = \frac{1}{N_B} \sum_{i=1}^{N_B} \frac{\partial^2 l_i}{\partial \theta \partial \theta} \), where \( N_B \) is the size of one mini-batch.

Solving Eq. 1 for a real learning problem (and not a simple model) is a very challenging task. Despite years of research, we have not yet been able to resolve several seemingly ad-hoc tricks that are required to converge (hopefully) to a good solution. Next, we briefly discuss the different popular optimization methods proposed in recent years to address the challenges associated with solving Eq. 1. This is by no means a comprehensive review, and we refer the interested reader to [7] for a thorough review.

### A. Adaptive First Order Methods

Due to their simplicity and effectiveness, first order optimization methods [18, 24, 28, 35, 41, 61] have become the de-facto algorithms used in deep learning. There are multiple variations, but these methods can be represented using the following general update formula:

\[
\theta_{t+1} = \theta_t - \eta_t m_t / v_t,
\]

where \( \eta_t \) is the learning rate, and \( m_t \), and \( v_t \) denote the so called first and second moment terms, respectively. A simple and popular update method is SGD, originally proposed in 1951 as a root-solving algorithm [41]:

\[
m_t = \beta m_{t-1} + (1 - \beta)g_t \quad \text{and} \quad v_t = 1.
\]

Here, \( g_t \) is the gradient of a mini-batch at \( t \)-th iteration and \( \beta \) is the momentum hyperparameter.

Using SGD to solve Eq. 1 is often very challenging, as the convergence of the iterative formulae in Eq. 2 is very sensitive to the right choice of the learning rate, its decay schedule, and the momentum parameter. To address this, several methods have been proposed to take into account the knowledge of the geometry of the data by scaling gradient coordinates, using the past gradient information. This can be viewed in one of two equivalent ways: either as automatically adjusting the learning rate in Eq. 2; or as an adaptive preconditioning of the gradient. One notable method is Adagrad [18, 31], which accumulates all the gradients from the first iteration and applies the square root of the result to precondition the current gradient.

The update formulae in this case become:

\[
m_t = g_t \quad \text{and} \quad v_t = \sqrt{\sum_{i=1}^{t} g_i^2}.
\]

While Adagrad works well for sparse settings, its performance significantly degrades for dense settings, which is the case for many machine learning tasks. In particular, this stems from the accumulation of all previous gradients for the preconditioner Eq. 4. This results in a monotonic increase in the magnitude of the second moment, \( v_t \), which effectively translates into a rapid decay of the learning rate. To address this, several methods have been proposed where the intuition is to limit the accumulation to a small window of past iterations, and in particular exponentially reduce the weight of earlier iterations. Notable works incorporating this method are RMSProp, ADADelta, and Adam [24, 48, 61]. In

\(^1\)Throughout the paper, without further notification, for two vectors, e.g., \( a \) and \( b \), we use both \( ab \) and \( a \odot b \) to denote the element-wise product, and \( \langle a, b \rangle \) denotes the inner product.
AdamW has the best performance by a large margin as AdamW has become the preferred optimizer for NLP. Weight decay from the update equation of Adam can sometimes refer to as first and second moment coefficients. In particular, note that the sum over past gradients is scaled by $\beta_2$ which exponentially reduces the contribution of early gradients. A notable variant here is AdamW [28], which shows that decoupling weight decay from the update equation of Adam can lead to a noticeable performance improvement. Recently, AdamW has become the preferred optimizer for NLP tasks, and in particular for training transformers [49]. There are also many other variants of adaptive first order methods [11, 27, 46, 47, 63].

Despite all these attempts, it is still not clear which optimizer should work for a new learning task/model. This is in fact one of the main baffling practical issues in machine learning, and one for which theory has little to say. For example, SGD is currently the best performing optimizer for some CV tasks. That is, using other variants such as AdamW leads to significantly worse generalization performance. However, for NLP tasks, AdamW has the best performance by a large margin as compared to SGD. The point here is that even the choice of the optimizer has effectively become a hyperparameter.

### B. Second Order Methods

Second order methods are among the most powerful optimization methods that have been designed, and there have been several attempts to use their many advantages for training NNs. Second order methods are designed to address ill-conditioned optimization problems by automatically rotating and rescaling gradient. This allows one to choose a better descent direction, and automatically adjust the learning rate for each parameter. There have also been multiple theoretical studies showing better convergence rate of second order based methods [2, 3, 5, 10, 12, 13, 42, 52–54, 56, 60]. In particular, second order methods can guarantee convergence to second order critical points, while the vast majority of first order methods lack such guarantees. For example, theoretically it has been shown that some first order methods can only converge to an approximate second order critical point [19, 23, 26, 40].

Newton’s method is a classical second order method where one solves a linear system, essentially meaning that the inverse of the local Hessian is used at every iteration to precondition the gradient vector. One major challenge with this approach is that it can be expensive to solve the linear system, naively requiring cubic computational complexity, not including the cost of forming the Hessian itself and the corresponding quadratic memory complexity. However, the overhead of such a naive implementation can be improved by using so-called matrix free methods, where the Hessian matrix is never explicitly formed (addressing quadratic memory cost), and its inverse is approximately and only implicitly applied (addressing the cubic computational complexity).

