PREDICTIVE DIFFERENTIAL TRAINING GUIDED BY TRAINING DYNAMICS

Anonymous authors
Paper under double-blind review

ABSTRACT

This paper centers around a novel concept proposed recently by researchers from the control community where the training process of a deep neural network can be considered a nonlinear dynamical system acting upon the high-dimensional weight space. Koopman operator theory (KOT), a data-driven dynamical system analysis framework, can then be deployed to discover the otherwise non-intuitive training dynamics. Taking advantage of the predictive power of KOT, the time-consuming Stochastic Gradient Descent (SGD) iterations can be then bypassed by directly predicting network weights a few epochs later. This "predictive training" framework, however, often suffers from gradient explosion especially for more extensive and complex models. In this paper, we incorporate the idea of "differential learning" into the predictive training framework and propose the so-called "predictive differential training" (PDT) for accelerated learning even for complex network structures. The key contribution is the design of an effective masking strategy based on a dynamic consistency analysis, which selects only those predicted weights whose local training dynamics align with the global dynamics. We refer to these predicted weights as high-fidelity predictions. PDT also includes the design of an acceleration scheduler to adjust the prediction interval and rectify deviations from off-predictions. We demonstrate that PDT can be seamlessly integrated as a plug-in with a diverse array of existing optimizers (SGD, Adam, RMSprop, LAMB, etc.). The experimental results show consistent performance improvement across different network architectures and various datasets, in terms of faster convergence and reduced training time (10-40%) to achieve the baseline's best loss, while maintaining (if not improving) final model accuracy. As the idiom goes, a rising tide lifts all boats; in our context, a subset of high-fidelity predicted weights can accelerate the training of the entire network!

1 INTRODUCTION

The advent of cutting-edge hardware (Li et al., 2014) and the development of parallel processing techniques (Li et al., 2020) have greatly accelerated the training process of Deep Neural Network (DNN). However, enhancing the fundamental techniques of DNN training continues to be a significant challenge. From the inception of Stochastic Gradient Descent (SGD) (Robbins & Monro, 1951), which has since become a mainstay in DNN training, numerous techniques have been proposed to increase the efficiency of the underlying optimization task, including, for example, learning rate annealing and momentum (Sutskever et al., 2013), RMSprop (Tieleman & Hinton, 2012), and Adam (Kingma & Ba, 2014). In addition to these first-order optimizers, second-order alternatives (Martens, 2010) utilizing curvature information or second-order derivatives of the loss function have been explored to potentially enable more efficient convergence. Despite these advancements, gradient-based methods are still inherently iterative, requiring repeated gradient computations and weight adjustments throughout the network. This iterative burden manifests a **fundamental limitation** of SGD and its variants, which lies at the core of the computationally expensive training process.

The concept of *differential learning*—where different parts of the network can exhibit different learning behaviors during training—has emerged as a promising direction to address this limitation. Differential learning can be layer-specific (Devlin et al., 2019; He et al., 2019) or parameter-specific (Tieleman & Hinton, 2012; Duchi et al., 2011a), allowing for more targeted optimization. The Adam optimizer (Kingma & Ba, 2014), for instance, adaptively computes individual learning rates for

different parameters. While differential learning takes adaptive approaches on how parameters are updated, it does not fundamentally address the limitation of the iterative optimization process itself.

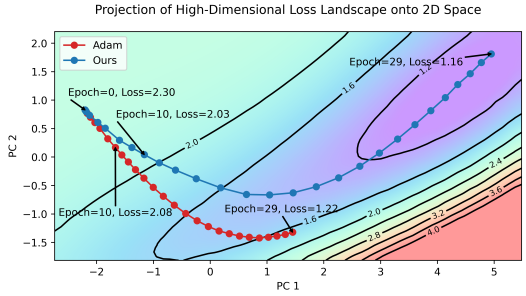


Figure 1: Comparison of training trajectories and loss landscapes between Adam and the proposed PDT. (Trained on CIFAR-10 using AlexNet.)

