Trainable Weight Averaging for Fast Convergence and Better Generalization

Tao Li¹, Zhehao Huang¹, Qinghua Tao², Yingwen Wu¹, Xiaolin Huang¹
¹Department of Automation, Shanghai Jiao Tong University
²ESAT-STADIUS, KU Leuven

Abstract

Stochastic gradient descent (SGD) and its variants are commonly considered as the de-facto methods to train deep neural networks (DNNs). While recent improvements to SGD mainly focus on the descent algorithm itself, few works pay attention to utilizing the historical solutions—as an iterative method, SGD has actually gone through substantial explorations before its final convergence. Recently, an interesting attempt is stochastic weight averaging (SWA), which significantly improves the generalization by simply averaging the solutions at the tail stage of training. In this paper, we propose to optimize the averaging coefficients, leading to our Trainable Weight Averaging (TWA), essentially a novel training method in a reduced subspace spanned by historical solutions. TWA is quite efficient and has good generalization capability as the degree of freedom for training is small. It largely reduces the estimation error from SWA, making it not only further improve the SWA solutions but also take full advantage of the solutions generated in the head of training where SWA fails. In the extensive numerical experiments, (i) TWA achieves consistent improvements over SWA with less sensitivity to learning rate; (ii) applying TWA in the head stage of training largely speeds up the convergence, resulting in over 40% time saving on CIFAR and 30% on ImageNet with improved generalization compared with regular training. The code is released at https://github.com/nblt/TWA.

1 Introduction

Training deep neural networks (DNNs) usually requires a large amount of time and computational resources. As the size of models and datasets grow larger, more efficient optimization methods together with better generalization capability are increasingly demanded. In the existing works, great efforts have been made to improve the efficiency of stochastic gradient descent (SGD) and its variants, which mainly focus on adaptive learning rates [7, 21, 26, 57, 17] or accelerated schemes [31, 28]. As an iterative descent method, SGD generates a series of solutions during optimization. These historical solutions provide dynamic information about the training and have brought many interesting perspectives, e.g., trajectory [25], landscape [11], and optimization [18, 42], to name a few. In fact, they can also be utilized to improve the training performance, resulting in the so-called stochastic weight averaging (SWA) [19], which shows significantly better generalization by simply averaging the tail stage explorations of SGD. The success of SWA encourages more in-depth investigations on the roles of historical solutions obtained during the training [11, 29, 56].

In this paper, our main purpose is to utilize the historical solutions in a relatively early stage (i.e. the head stage) to speed up the convergence and meanwhile improve the generalization capability. The idea of utilizing these early solutions in DNNs’ training is mainly inspired by two facts. On the one hand, high test accuracy commonly starts appearing at an early stage. For example, a PreAct ResNet-164 model [16] achieves over 80% test accuracy within 10 training epochs on CIFAR-10 [22], while requiring to complete the whole 200 epochs to reach its final 95% accuracy. This observation also

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Input: Sampled weights \( \{ w_i \}_{i=1}^n \), Batch size \( b \), Loss function \( L : \mathcal{W} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+ \), Learning rate \( \eta \).

Output: Model trained with TWA

Orthogonalize \( \{ w_i \}_{i=1}^n \) to \( \{ e_i \}_{i=1}^n \);

Initialize \( w_{twa}^{(0)} \), \( t = 0 \), \( P = [e_1, e_2, \ldots, e_n] \);

while not converged do
  Sample batch data: \( B = \{ (x_i, y_i) \}_{i=1}^b \);
  Compute gradient: \( g = \nabla w L_B(w_{twa}^{(t)}) \);
  Update weights: \( w_{twa}^{(t+1)} = w_{twa}^{(t)} - \eta P (P^T g) \);
  \( t = t + 1 \);
end while

Return \( w_{twa}^{(t)} \)

Algorithm 1: TWA algorithm.

Figure 1: TWA intuition.

coincides with the recent findings that the key connectivity patterns of DNNs emerge early in training [38][10], indicating a well-explored solution space formed. On the other hand, simply averaging the solutions collected at the SWA stage immediately provides a huge accuracy improvement (e.g. over 16% on CIFAR-100 with Wide ResNet-28-10 [39]) than before averaging [19]. These facts point out a promising direction that sufficiently utilizing these early explorations may be capable of quickly composing the final solution while obtaining good generalization.