One seminal work here is the limited memory BFGS (LBFGS) [9] method which has a desirable linear computational and memory complexity. This approach approximates the Hessian as a series sum of first order information from prior iterations. As such, these approaches that do not directly use the Hessian operator are referred to as Quasi-Newton methods. While this approach works well for many optimization problems, it does not work well for many machine learning problems. One reason for this is that LBFGS method requires full batch gradients, as stochastic gradients can lead to drastic errors in the approximation [6]. This is one of the main challenges with Quasi-Newton methods applied to ML problems. Other approaches such as approximating the Hessian as the Kronecker product of vectors has also been explored [30].

There has also been work on enhancing first order methods by incorporating the Fisher information matrix [20]. The main idea is to use the Fisher information instead of the squared norm of the gradient. A naive use of Fisher information has computational and memory overhead, but it is possible to also approximate the Fisher information matrix using low rank decomposition [20].

Another line of work has been to directly incorporate the Hessian operator itself, instead of approximating it using first order information. A seminal work here is [45] which uses Gauss-Newton Hessian diagonal to adaptively adjust the learning rate. The work of [53] also directly incorporates the Hessian using a trust region method.

While the above approaches are very interesting and result in a good performance for simple models, they do not achieve comparable results for more complex...
Table I: Summary of the first and second moment used in different optimization algorithms to update parameters \((\theta_{t+1} = \theta_t - \eta_t m_t / v_t)\).

| Optimizer   | \(m_t\)                                      | \(v_t\)                                      |
|-------------|----------------------------------------------|----------------------------------------------|
| SGD [41]    | \(\beta m_{t-1} + (1 - \beta)g_t\)          | 1                                            |
| Adagrad [18]| \(g_t\)                                      | \(\sqrt{\sum_{i=1}^{t-1} g_r g_t}\)          |
| Adam [24]   | \((1 - \beta_1) \sum_{i=1}^{t} \beta_1^{i-1} g_t\) | \(\sqrt{(1 - \beta_2) \sum_{i=1}^{t} \beta_2^{i-1} g_r g_t}\) |
| RMSProp [48]| \(g_t\)                                      | \(\sqrt{v_{t-1}^2 + (1 - \beta)g_r g_t}\)    |
| ADAHESSIAN  | \((1 - \beta_1) \sum_{i=1}^{t} \beta_1^{i-1} g_t\) | \(\sqrt{(1 - \beta_2) \sum_{i=1}^{t} \beta_2^{i-1} D_r D_t}\) |

NN architectures. One of the reasons that second order methods have not been successful yet for machine learning, as opposed to other domains such as scientific computing, is due to the stochastic nature of the problem. Such stochastic noise leads to an erroneous approximation of the Hessian, leading to suboptimal descent directions. SGD is more robust to such noise since we can efficiently incorporate moving averages and momentum. Ideally, if there was a way to apply the same moving average method to the Hessian, then that would help smooth out local curvature noise to get a better approximation to the non-noisy curvature of the loss landscape. However, such an approximation is challenging since the Hessian is a matrix that cannot be explicitly formed to be averaged, whereas it is easy to form the gradient vector.

As we show below, ADAHESSIAN addresses this problem by incorporating the Hutchinson’s method along with spatial averaging to reduce the impact of the stochastic noise. The result exceeds the performance of all the above methods for machine learning tasks. Next, we formally introduce the ADAHESSIAN algorithm.

### III. Methodology

Here, we first derive a general Hessian based descent direction. Afterwards, we discuss how one could efficiently approximate the Hessian operator instead of using full Hessian which is computationally infeasible. Finally, we introduce ADAHESSIAN algorithm.

**A. A General Hessian Based Descent Direction**

Assume \(f(w)\) is a strongly convex and strictly smooth function in \(\mathbb{R}^d\), such that there exists positive constants \(\alpha\) and \(\beta\) so that \(\alpha I \preceq \nabla^2 f(w) \preceq \beta I\) for all \(w\). Let us denote the corresponding gradient and Hessian of \(f(w_t)\) as \(g_t\), and \(H_t\) at iteration \(t\). A general Hessian based descent direction can then be written as follows:

\[
\Delta w_t = H_t^{-k}g_t,
\]

where we refer to \(0 \leq k \leq 1\) as Hessian power. The power of a positive definite matrix is defined as

\[
H^a = U^T \Lambda^a U,
\]

where \(U^T \Lambda U\) is the eigen-decomposition of \(H\). Note that for \(k = 0\) we recover the gradient descent algorithm, and for \(k = 1\) we retrieve the so-called Newton method. For a strongly convex function, we can show that the update formulation of Eq. 6 is a converging algorithm. Particularly, we can show that with the proper learning rate we have:

\[
f(w_{t+1}) - f(w_t) \leq -\frac{\alpha^k}{2\beta^{1+k}}\|g_t\|^2.
\]

The proof can be found in Appendix A. Note that when \(k = 0\) or 1, the convergence rate is the same as gradient descent or Newton method\(^4\) [8], respectively.

The basic idea of Hessian based methods is to precondition the gradient with the \(H^{-k}\) matrix and use \(H^{-k}g\) for the descent direction, instead of naively using the bare \(g\) vector. The preconditioner automatically rotates and rescales the gradient vector. As discussed before (Figure 1) this is important since the loss landscape curvature is generally different across different directions/layers. Thus, ideally we need a different step size per dimension. This is further illustrated in Figure 2 where we show a 2D schematic plot of the loss landscape for different convolution channels. Each channel can have a different loss landscape topology. In this illustration, the last channel has a much flatter loss landscape as compared to other layers. As a result, it is preferred to take a larger step size for the last channel, as opposed to the first channel, which has a very “sharp” loss landscape. Problems that exhibit this behaviour are ill-conditioned.