Recently, a novel interpretation of the DNN training process has been proposed, mainly by researchers from the control community (Redman et al., 2022; Dogra & Redman, 2020; Manojlovic et al., 2020; Tano et al., 2020; Redman et al., 2024) – If it is intuitive to consider a pre-trained DNN as an inherently nonlinear static system acting upon the inputs, then *the DNN "training process" itself is a "nonlinear" dynamical system acting upon the high-dimensional "weight space"*! It is a discrete dynamical system since the weights of a DNN evolve over each iteration (or epoch) according to the optimization process adopted. This drastically different interpretation has led to the establishment of a novel mathematical framework for learning. Koopman Operator Theory (KOT) (Mezić, 2005), a powerful data-driven dynamical system analysis tool, is often adopted to exploit the underlying dynamics in the seemingly non-intuitive training process of a DNN. Taking advantage of the predictive power of KOT, the time-consuming SGD iterations can be bypassed by directly predicting network weights a few epochs later (Dogra, 2020; Dogra & Redman, 2020; Tano et al., 2020). We refer to these approaches as *predictive training*.

However, practical challenges quickly emerge. The absence of actual gradient descent means that convergence cannot be guaranteed, and the framework is sensitive to disturbances in the weight space, leading to error accumulation across iterations. As the network scales, the previous Koopman-based predictive training framework becomes increasingly ineffective. This issue is mostly due to the lack of adaptive mechanisms when applying prediction-based acceleration. That is, existing predictive training approaches tend to accept *all* predicted weights without checking if the prediction is of "high-fidelity" or not. This often leads to gradient explosion, especially for more extensive and complex models.

The **key observation** is that even though KOT is a powerful predictive tool for studying traditional small-scale control problems, when dealing with DNN whose parameter dimension reach into the millions or even billions, the quality of prediction tends to be highly inhomogeneous across the entire weight space. Hence, the predictive learning has to be "selective" – only high-fidelity predictions should be selected to effectively accelerate learning.

In this paper, we propose *predictive differential training* (PDT), where acceleration by prediction is selectively applied based on a dynamic consistency analysis. This principled approach identifies parameters that are in a stable, predictable phase of their evolution by ensuring their local dynamics align with the global system dynamics modeled from the training history. This selective acceleration is conceptually similar to various adaptive learning rate methods. For instance, Adagrad (Duchi et al., 2011b) targets acceleration at rare features; Momentum (Rumelhart et al., 1986) prioritizes weights with the largest recent velocity; and the popular Adam optimizer (Kingma & Ba, 2014) employs a combined strategy. Fig. 1 illustrates the compelling effectiveness of PDT over Adam through a visual comparison of the training trajectory and loss landscape. The contributions of the proposed PDT can be summarized as follows:

- We propose the Predictive Differential Training (PDT) framework that selectively applies predictive updates to effectively accelerate training.

- We design a dynamic consistency analysis as a masking strategy to conduct prediction. It selects parameters whose local training dynamics align with the global dynamics, allowing PDT to identify parameters that are in a stable, predictable phase of their evolution.
- We demonstrate that PDT can be seamlessly integrated as a plug-in with numerous existing optimizers, such as SGD, Adam, RMSprop, Shampoo, and LAMB, while maintaining computational efficiency through epoch-level predictions.
- We validate PDT's effectiveness across a wide range of network architectures (from FCN to ViT-Huge), datasets (from CIFAR-10 to ImageNet), and learning paradigms (from supervised to self-supervised), demonstrating its scalability and robustness under various training conditions.

2 Background and Related Work

The key notion of Koopman analysis is the representation of a (possibly nonlinear) dynamical system as a linear operator on a typically infinite-dimensional space of functions (Mezić, 2021; 2005; Mezić & Banaszuk, 2004). Koopman-based approaches directly contrast with standard linearization techniques that consider the dynamics in a close neighborhood of some nominal solution. Indeed, Koopman analysis can yield linear operators that accurately capture fundamentally nonlinear dynamics.

Koopman Operator Theory. As a brief description, consider a discrete-time dynamical system $\mathbf{x}_{i+1} = T(\mathbf{x}_i)$, where $\mathbf{x}_i \in \mathbb{R}^n$ is the current state and $\mathbf{x}_{i+1}$ is the next state after applying the potentially nonlinear mapping T. Consider also a vector-valued observable $\mathbf{g}(\mathbf{x}) \in \mathbb{R}^m$. The evolution of observables under this mapping can be described as

$$\mathbf{g}(\mathbf{x}_{i+1}) = \mathbf{g}(T(\mathbf{x}_i)) = \mathcal{K}\mathbf{g}(\mathbf{x}_i). \tag{1}$$