As the model parameters go through a rapid evolution at the early stage of training, a simple averaging strategy with the same weighting coefficient assigned to each historical solution as in SWA can cause large estimation errors. We here introduce a Trainable Weight Averaging (TWA), which allows explicit adjustments for the averaging coefficients in a trainable manner. Specifically, we construct a subspace that contains all sampled solutions during the training and then conduct efficient optimization therein. As optimization in such a subspace takes into account all possible averaging choices, we are able to adaptively search for a good set of averaging coefficients without the influence of outliers (e.g. less effective historical solutions) and largely reduce the estimation variance. The proposed optimization scheme is essentially the gradient projection onto a tiny subspace. Hence, the degree of freedom for training is substantially reduced from the original millions to dozens or hundreds (equal to the number of averaging points), making TWA enjoy fast convergence and better generalization. In extensive experiments with different tasks and various network architectures, we reach superior performance when applying TWA to the head stage of training. For instance, we attain 1.5 – 2.2% accuracy improvement on CIFAR-100 and 0 – 0.1% on ImageNet with over 40% and 30% training epochs reduced, respectively, compared with the regular training.

In summary, we make the following contributions:

- We propose Trainable Weight Averaging (TWA) that allows explicit adjustments for the averaging coefficients with a proper regularization. It brings consistent improvements over SWA with reduced estimation error.
- We firstly apply weight averaging to the head stage of training, resulting in a great time saving (e.g. over 40% on CIFAR and 30% on ImageNet) compared to regular training along with improved generalization and reduced generalization gap.
- Our TWA is easy to implement and could be flexibly plugged into different parts of training. It provides a new scheme for efficient DNNs’ training by sufficiently utilizing historical explorations, which may enlighten more powerful optimization methods.

2 Method

In this section, we first formulate the optimization target of TWA, where the averaging coefficients are optimized with a proper regularization. Then, the detailed training algorithm is introduced which consists of two phases: Schmidt orthogonalization to construct the subspace and projected optimization to search for a good set of averaging coefficients. Note that in this paper, the model’s weights are aligned as a vector, i.e., \( w \in \mathbb{R}^D \), where \( D \) denotes the number of parameters.
2.1 Optimization Target

In SWA, the weight averaging is simply given by $w_{\text{swa}} = \frac{1}{n} \sum_{i=1}^{n} w_i$, where $n$ solutions of the network collected during the training are equally weighted. Such averaging strategy is quite effective when being applied at the tail of training, however, may be inadequate at the head stage. This is because the network’s solutions have not stepped into a stationary distribution at that time and equally averaging will result in a large estimation error. Therefore, we propose to train the averaging coefficients with the hope of correcting the estimation error. Specifically, the set of possible TWA solutions, i.e., $w_{\text{twa}}$, can be represented as follows:

$$A = \{ \alpha_1 w_1 + \alpha_2 w_2 + \cdots + \alpha_n w_n \mid \alpha_1 + \alpha_2 + \cdots + \alpha_n = 1 \}.$$  \hfill (1)

Then we search for a good solution in this set by optimizing the following problem,

$$\min_{w_{\text{twa}} \in A} E_{(x,y) \sim D} [\mathcal{L}(f(w_{\text{twa}}; x), y)] + \lambda \cdot \frac{1}{2} \sum_{i=1}^{n} \alpha_i^2,$$  \hfill (2)

where $\mathcal{L}(\cdot, \cdot)$ is the loss function as in a regular training and the second term is a regularization with a pre-given coefficient $\lambda > 0$. Obviously, SWA ($w_{\text{swa}}$) is actually a special solution of (2) with determined $\alpha_i = 1/n$. Optimizing over $\alpha_i$ will bring benefits in the view of training loss, and a good generalization capability can also be expected: in regular training, the number of optimization variables equals the number of parameters $D$, which is usually very large, but here there are only $n$ averaging coefficients $\{\alpha_i\}_{i=1}^{n}$ to be optimized. The significant reduction in dimensionality leads to better generalization. Further, we control the model complexity by introducing the $l_2$-norm regularization term. Notice that weights with good performance have a quite similar norm ($\|w\|_2$). Thus, the first term in (2) that minimizes the training loss has already implicitly required the norm of $w_{\text{twa}}$ to be close as $w_i$, i.e., the sum-one constraint in (1) can be naturally satisfied and we do not require explicitly imposing it in optimizing (2).