The role of the Hessian preconditioner is to automatically normalize the ill-conditioned problem by stretching and contracting different directions to accommodate for the curvature differences.

However, there are two major problems with this approach. The first problem is that a naive use of the Hessian preconditioner comes at the prohibitively high

\(^3\)Without confusion, we use the naive use of the Hessian preconditioner comes at the prohibitively high power of a positive definite matrix is defined as

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\(^4\)The convergence rate here denotes the global convergence rate of Newton’s method.
We illustrate a simple model with $N$ layers on the left, with convolutional blocks of the $N-1$ layer shown in the second column. We also show the loss landscape of each block, which can be calculated by perturbing the convolutions’ parameters in two different directions while keeping all the other parameters constant. Note the different loss landscape topology. First order methods do not explicitly capture this difference. We also show a schematic for the gradient $\mathbf{g} \in \mathbb{R}^d$, which is a vector, and the Hessian $\mathbf{H} \in \mathbb{R}^{d \times d}$ which is a matrix. The entries (3D tensors) colored in blue show the components used for calculating the block diagonal average of Hessian. The part of the gradient highlighted in the orange box is the corresponding gradient of the blue convolution kernel. The part of the Hessian diagonal highlighted in the orange is used to compute the spatial average.

cost of applying Hessian inverse to the gradient vector at every iteration ($\mathbf{H}^{-k} \mathbf{g}$ term). The second problem and more challenging problem is that local Hessian (curvature) information can be very misleading for a noisy loss landscape. A simple example is illustrated in Figure 4, where we plot a simple parabola with a small sinusoidal noise as the loss landscape (shown in green). As one can see, the local Hessian (curvature) information is completely misleading, as it computes the curvature of the sinusoidal noise instead of global Hessian information for the parabola. Applying such misleading information as the preconditioner would actually result in very small steps to converge to one of the many local minima created by the sinusoidal noise. The same problem exists for the gradient as well, but that can be resolved by exploiting the stochasticity of the batches or using momentum instead of local gradient information. However, it is computationally infeasible to compute a Hessian momentum. The reason is that we cannot form the Hessian matrix and average it throughout different iterations, as such an approach has quadratic memory complexity in the number of parameters along with a prohibitive computational cost. However, as we discuss next, both problems can be resolved by using our inexact Newton method.

### B. Hessian Diagonal: Inexact Newton Method

As mentioned above, applying the inverse Hessian to the gradient vector at every iteration is computationally infeasible, as NNs often contain millions of parameters. To resolve this, one could use inexact Newton method, where an approximate Hessian operator is used instead of the Full Hessian inverse [5, 15, 54, 55, 60]. The most simple and computationally efficient approach is to approximate the Hessian as a diagonal operator in Eq. 6:

$$\Delta \mathbf{w} = \text{diag}(\mathbf{H})^{-k} \mathbf{g}, \quad (9)$$

where $\text{diag}(\mathbf{H})$ is the Hessian diagonal which we denote as $\mathbf{D}$. We theoretically show that using Eq. 9 has the same convergence rate as using Eq. 6; see Appendix B.

The Hessian diagonal can be efficiently computed using the Hutchinson method. The two techniques we used for the approximation are: (i) a Hessian-free method [58]; and (ii) a randomized numerical linear algebra (RandNLA) method [4, Figure 1]. Particularly, the Hessian-free method is an oracle to compute the multiplication between the Hessian matrix $\mathbf{H}$ with a random vector $z$, i.e.,

$$\frac{\partial \mathbf{g}^T z}{\partial \theta} = \frac{\partial \mathbf{g}^T}{\partial \theta} z + \mathbf{g}^T \frac{\partial z}{\partial \theta} = \frac{\partial \mathbf{g}^T}{\partial \theta} z = \mathbf{H} z. \quad (10)$$

$\mathbf{D}$ can also be considered as a vector so that $\mathbf{D}^{-k} \mathbf{g}$ is an element-wise product.
As mentioned above, we adopt the momentum for both Hutchinson method. The diagonal is approximated by drawing an i.i.d. random vector \(z\) sampled from a Rademacher distribution. This vector is then multiplied by Hessian using the matrix free method of Eq. 9. The dot product of the result is then computed with \(z\). It is easy to show that the expectation of the result converges to the diagonal of the Hessian.

\[
D = \text{diag}(H) = \mathbb{E}[z \odot (Hz)],
\]

where \(z\) is a random number with Rademacher distribution, and \(Hz\) is computed by the Hessian matvec oracle given in Eq. 10. This process is schematically shown in Figure 3. It can be proved that the expectation of \(z \odot (Hz)\) converges to the Hessian diagonal with sufficiently many random samples [4].

Besides computational efficiency, another important advantage of using the Hessian diagonal is that we can compute its moving average to resolve the local versus global curvature problem mentioned above. This is critical as it allows us to smooth out noisy local curvature information, and use global Hessian information instead. In fact, one of the important differentiators of ADAHESSIAN with previous second order methods such as [45] is the use of a root mean square averaging in time and space which is described below.

### C. ADAHESSIAN

Now that we have described how an approximate Hessian can be efficiently computed, we will describe how it can be used to precondition the gradient vector. As mentioned above, we adopt the momentum for both gradient and diagonal Hessian in ADAHESSIAN. More specifically, let \(\bar{g}_t\) and \(\bar{D}_t\) denote the accumulated gradient and Hessian diagonal at the t-th step. We use the exponential moving average as well as a bias correction to compute \(\bar{g}_t\) and \(\bar{D}_t\), i.e.,

\[
\bar{g}_t = \frac{(1 - \beta_1) \sum_{i=1}^{t} \beta_1^{t-i} g_i}{1 - \beta_1^t},
\]

\[
\bar{D}_t = \sqrt{\frac{(1 - \beta_2) \sum_{i=1}^{t} \beta_2^{t-i} D_i D_i}{1 - \beta_2^t}},
\]

where \(0 < \beta_1, \beta_2 < 1\) are the first and second moment hyperparameters that are also used in Adam. We here use root mean square averaging (RMS) in ADAHESSIAN to compute \(\bar{D}_t\) to help smooth out the noise [24, 48].

#### Algorithm 1: ADAHESSIAN

| Require: Initial Parameter: \(\theta_0\) |
| Require: Learning rate: \(\eta\) |
| Require: Exponential decay rates: \(\beta_1, \beta_2\) |
| Require: Block size: \(b\) |
| Require: Hessian Power: \(k\) |

Set: \(\bar{g}_0 = 0, \bar{D}_0 = 0\)

for \(t = 1, 2, \ldots\) do // Training Iterations

\[
g_t \leftarrow \text{current step gradient}
\]

\[
D_t \leftarrow \text{current step estimated diagonal Hessian}
\]

Update \(\bar{g}_t, \bar{D}_t\) based on Eq. 12

\[
\theta_t = \theta_{t-1} - \eta \bar{D}_t^{-k} \bar{g}_t
\]

As mentioned above, the incorporation of the moving average for Hessian is critical to avoid misleading
local Hessian information which can be catastrophic. Incorporating a moving average enables us to smooth the noisy curvature information and get an approximation to the global curvature information. To illustrate this, we provide a simple example in 1D by considering $f(x) = x^2 + 0.1x \sin(20\pi x)$, as shown in Figure 4. It can be clearly seen that the method without the second order momentum gets trapped at a local minima even with more than 1000 iterations (orange trajectory). On the contrary, the optimization converges within 7 iterations with Hessian momentum (blue trajectory). (While this example is over-simplified in certain ways, we are using it here only to convey the importance of momentum.)

Another important dimension to smooth out Hessian is the spatial dimension. Recall that the Hessian varies for each single dimension of the problem. For example, for a convolutional layer, each convolution parameter can have its own Hessian. We found that it is helpful to group the parameters into blocks and use the average Hessian for all of them. This helps to smooth out variations further. This is illustrated in Figure 2. For example, for a convolutional neural network, we can group one output channel as one block and compute the average as their diagonal estimation values. In general, the block size (denoted as $b$) is a hyperparameter that can be tuned for different tasks. (The effectiveness of this spatial averaging will be illustrated in Section V-A.)

To summarize, ADAHESSIAN uses both the RMS averaging over iterations as well as the spatial averaging to smooth out curvature noise throughout optimization and parameter space. Our main algorithm, ADAHESSIAN, is depicted in Algorithm 1.

The main overhead of ADAHESSIAN is the Hutchinson’s method to approximate Hessian diagonal. The cost of each Hutchinson step is equivalent to the cost of one Hessian matvec product. The key observation is that the cost of each Hessian matvec is equivalent to one gradient backpropagation [57]. To get an accurate approximation, we need to approximate the diagonal many times for each iteration and compute their average. However, doing more than one diagonal computation per iteration is actually unnecessary and the multiple calculations could be performed as optimization iterations proceed. In particular, we only approximate the Hessian diagonal with one Hutchinson step per optimization iteration. (Later, in Section V-B, we will actually show that even this can be further relaxed to only computing it every multiple iterations to further reduce the overhead.)

IV. RESULTS

A. Experiment Setup

One of the problems with several formerly proposed optimization methods is that the methods were originally tested with very simple models on very few tasks. When those methods were later tested by the community on more complex models the results were often worse than popular optimization methods. To avoid such a scenario, we extensively test ADAHESSIAN on a wide range of learning tasks, including image classification, neural machine translation (NMT), language modeling (LM), and recommendation system (RecSys). We compare the ADAHESSIAN performance with SGD, Adam, AdamW [28], and Adagrad. Moreover, to enable a fair comparison we will use the same $\beta_1$ and $\beta_2$ parameters in ADAHESSIAN as in Adam/AdamW for each task, even though those default values may favor Adam (or AdamW) and disfavor ADAHESSIAN. Furthermore, we will use the exact same weight decay and learning rate schedule in ADAHESSIAN as that used by other optimizers. Below we briefly explain each of the learning tasks tested.

a) Image Classification: We experiment on both Cifar10 (using ResNet20/32) and ImageNet (using ResNet18) datasets. Cifar10 consists of 50k training images and 10k testing images. ImageNet has 1.2M training images and 50k validation images. We follow the settings described in [22] for training. We run each experiment 5 times on Cifar10 and report the mean and standard deviation of the results.