2.2 Training Algorithm

Directly optimizing the averaging coefficients is difficult, as the gradients can not be explicitly passed to them through back-propagation. The key issue lies in that network’s parameters ($w$) and averaging coefficients ($\alpha_i$) are from different spaces, which blocks the propagation of gradients. However, notice that there exists a bijection between the coefficient space and parameter space, i.e., each set of the averaging coefficients is uniquely mapped to a point of the parameter space, which essentially forms a complete subspace. We could alternatively optimize these coefficients in such a subspace.

We first focus on constructing such a subspace in which the optimization proceeds. Specifically, we need to find a set of orthogonal bases $\{e_i\}_{i=1}^{n}$ to cover the subspace spanned by $\{w_i\}_{i=1}^{n}$. This is a standard Schmidt orthogonalization, which sequentially takes the following steps:

$$\left\{ \begin{array}{l}
e_k = w_k - (w_k^\top e_1) e_1 - (w_k^\top e_2) e_2 - \cdots - (w_k^\top e_{k-1}) e_{k-1}, \\
e_k = e_k/\|e_k\|_2.
\end{array} \right.$$  \hfill (3)

We then initialize the TWA solution as one point in the subspace (e.g. $\frac{1}{n} \sum_{i=1}^{n} w_i$), and optimize the network’s parameters therein. Let $P = [e_1, e_2, \cdots, e_n]$, such optimization can be easily achieved by projecting the gradient onto the subspace using projection matrix $PP^\top$. We summarize the detailed training procedures of the proposed TWA in Algorithm [1] with an intuitive illustration in Figure [1].

**Implementation** The regularization in (2) can be seamlessly integrated into subspace training as weight decay and result in very easy implementation, which we will elaborate on in Appendix B.

**Computational complexity** TWA introduces additional constant computational overhead due to the gradient projection operation, but it is negligible compared with the network’s forward and backward propagation. The wall-clock time comparison of TWA and SGD is presented in Table [6]. For memory, TWA needs to store models’ historical checkpoints (usually dozens or hundreds) for composing the final solution. This is affordable since in DNNs’ training, the memory consumption is dominated by activations rather than weights, and we have actually conducted extensive experiments on large-scale datasets with standard backbones.
3 Variance Analysis

In this section, we analyze how TWA improves the SWA solution from the perspective of variance reduction. Mandt et al. [27] demonstrated that under appropriate assumptions, running SGD with a constant learning rate is equivalent to sampling from a stationary Gaussian distribution, and the variance of the distribution is controlled by the learning rate. Accordingly, we assume the solutions at the tail stage of SGD training are sampled from a Gaussian distribution \( N(\mu, \Sigma) \) centered at the minimum \( \mu \) with covariance \( \Sigma \). Denote the eigenvalues of \( \Sigma \) in descending order, i.e., \( \sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_n^2 \). Then we have the spectral decomposition of \( \Sigma \) as \( \Sigma = Q \text{diag}(\sigma_1^2, \sigma_2^2, \cdots, \sigma_n^2)Q^\top \).

Approximately, the sampled solutions \( \{w_i\}_{i=1}^n \) are independent random variables from \( N(\mu, \Sigma) \), as long as there are sufficient iterations between adjacent samplings. SWA and TWA provide two estimators for the minimum \( \mu \), \( w_{\text{swa}} \) and \( w_{\text{twa}} \). As an averaged solution, \( w_{\text{swa}} \) has statistically better estimation than any single solution due to the effect of variance reduction, while \( w_{\text{twa}} \) is approaching the center by minimizing the loss. Thus, \( w_{\text{twa}} \) is the best solution in the subspace \( V = \text{span}\{w_i\}_{i=1}^n \), and actually the projection of \( \mu \) onto \( V \), i.e., \( w_{\text{twa}} = \text{Proj}_V(\mu) \). As illustrated in Figure 2, we could see clearly that \( w_{\text{twa}} \) is always closer to the center \( \mu \). Both \( w_{\text{swa}} \) and \( w_{\text{twa}} \) are unbiased estimators for \( \mu \), but \( w_{\text{twa}} \) has a lower expected variance:

\[
\mathbb{E}(\|w_{\text{twa}} - \mu\|_2^2) \leq \mathbb{E}(\|w_{\text{swa}} - \mu\|_2^2).
\]

Figure 2: (a) We give an illustration of the variance reduction of TWA, i.e., projection onto the subspace always minimizes the distance to \( \mu \); (b) and (c) The variance ratio distribution of each components and total variance for PCA on samples collected at the head of training (epoch 0 - 100 in SGD) and tail of training (epoch 126 - 225 in SWA). The variance ratio shows a fast decay for both cases. The experiments are conducted on CIFAR-100 with PreAct ResNet-164 model.