b) Neural Machine Translation (NMT): We use IWSLT14 German-to-English (De-En) and WMT14 English-to-German (En-De) datasets. Transformer base architecture is used for WMT14 (4.5M sentence pairs), and small architecture is used for IWSLT14 (0.16M sentence pairs). We follow the settings reported in [37] and use pre-normalization described in [50]. The length penalty is set to 0.6/1.0 and the beam size is set to 4/5 for WMT/IWSLT [36]. We report the average results of the last 10/5 checkpoints respectively. For NMT, BLEU score is used [38]. In particular, we report tokenized case-sensitive BLEU on WMT14 En-De and case-insensitive BLEU IWSLT14 De-En. Furthermore, we use AdamW for this task instead of Adam since the former is the standard optimizer (Adam consistently scores lower).

c) Language Modeling: We use PTB [33] and Wikitext-103 [32] datasets, which contain 0.93M and 100M tokens, respectively. Following [29], a three-layer tensorized transformer core-1 for PTB and a six-layer tensorized transformer core-1 for Wikitext-103 are used.
Table II: Results of ResNet20/32 on Cifar10 (left two columns) and ResNet18 on ImageNet (last column). On Cifar10: Adam performs consistently worse than SGD; AdamW has slightly worse performance than SGD; and ADAHESSIAN outperforms AdamW and even gets accuracy comparable to SGD. On ImageNet: ADAHESSIAN has significantly better accuracy than Adam (5.53%), AdamW (2.67%), and has similar performance to SGD.

| Dataset       | Cifar10 | ImageNet |
|---------------|---------|----------|
|               | ResNet20 | ResNet32 | ResNet18 |
| SGD [43]      | 92.08 ± 0.08 | 93.14 ± 0.10 | 70.03 |
| Adam [24]     | 90.33 ± 0.13 | 91.63 ± 0.10 | 64.53 |
| AdamW [28]    | 91.97 ± 0.15 | 92.72 ± 0.20 | 67.41 |
| **ADAHESSIAN**| **92.13 ± 0.18** | **93.08 ± 0.10** | **70.08** |

AdaHessian 92.13 ± 0.18 is significantly better than Adam (5.53%), AdamW (2.67%) and has similar performance to SGD.

Table III: NMT performance (BLEU) on IWSLT14 De-En and WMT14 En-De testsets (higher is better). Unlike in Table II SGD has significantly worse results than AdamW. Note that ADAHESSIAN outperforms the default and heavily tuned optimizer AdamW by 0.27 and 0.33 on IWSLT14 and WMT14, which is significant for this task.

| Model         | IWSLT14 | WMT14 |
|---------------|---------|-------|
| SGD           | 28.45   | 26.04 |
| AdamW [28]    | 35.60   | 28.19 |
| ADAHESSIAN    | **35.87** | **28.52** |

testing curves of different optimizers for ResNet20/32 on Cifar10 are shown in Figure A.8, respectively.

Next, we use the best learning rate obtained by training ResNet20/32 on Cifar10 to optimize ResNet18 on ImageNet for all four optimizers. We try two different learning rate schedules for all four optimizers, and we use the one with the better result. The two learning rate schedules are quite standard, i.e., the step decay schedule and the plateau based schedule [39]. The final result is reported in Table II. Again note that the final performances of Adam and AdamW are much worse than that of SGD and ADAHESSIAN. We plot the training and testing curve in Figure A.9.

It is worthwhile to note that our learning rate tuning is performed at an academic scale, but ADAHESSIAN still significantly exceeds other adaptive methods and reaches the same performance level as SGD which has been tuned at the industrial scale.

C. Neural Machine Translation

We report the NMT results in Table III. The first interesting observation is that here SGD performs much worse than AdamW (which is opposite to the image classification tests). As pointed out in the introduction, even the choice of the optimizer has become another hyperparameter. In particular, note that the BLEU scores of SGD are 7.15 and 2.15 lower than AdamW on IWSLT14 and WMT14, which is quite significant. Similar observations about SGD were also reported in [62].

Despite this, ADAHESSIAN achieves state-of-the-art performance for NMT. In particular, ADAHESSIAN outperforms AdamW by 0.28 BLEU score on IWSLT14. Furthermore, the accuracy of ADAHESSIAN on WMT14 is 28.52, which is 0.33 higher than that of AdamW. We plot the training losses of AdamW and ADAHESSIAN on IWSLT14/WMT14 in Figure 5. As one can see, ADAHESSIAN consistently achieves lower training loss. These improvements are quite significant for NMT, and importantly achieved even though ADAHESSIAN uses the
Fig. 5: Training loss curves of AdamW and ADAHessian for Transformer on IWSLT14 and WMT14. The training loss of ADAHessian is lower than that of AdamW on both IWSLT14 and WMT14. Testing results are reported in Table III.

Table IV: LM performance (PPL) on PTB and Wikitext-103 test datasets (lower is better). The PPL of ADAHessian is 1.8 and 1.0 lower than that of AdamW.

| Model       | PTB Three-Layer | PTB Six-Layer | Wikitext-103 |
|-------------|-----------------|---------------|--------------|
| SGD         | 59.7            | 78.5          |              |
| AdamW [28]  | 53.2            | 20.9          |              |
| ADAHessian  | **51.4**        | **19.9**      |              |

Fig. 6: Training PPL curves of AdamW and ADAHessian for Transformer on PTB and Wikitext-103. The losses of ADAHessian are consistently lower than AdamW from the beginning of the training. ADAHessian achieves 29.56/23.51 final training perplexity (PPL) on PTB/Wikitext-103 as compared to AdamW (31.72/24.01). Testing results are reported in Table IV.

D. Language Modeling

We report the language modeling results in Table IV, using the tensorized transformer proposed in [29]. Similar to NMT, note that the PPL of SGD is 57.6 worse than AdamW on Wikitext-103. However, ADAHessian achieves state-of-the-art, with more than 1.8/1.0 better PPL than that of AdamW on PTB/Wikitext-103, respectively. The detailed training loss curves are shown in Figure 6. ADAHessian achieves consistently lower loss values than AdamW throughout the training process, on both PTB and Wikitext-103. Similar to NMT, the $\beta_1/\beta_2$ as well as the warmup phase of ADAHessian are kept the same as AdamW.

E. Recommendation System

We solely focus on modern recommendation systems, and in particular DLRM model widely adopted in industry [34]. These systems include a large embedding layer followed by a series of dense FC layers. In training, a sparse set of rows of the embedding layer is used and only those rows are updated. These rows do change from one iteration to the next. For such a sparse setting, we use Adagrad to update the embedding table, and we use ADAHessian to update the rest of the FC network in the experiments. (Pytorch currently does not support second order backpropagation for the sparse
Fig. 7: Training and Testing Accuracy curves of Adagrad and ADAHESSIAN on Criteo Ad Kaggle dataset. As can be seen, the test accuracy of ADAHESSIAN is better (0.032%) than that of Adagrad. This is quite significant for this task.

As reported in the previous section, ADAHESSIAN achieves state-of-the-art performance on a wide range of tasks. Two important issues are the sensitivity of ADAHESSIAN to the hyperparameters of learning rate and block size which are discussed next.

A. Learning Rate and Block Size Effects

Here, we explore the effects of the learning rate and block size parameters on ADAHESSIAN’s performance. We first start with the learning rate and test the performance of ADAHESSIAN and AdamW with different learning rates. The results are reported in Table V for IWSLT14 dataset, where we scale the original learning rate with a constant factor, ranging from 0.5 to 5 (the original learning rate is the same as in Section IV-C). It can be seen that ADAHESSIAN is more robust to the large learning rates. Even with $4 - 5\times$ learning rate scaling, ADAHESSIAN still achieves 34.11/33.32 BLEU score as compared to 13.75/0.50 of AdamW.

We also test the effect of the block size which is used for spatial averaging of the Hessian, shown in Figure 2 (parameter $b$ in Algorithm 1). The results are shown in Table VI where we vary the block size from 2 to 128. While the best performance is achieved for the block size of 32, the performance variation for other block sizes is small. Moreover, all the results are still no worse than AdamW.

### V. Discussion

One widely-held (incorrect) belief is that second order methods are orders of magnitude slower than first order methods. However, this is simply not accurate generally, and specifically for ADAHESSIAN. Of course, that belief is true when second order methods are implemented naively, but ADAHESSIAN uses an efficient inexact Newton method. Based on the computational complexity analysis, ADAHESSIAN requires twice the flops as compared to SGD. This $2\times$ overhead comes from the cost of computing the Hessian diagonal, which is performed with one Hutchinson step per optimization iteration, via Eq. 11. This step requires one more gradient backpropagation, hence leading to twice the theoretical complexity. We have also measured the actual runtime of ADAHESSIAN in Pytorch on a single Titan RTX 2080 GPU machine, as reported in the second column of Table VII. For ResNet20, ADAHESSIAN is 2.42× slower than SGD (and 2.27× slower than Adam). As one can see, ADAHESSIAN is not orders of magnitude slower than first order methods.

Another point is that the theoretical complexity does not include the cost of additional data movements and caches that add overhead to the run time. However, it may be possible to approach the theoretical run time by further performance engineering. We leave this for future work.

There are several orthogonal approaches that can be used to further reduce the ADAHESSIAN overhead. While
We also measured the speed up for different Hessian computation frequencies. As one can see, ADAHESSIAN is not orders of magnitude slower than SGD, despite the widely-held incorrect belief about the efficiency of Hessian based methods. Furthermore, by increasing the Hessian computation frequency, the run time can improve from 3.23× to 1.45×, as compared to SGD for ResNet32. The real measurement is performed on one Titan RTX 2080 GPU.