Let us investigate the advantages of optimizing the averaging coefficients in more detail. Intuitively, with \( n \) samples collected, TWA is able to eliminate the estimation errors along with \( n \) principal directions via optimizing the \( n \) coefficients. Although the number of parameters is quite large and \( n/D \) is very small, eliminating along the largest \( n \) principal directions is still quite significant due to the fast eigenvalue decay of \( \Sigma \) [13, 8]. As an example, we perform principal component analysis (PCA) on the solutions collected at the head/tail stages of training and plot the variance ratio distribution in Figure 2. The variance ratio becomes vanishingly small (< 1%) after the 8th component for the head stage and after the 15th for the tail, showing that the majority of errors exist along with a few principal directions and optimizing over them can largely reduce the errors. We also plot the total variance in the top right corner, from which one can see that the head stage contains significantly greater variance than the tail stage since the solutions have not fully converged. Moreover, in the head stage, the eigenvalue decay is more prominent, i.e., canceling the errors in the top principal directions has more benefits. This partially explains why SWA may fail in the head stage but TWA is quite efficient there. The above is discussing the empirical loss and the conclusion that TWA is closer to the optimum can be well generalized to the test error, as will be shown in Figure 5 and 6, since the optimization of TWA is in a very low-dimensional space.

4 Related Work

Improving the model’s generalization capability is of great importance and has received wide attention from researchers. The recent efforts mainly focus on two aspects: (1) proper regularization terms to search for more flat minimum [20, 24], such as weight decay [23], dropout [33], label smoothing [34],
Shake-Shake [12], MixUp [41], SAM [9] and AMP [43]; (2) effective data augmentation to diversify the dataset, such as Cutout [6], AutoAugment [3] and RandAugment [4]. Different from these techniques, we improve the model’s generalization by constraining the network’s training in a low-dimensional hyper-plane spanned by historical explorations along the optimization trajectory, which is a novel approach to regularizing the model complexity. We also note that TWA is orthogonal to these methods, and it is possible to combine them together to boost further improvements. Stochastic weight averaging (SWA, [19]) is one of the most effective methods to yield a flat minimum and enhance the model’s generalization via averaging the weights at the tail stage of the training. It has found a wide range of applications [1, 29, 36, 15]. Instead of the equal averaging simply used in SWA, we introduce trainable averaging coefficients by casting it as an optimization problem and, for the first time, apply the weight averaging in the head stage of training to boost fast convergence.

A lot of efforts have been made to speed up the convergence of DNNs’ training. Apart from the well-known methods on adaptive learning rates (e.g. Adam [21]) and accelerated schemes (e.g. Nesterov momentum [28]), Zhang et al. [42] proposed a new method that utilizes a look-ahead search direction generated by another “fast” optimizer, achieving faster convergence and better learning stability. Goyal et al. [14] adapted a large mini-batch to speed up the training and introduced a scaling rule for adjusting the learning rates. In this paper, we accelerate the convergence from a different perspective that the degree of freedom for training is substantially reduced from original millions (the number of parameters) to hundreds or even dozens, thus allowing very efficient training.

For utilizing historical explorations, SWA [19] is a simple strategy that averages the weights of tail explorations to achieve better generalization. Cha et al. [2] extended it to the domain generalization task with a dense and overfit-aware stochastic weight sampling strategy. We firstly propose to utilize the explorations at the head stage of training to achieve training efficiency. Exponentially decaying running average [18] is a common technique adopted by practitioners to smooth the trajectory, but it virtually utilizes a very short period of explorations due to the exponential decay properties and only performs comparably as SGD [19]. Another closely related work is model soups [35], which improves the model performance by averaging the weights of multiple models fine-tuned with different configurations. We differ in that the historical explorations used are from one single configuration instead of different fine-tuned models. We also mainly focus on training efficiency and do not require a validation set since we adopt a trainable manner.

5 Experiments

In this section, we numerically demonstrate the effectiveness of our proposed TWA for fast convergence and better generalization. First, we show that TWA improves the SWA solutions in the original SWA settings, i.e., the tail stage of training. Second, we apply TWA to the head stage of training, which brings significant efficiency together with improved generalization. We finally visualize the training trajectory as well as loss/accuracy surfaces.

5.1 Experimental settings

Datasets. We experiment over three benchmark image datasets, including CIFAR-10, CIFAR-100 [22], and ImageNet [5]. Following prior works [19, 36], we apply standard preprocessing and data augmentation for experiments on CIFAR datasets. For ImageNet, we adopt the preprocessing and data augmentation in the public Pytorch example [30].