Table VII: Comparison between ADAHESSIAN theoretical and measured speed, as compared to Adam and SGD, tested on Cifar10.

| Hessian Computation Frequency | 1   | 2   | 3   | 4   | 5   |
|------------------------------|-----|-----|-----|-----|-----|
| Theoretical Per-iteration Cost (×SGD) | 2×  | 1.5×| 1.33×| 1.25×| 1.2×|
| ResNet20 (Cifar10)           | 92.13 ± .08 | 92.40 ± .04 | 92.06 ± .18 | 92.17 ± .21 | 92.16 ± .12 |
| Measured Per-iteration Cost (×SGD) | 2.42× | 1.71× | 1.47× | 1.36× | 1.28× |
| Measured Per-iteration Cost (×Adam) | 2.27× | 1.64× | 1.42× | 1.32× | 1.25× |
| ResNet32 (Cifar10)           | 93.08 ± .10 | 92.91 ± .14 | 92.95 ± .17 | 92.93 ± .24 | 93.00 ± .10 |
| Measured Per-iteration Cost (×SGD) | 3.23× | 2.12× | 1.74× | 1.56× | 1.45× |
| Measured Per-iteration Cost (×Adam) | 2.91× | 1.96× | 1.64× | 1.48× | 1.38× |

A detailed exploration of such approaches is outside the scope of this paper, but we have performed initial experiments to reduce the ADAHESSIAN overhead even further. One simple idea is to delay the frequency of computing the Hutchinson step from every 1 iteration to every multiple iterations. For example, for a frequency of 2, we perform the Hutchinson step every other iteration. This reduces the theoretical computation cost to 1.5× from 2×. The corresponding accuracy results are reported in Table VII for frequency of 2 to 5. As one can see, there is a small performance degradation, but the ADAHESSIAN overhead significantly decreases as compared to SGD and Adam. Other possible efficiency optimizations include using stale gradients to overlap the Hutchinson step with gradient computation completely, or incorporating parallel resources in a more fine-grained manner. We leave these as future work.

VI. CONCLUSIONS

In this work, we proposed ADAHESSIAN, an adaptive Hessian based optimizer. ADAHESSIAN uses an inexact Newton method and incorporates approximate Hessian diagonal to precondition the gradient vector. This automatically rescales and rotates the gradient vector resulting in better descent directions. One of the key novelties in our approach is the incorporation of an exponential root mean square moving average in time; and another novelty is the spatial averaging for Hessian computations. These enable us to avoid noisy local Hessian information which could be highly misleading. We extensively tested ADAHESSIAN on various datasets and tasks, using state-of-the-art models. These include Cifar10 and ImageNet for image classification, IWSLT14 and WMT14 for neural machine translation, PTB and Wikitext-103 for language modeling, and Criteo Ad Kaggle for recommendation system. ADAHESSIAN consistently achieves the new state-of-the-art generalization performance as compared to the highly tuned default optimizers used for different tasks.

Stepping back, it is important for every work to state its limitations (in general, but in particular in this area). We made sure to repeat all the reported results multiple times, and we made sure to perform an extensive test with multiple modern networks on different tasks. The current limitation of ADAHESSIAN is that it is 2—3× slower than first order methods such as SGD and Adam. However, ADAHESSIAN consistently achieves comparable or better accuracy. For example, for LM task, ADAHESSIAN achieves up to 1.8/58.0 better PPL, as compared to AdamW/SGD, which is significant for this task. We briefly explored how this overhead could be reduced, but more work is needed in this area.

Finally, from a higher-level perspective, we should note that there has been significant development within second order methods, both theory and practice, even though these methods were widely viewed as inapplicable for ML even just a few years ago. Some examples include Hessian based model compression [16, 17, 21, 25], adversarial attacks [59], and studies of the loss landscape topology for different NN architectures [44, 57], just to name a few. ADAHESSIAN is an important step in this area, and we expect that it will enable still further progress. We have open sourced ADAHESSIAN and we hope that it would help this progress [1].

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APPENDIX

A. Descending Property of Eq. 6

Here, we prove that the statement provided in Eq. 8. Let us define \( \lambda(w_t) = (g_t^T H_t^{-k} g_t)^{1/2} \). Since \( f(w) \) is strongly convex, we have

\[
\begin{align*}
    f(w_t - \eta \Delta w_t) &\leq f(w_t) - \eta g_t^T \Delta w_t + \frac{\eta^2 \beta \| \Delta w_t \|^2}{2} \\
    &\leq f(w_t) - \eta \lambda(w_t)^2 + \frac{\beta}{2 \alpha k} \eta^2 \lambda(w_t)^2.
\end{align*}
\]

The last inequality comes from the fact that

\[
\lambda(w_t)^2 = \Delta w_t^T H_t^k \Delta w_t \geq \alpha k \| \Delta w_t \|^2.
\]

Therefore, the step size \( \hat{\eta}_t = \frac{\alpha}{\beta} \) will make \( f \) decreases as follows,

\[
    f(w_t - \hat{\eta}_t \Delta w_t) \leq f(w_t) - \frac{1}{2} \hat{\eta}_t \lambda(w_t)^2.
\]

Since \( \alpha \leq H_t \leq \beta \), we have

\[
\lambda(w_t)^2 = g_t^T H_t^{-k} g_t \geq \frac{1}{\beta k} \| g_t \|^2.
\]

Therefore,

\[
    f(w_t - \hat{\eta}_t \Delta w_t) - f(w_t) \leq - \frac{1}{2 \beta k} \hat{\eta}_t \| g_t \|^2 = - \frac{\alpha k}{2 \beta (1 + \epsilon)} \| g_t \|^2.
\]

B. Descending Property of Eq. 9

Here we prove that Eq. 9 has the same convergence rate as Eq. 6. First of all, it is not hard to see the diagonal elements in \( D \) are all positive since \( f(w) \) is a strongly convex problem. That is,

\[
\alpha < e_i^T H_i e_i = e_i^T D e_i = D_{i,i},
\]

where \( e_i \) is the vector whose coordinates are all zero, except the i-th one that equals 1. Similarly, we have

\[
D_{i,i} = e_i^T D e_i = e_i^T H e_i \leq \beta.
\]

Therefore, the diagonal elements in \( D \) are in the range \([\alpha, \beta]\). Using the same proof as in Appendix A, we will get the result.

C. Experimental Setup

Here, we provide more details on the experimental setup for the empirical evaluation.

a) Image Classification: The training/test sets for Cifar10 dataset contain 50k/10k images, respectively. The models used on Cifar10 are standard ResNet20/32. We train both models with 160 epochs and decay the learning rate by a factor of 10 at epoch 80 and 120. For SGD/Adam/AdamW, the initial learning rates are tuned and set to be 0.1/0.001/0.005. For ADAHESSIAN, we set the block size as 9, \( k \) to be 1, and learning rate as 0.15 for both ResNet20/32. For Adam/AdamW/ADAHESSIAN, \( \beta_1 = 0.9 \) and \( \beta_2 = 0.999 \). The training/test sets for ImageNet dataset contain 1.2M/50k images, respectively. Our code is modified from the official PyTorch example\(^7\). We train ResNet18 for 90 epochs. All the settings of different optimizers are the same as used in Cifar10 example.

\(^7\)https://github.com/pytorch/examples/tree/master/imagenet
b) Neural Machine Translation: The training/validation/test sets for the IWSLT14 dataset contain about 153K/7K/7K sentence pairs, respectively. We use a vocabulary of 10K tokens via a joint source and target byte pair encoding (BPE). For the WMT14 dataset, we follow the setting of [49], which contains 4.5M parallel sentence pairs for training. We use Newstest2014 as the test set, and Newstest2013 as the validation set. The 37K vocabulary for WMT14 is also via a joint source and target BPE factorization. We set dropout as 0 for Transformer base/small model. For AdamW, we follow the optimizer setting and learning rate schedule in [50]. For ADAHESSIAN, we set the block size as 32 for IWSLT/WMT, k to be 1.0, and learning rate as 0.047/1.0 for IWSLT/WMT. For both AdamW/ADAHESSIAN, we set $\beta_1 = 0.9$ and $\beta_2 = 0.98$. We fix the label smoothing value as $\epsilon_{ls} = 0.1$ in all experiments. We implement our code for MT based on fairseq-py [36]. We employ BLEU [38] as the evaluation metric for MT. Following standard practice, we measure tokenized case-sensitive BLEU and case-insensitive BLEU for WMT14 En-De and IWSLT14 De-En, respectively. For a fair comparison, we do not include other external datasets. We train 130/55 epochs for WMT/IWSLT, respectively. For inference, we average the last 10 checkpoints, and we set the length penalty as 0.6/1.0 and beam size as 4/5 for WMT/IWSLT, following [36].

c) Language Modeling: PTB [33] has 0.93M training tokens, 0.073M validation tokens, and 0.082M test tokens. Wikitext-103 [32] contains 0.27M unique words, and 100M training words from 28K articles, with an average length of 3.6K words per article. We use the same evaluation scheme following [14]. We use a three-layer tensorized transformer core-1 for PTB and a six-layer tensorized transformer core-1 for Wikitext-103, following [29]. We set the dropout rate as 0.3 in all the LM experiments. The model is trained for 30 epochs on both PTB and WikiText-103. For AdamW, we follow the learning rate setting in [29]. For ADAHESSIAN, we set the block size as 4 and k as 0.5 for PTB and WikiText-103. We set the learning rate as 2.0/1.0 for PTB/Wikitext-103, respectively. For AdamW/ADAHESSIAN, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. We set the warmup steps to be 4000 and label smoothing to be $\epsilon_{ls} = 0.1$ in all LM experiments.

d) Recommendation System: The Criteo Ad Kaggle dataset consists of click logs for ad CTR prediction for 7 days. Each data set contains 13 continuous and 26 categorical features. The dataset contains about 45 million samples over 7 days. In experiments, we follow the setting from [34]. Our code is also modified from [34]9. For Adagrad, the learning rate is set to be 0.01. For ADAHESSIAN, we set the block size as 1, k as 0.5, learning rate as 0.043, $\beta_1 = 0.9$, and $\beta_2 = 0.98$.

e) Delayed Hessian Update: For ResNets on Cifar10, we use 5 epochs for warmup. In particular, within 5 epochs, the Hessian diagonal is still computed for every iteration. After that, the Hessian diagonal computation frequency is set between 1 to 5 iterations.

D. Additional Results

In this section, we present additional empirical results that were discussed in Section IV. See Figure A.8, and A.9.

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9https://github.com/moses-smt/mosesdecoder/blob/master/scripts/generic/multi-bleu.perl

9https://github.com/facebookresearch/dlrm
**Fig. A.8:** Training and testing loss curves of SGD, Adam, AdamW, AdaHessian for ResNet20/32 on Cifar10. SGD and AdaHessian consistently achieve better accuracy as compared to Adam and AdamW. The final accuracy results are reported in Table II.

**Fig. A.9:** Training/Test loss curve of SGD, Adam, AdamW, AdaHessian for ResNet18 on ImageNet. SGD and AdaHessian consistently achieve better accuracy as compared to Adam and AdamW. The final accuracy results are reported in Table II.