Architectures. We use two representative architectures, VGG-16 [32] and PreAct ResNet-164 [16] on CIFAR experiments. For ImageNet, we use ResNet-18 and ResNet-50 [16].

Training. The main body of experiments contains two parts: (1) for the tail stage of training, we use the same hyper-parameters as in SWA [19] and then a larger tail learning rate is also tried. (2) for the head stage of training, we adopt the standard training protocol with a step-wise learning rate. For CIFAR, we run all experiments with 3 seeds and use SGD optimizer with momentum 0.9, weight decay $1 \times 10^{-4}$, and batch size 128. We train the models for 200 epochs with an initial learning rate 0.1 and decay it by 10 at the 100th and the 150th epoch. For ImageNet, we follow official PyTorch implementation.

For TWA, we collect solutions after every epoch training for CIFAR and uniformly 5 times per epoch for ImageNet. We use a condensed learning rate (Figure 4), which takes 10 epochs

https://github.com/pytorch/examples/tree/main/imagenet
of training for CIFAR and 2 epochs for ImageNet for fast convergence. The regularization coefficient \( \lambda \) defaults to \( 1 \times 10^{-5} \). More details can be found in Appendix A.

5.2 Improving SWA solutions

First, we will compare SWA and TWA in the original SWA settings. Specifically, TWA and SWA use the same weights sampled from the tail stage of training. For CIFAR, we try two kinds of tail learning rates: 0.05, the recommended one adopted in [19], and 0.10, a larger one for the case with greater variance. From the results in Table 1, we observe that TWA brings consistent improvements over SWA. Especially when the learning rate is not well-tuned, SWA’s performance will suffer a dramatic drop, but TWA is much less sensitive since the estimation error could be well controlled through training. One example is on CIFAR-100 dataset with VGG-16 architecture and a tail learning rate 0.10. In this case, the estimation error of SWA substantially increases and TWA achieves a significant accuracy improvement, i.e., 4.18\%, over SWA. Notice that in this comparison, TWA starts from the last sampled weights, not the averaged solution of SWA for a fair comparison.

![Figure 3: Performance comparisons on before and after TWA w.r.t. different epochs of weights used. “SGD final” indicates the accuracy reached by regular SGD training and “TWA” is the corresponding accuracy reached by Algorithm 1 with these epochs of weights. The final accuracy of SGD training is plotted for reference. TWA dramatically lifts the SGD accuracy and outperforms the final accuracy of SGD within 100 epochs. The experiments are repeated over 3 trials.](image)

| DATASET | MODEL       | SWA_\text{LR} = 0.05 | TWA | SWA_\text{LR} = 0.10 | TWA |
|---------|-------------|-----------------------|-----|-----------------------|-----|
| CIFAR-10 | VGG16       | 94.01 ± 0.04          | 94.16 ± 0.14 | 91.03 ± 0.14          | 92.41 ± 0.15 |
|         | PreResNet-164 | 95.58 ± 0.09          | 95.65 ± 0.13 | 91.58 ± 0.45          | 92.61 ± 0.09 |
| CIFAR-100 | VGG16      | 74.71 ± 0.03          | 75.73 ± 0.18 | 65.52 ± 0.25          | 69.70 ± 0.45 |
|         | PreResNet-164 | 80.20 ± 0.41          | 80.35 ± 0.27 | 78.14 ± 0.48          | 78.87 ± 0.27 |

On ImageNet, we experiment with ResNet-18 / 50 [19]. Following [19, 50], we start from pre-trained models (they are from torchvision.models) and collect weights by running SGD optimizer up to 10 epochs (with a constant learning rate 0.005). In Table 2, we report the test accuracy and observe that with more sampling epochs, both TWA and SWA achieve better performance. Notably, TWA performs significantly better than SWA by 0.1 – 0.3\%, and such improvements are more obvious in “5 EPOCHS” case. For example, using 5 epochs of weights, TWA achieves 70.23\% accuracy with ResNet-18 and 76.78\% accuracy with ResNet-50, outperforming the SWA counterparts with 10 epoch weights. This indicates that TWA requires fewer weight samples to achieve a comparable or even better performance than SWA, due to its ability to reduce the estimation variance.

| MODEL      | PRETRAINED | 5 EPOCHS | 10 EPOCHS | 5 EPOCHS | 10 EPOCHS |
|------------|------------|----------|-----------|----------|-----------|
|            |            | SWA      | TWA       | SWA      | TWA       |
| ResNet-18  | 69.76      | 70.02    | 70.28     | 70.12    | 70.32     |
| ResNet-50  | 76.13      | 76.62    | 76.78     | 76.74    | 76.93     |
5.3 Fast convergence and better generalization

We then move on to the head stage of training, where SWA usually fails due to large estimation variance from the fast-evolving solutions and a large learning rate. Since TWA could better reduce the variance and be much less sensitive to the learning rate, we expect that it will work well in this stage. If so, it is promising to simultaneously attain generalization improvements and training efficiency.

We first focus on CIFAR datasets. The original training schedule contains 200 epochs and we take the first 100 epoch explorations for TWA. The results are given in Table 3, where we observe that TWA achieves better performance compared with the original SGD training with a significantly reduced generalization gap — for instance, we attain $+1.52\%$ accuracy improvement on CIFAR-100 with VGG-16 model while the generalization gap is reduced by $9.56\%$. This suggests that a better solution could already be composed using these historical solutions without further training by more delicate learning rates, which instead may bring overfitting problems and harm the generalization. By comparison, SWA averages these samples equally and shows degraded performance due to the existence of estimation error. Apart from the good performance obtained, TWA also manifests its great potential in improving the training efficiency: we use only 10 epochs to complete the convergence, which takes the original SGD additional 90 epochs. Considering that TWA and SGD have almost the same computation overhead per epoch, the time-saving is around 45%.

### Table 3: Test accuracy (%) and generalization gap (%) on CIFAR-10/100 for head training

| Dataset     | Model            | SGD (200 EPOCHS) | SWA (100 EPOCHS) | TWA (100 + 10 EPOCHS) |
|-------------|------------------|------------------|------------------|-----------------------|
|             |                  | ACCURACY         | GAP              | ACCURACY              | ACCURACY              | GAP              |
| CIFAR-10    | VGG16            | 93.54 ± 0.11     | 6.42             | 92.40 ± 0.08          | 93.79 ± 0.18          | 5.50 (4.08)     |
|             | PreResNet-164    | 95.11 ± 0.17     | 4.86             | 92.52 ± 0.04          | 95.19 ± 0.04          | 4.11 (4.75)     |
| CIFAR-100   | VGG16            | 72.72 ± 0.17     | 26.70            | 69.18 ± 0.24          | 74.24 ± 0.24          | 17.14 (4.96)    |
|             | PreResNet-164    | 75.85 ± 0.18     | 24.10            | 73.36 ± 0.34          | 78.11 ± 0.19          | 20.02 (4.08)    |

We then study the effects of different averaging epochs. Generally, utilizing more epochs of explorations could provide a better estimation for the center minimum and hence lead to better performance. We illustrate the results in Figure 4, where the final accuracy of SGD and the accuracy reached by SGD before averaging are also given as references. It could be observed that the model’s performance is consistently improved with more epochs of explorations, and with optimized coefficients, averaging these historical solutions largely lifts the performance of SGD. Notably, although one single solution in a relatively short period of explorations is not good, satisfied solutions have actually emerged in the subspace spanned by those solutions. Then through proper optimization in subspace, TWA could find it out, e.g., on CIFAR-100 with PreAct ResNet-164 model, averaging over 50 epochs via TWA has already matched the final performance of regular SGD training.

For ImageNet, the efforts required for each epoch training are much greater, and hence efficient methods to reduce the training epochs are highly desirable. The comparison results of SGD/SWA/TWA are shown in Table 4. We observe that besides the reduced generalization gap, TWA takes only 2 epochs for quickly averaging the first 60 epochs of solutions, reaching comparable or even better
We then visualize the optimization trajectory of regular training. Due to the very high-dimensional nature of DNNs, it is generally hard to illustrate their training process. Nevertheless thanks to the fast eigenvalue decay property discussed in Section 3, we are able to visualize it with most variance information kept. Specifically, we take the first two principal directions of PCA on $[w_0, \cdots, w_{100}]$ as $x/y$-axis with mean as the origin. We then project the solutions along the trajectory as well as the TW A solution onto the plane and display them in Figure 6. We have the following observations: (1) SWA, which is the origin due to the centralization of PCA, is not a good solution for the head training stage; (2) TW A effectively finds the minimum of training loss; (3) The minimal test error on this 2-D plane is already close to that of TW A solution, coinciding with the fast eigenvalue decay and also verifying that a good solution has emerged as a combination of the historical solution (notice

| Model  | SGD (90 epochs) | SWA (60 epochs) | TWA (60 + 2 epochs) |
|--------|----------------|-----------------|---------------------|
|        | Accuracy       | Gap             |         Accuracy     |         Accuracy | Gap           |
| RESNET-18 | 69.82   | -1.59           | 62.19     | 69.82            | -2.36        |
| RESNET-50 | 75.82    | 0.25            | 67.66     | 75.90            | -0.68        |

Table 6: Wall-clock time per epoch

| Optimizer | Time per epoch |
|-----------|----------------|
| SGD       | 59.04s         |
| TWA       | 60.20s         |

5.4 Landscape visualization

Following [11, 19], we visualize the training loss and test error surfaces of SWA and TWA for CIFAR-100 dataset and PreAct ResNet-164 in Figure 5. We set the SGD solution after 125 training epochs as the origin and plot the TW A and SW A solutions on the plane. For the case with a default learning rate 0.05, we observe TW A achieves slightly better test accuracy with lower training loss. This shows that in the subspace, minimizing the training loss is meaningful and results in lower test error due to the good generalization capability. Especially for the case with a larger learning rate, the superiority of TW A over SW A is more significant (over 0.7% improvement on test accuracy), since the variance becomes larger and the variance reduction effect of TW A is more obvious.

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Figure 5: Train loss and test error surface of TWA and SWA with different SWA\_LR.

Figure 6: Training trajectory visualization on CIFAR-100 with PreAct ResNet-164 model. We take the first two principal directions of PCA on $[w_0, \ldots, w_{100}]$ and set them as $x/y$-axis, respectively, with the mean as the center. 79.9\% of the variance is retained.

that the principal direction is virtually a linear combination of the weight points); (4) The landscape of training loss and test error is quite similar, implying good generalization capability in subspace.

6 Conclusion

In this work, we have introduced TWA, a novel optimization method that utilizes historical solutions of DNNs’ training to achieve fast convergence and better generalization. It allows explicit adjustment of the averaging coefficients in a trainable manner, which is essentially an optimization in a reduced low-dimensional subspace that manifests many favorable properties, such as fast convergence, good generalization, and less sensitivity to the learning rate. We show strong empirical results on benchmark computer vision tasks with various architectures, highlighting that good weights of DNNs’ model could be composed by averaging the head stage solutions with optimized coefficients.

Broader Impact

Our work focuses on utilizing the historical solutions of DNNs’ training to achieve efficiency and better performance, which may have a real impact on promoting more energy-efficient model training.
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A  Training Details

For SW A experiments, we replicate the SW A baseline by using the publicly released implementation of [19]. We use VGG-16 architecture with batch normalization for a unified learning rate setting as PreAct ResNet-164. For ImageNet experiments, we follow official PyTorch implementation\footnote{https://github.com/pytorch/examples/tree/main/imagenet}. We use a condensed learning rate for TWA training with 20x and 30x factors on CIFAR and ImageNet, respectively (e.g. the original learning rate of 0.1 is scaled up to 2 on CIFAR). CIFAR experiments are performed on one Nvidia Geforce GTX 2080 TI GPU, while ImageNet experiments are on four NVIDIA Tesla A100.

We now disclose the specific hyper-parameters in the following.

A.1  SWA training

A.1.1  CIFAR

We use the same schedule and hyper-parameters as in [19]. For VGG-16, we use weight decay of $5 \times 10^{-4}$ and train the model for 300 epochs with weight averaging at 161 to 300 epochs. For PreAct ResNet-164, we use weight decay of $3 \times 10^{-4}$ and train the model for 225 epochs with weight averaging at 126 to 225 epochs. The batch size is set to 128.

For TWA training, we use the same weights as SWA and initialize $w_{twa}$ as the last checkpoint (i.e. 300 / 225 epochs). We train the models for 10 epochs with an initial learning rate of 2 and decay it by 10 at the 5th and 8th epochs. The regularization coefficient $\lambda$ is set to $5 \times 10^{-5}$.

A.1.2  ImageNet

Following [19, 36], we start from pre-trained models (they are from torchvision.models) and collect weights by running SGD optimizer up to 10 epochs (with a constant learning rate 0.005, weight decay $1 \times 10^{-4}$, batch size 256). We uniformly sample the solutions 5 times per epoch.

For TWA training, we use the same weights as SWA and initialize $w_{twa}$ as the pre-trained model. For ImageNet, there are many iterations in one epoch, and hence we conduct TWA training for one epoch, in which we linearly decay the learning rate from 0.03 to 0. The regularization coefficient $\lambda$ is set to $1 \times 10^{-5}$.

A.2  Regular training

A.2.1  CIFAR

For regular training, we train the models for 200 epochs with an initial learning rate of 0.1 and decay it by 10 at the 100th and the 150th epoch. We use SGD optimizer with momentum 0.9, weight decay $1 \times 10^{-4}$, and batch size 128 by convention.

For TWA training, we initialize $w_{twa}$ as $\frac{1}{n} \sum_{i=1}^{n} w_i$, i.e., the center of sampled solutions. We train the models for 10 epochs with an initial learning rate of 2 and decay it by 10 at the 5th and 8th epochs. The regularization coefficient $\lambda$ is set to $1 \times 10^{-5}$.

A.2.2  ImageNet

We follow the training protocol described in [16]. Specifically, we train the models for 90 epochs with an initial learning rate of 0.1 and decay it by a factor of 10 every 30 epochs. We use SGD optimizer with momentum 0.9, weight decay $1 \times 10^{-4}$, and batch size 256.

For TWA training, we uniformly sample solutions 5 times per epoch and initialize $w_{twa}$ as $\frac{1}{n} \sum_{i=1}^{n} w_i$. We train the models for 2 epochs with a learning rate of 0.3 and 0.03, respectively.

For the extra one epoch training, we use the same training protocol as in subsection A.1.2, i.e., linearly decaying the learning rate from 0.03 to 0. The regularization coefficient $\lambda$ is set to $1 \times 10^{-5}$.
B Implementation

The optimization target for TWA is given by

\[
\min_{w_{twa} \in A} L (w_{twa}) = \mathbb{E}_{(x,y) \sim D} [\mathcal{L} (f (w_{twa}; x), y)] + \lambda \cdot \frac{1}{2} \sum_{i=1}^{n} \alpha_i^2,
\]

(5)

where \(A = \{\alpha_1 w_1 + \alpha_2 w_2 + \cdots + \alpha_n w_n \mid \alpha_1 + \alpha_2 + \cdots + \alpha_n = 1\}\) is the possible solution set of \(w_{twa}\). We have discussed in the main paper that the averaging coefficients could be alternatively optimized in the parameter space, and the sum-one constrain can be naturally satisfied in optimizing the left term of (5) (the empirical loss on training data). Hence, we do not need to explicitly impose the constraint and the solution set \(A\) could be relaxed to \(\text{span}\{w_i\}_{i=1}^{n}\). In the following, we first convert the gradients w.r.t. averaging coefficients into the parameter space.

The derivative of the regularization term w.r.t. the averaging coefficient \(\alpha_i\) in the loss function \(L\) is \(\lambda \alpha_i\). Since there exists a bijection between \(\{\alpha_i\}_{i=1}^{n}\) and \(\text{span}\{w_i\}_{i=1}^{n}\), mapping the derivatives into the parameter space and we have

\[
(\lambda \alpha_1, \lambda \alpha_2, \cdots, \lambda \alpha_n) \mapsto \sum_{i=1}^{n} \lambda \alpha_i w_i = \lambda \left( \sum_{i=1}^{n} \alpha_i w_i \right) = \lambda w_{twa}.
\]

(6)

Let \(\frac{dL}{dw}\) be the gradient of the empirical loss w.r.t. the model parameters \(w\) and \(P = [e_1, e_2, \cdots, e_n]\) be the orthogonal basis vectors of the subspace \(\text{span}\{w_i\}_{i=1}^{n}\). To conduct optimization in subspace, we project the gradient \(\frac{dL}{dw}\) (in full parameter space) onto the subspace via the projection matrix \(PP^\top\) and obtain the complete gradient of loss function \(L\) w.r.t. \(w_{twa}\) as following:

\[
\frac{\partial L}{\partial w_{twa}} = PP^\top \frac{dL}{dw_{twa}} + \lambda w_{twa}.
\]

(7)

Thus, we could optimize (2) with the following gradient descent:

\[
w_{twa}^{(t+1)} = (1 - \lambda) w_{twa}^{(t)} - \eta \left(PP^\top\right) \frac{dL}{dw_{twa}},
\]

(8)

where one could see clearly that the \(\ell_2\)-norm regularization on averaging coefficients is equivalent to weight decay on model parameters in reduced subspace.