where $\mathcal{K}$ operates on the vector space of observables and maps $\mathbf{g}(\mathbf{x}_i)$ to $\mathbf{g}(\mathbf{x}_{i+1})$. $\mathcal{K}$ is referred to as the "Koopman operator" that is associated with the fully nonlinear dynamical system. The Koopman operator is linear, but also infinite-dimensional. As such, for dynamical systems with a pure point spectrum for observables (Mezić, 2020), its action can be decomposed according to

$$\mathbf{g}(\mathbf{x}_{i+1}) = \mathcal{K}\mathbf{g}(\mathbf{x}_i) = \sum_{k=1}^{\infty} \lambda_k \phi_k(\mathbf{x}_i)\mathbf{c}_k, \tag{2}$$

where λ_k is an eigenvalue associated with the eigenfunction $\phi_k(\mathbf{x})$, which can be evaluated at either the initial state $\mathbf{x}_0$ or any intermediate state $\mathbf{x}_i$. $\mathbf{c}_k$ is the reconstruction coefficient, also known as the "Koopman mode", which represents the projection of the observable function $\mathbf{g}$ onto the eigenspace. It immediately follows that $\mathbf{g}(\mathbf{x}_{i+\tau}) = \sum_{k=1}^{\infty} \lambda_k^{\tau} \phi_k(\mathbf{x}_i)\mathbf{c}_k$ for any $\tau \in \mathbb{N}$. This has provided a convenient and general framework to "predict and control" a given dynamical system. Each Koopman mode evolves over time with its frequency and decay rate governed by the imaginary and real components, respectively.

Koopman-based techniques are particularly useful in a data-driven setting because they only require measurements of observables. As such, they can be implemented even when the underlying model dynamics are unknown.

Dynamic Mode Decomposition (DMD). When using Koopman-based approaches, it is critical to identify a suitable *finite* basis for representing the infinite-dimensional Koopman operator. Dynamic Mode Decomposition (DMD) (Schmid, 2010) is one standard approach for inferring Koopman-based models. It uses least-squares fitting techniques to approximate a finite-dimensional linear matrix operator, A, that advances high-dimensional measurements of a system forward in time:

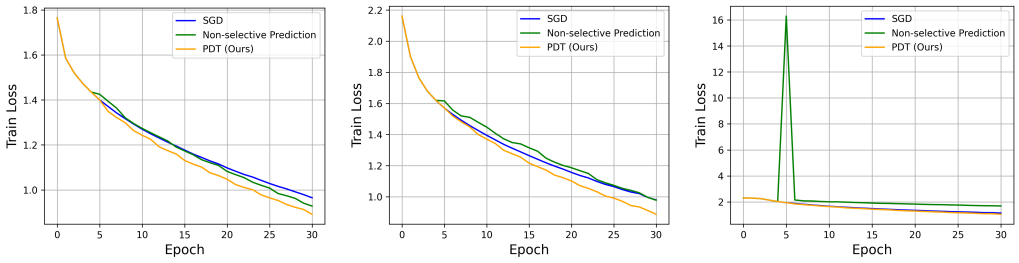
$$\mathbf{g}(\mathbf{x}_{i+1}) \approx A\mathbf{g}(\mathbf{x}_i) \tag{3}$$

where A is an approximation of the Koopman operator, $\mathcal{K}$, in Eq. 1, restricted to a measurement subspace spanned by direct measurements of the state $\mathbf{x}$. Since the weight space of a neural network is a *fully observable* system, we define $\mathbf{g}(.)$ to be the identity function in this work. That is, $\mathbf{w}_i = \mathbf{g}(\mathbf{w}_i)$. In practice, we often use "snapshots" of the system arranged into two data matrices, W_i and W_{i+1}, where columns of these matrices indicate measurements (i.e., network weights) taken at a certain time, and W_{i+1} is W_i shifted by one time step. Hence,

$$W_{i+1} \approx AW_i, \tag{4}$$

and A can be solved by $A = W_{i+1}W_i^\dagger = W_{i+1}V\Sigma^{-1}U^T$, where $W_i = U\Sigma V^T$ is the Singular Value Decomposition (SVD), and $W_i^\dagger$ denotes the pseudo-inverse of W_i. A comprehensive discussion of DMD and its variants has been provided in Kutz et al. (2016).

DNN Training as a Dynamical System. There have been a few works in recent years that adopt Koopman-based approaches to accelerate the training process of a general-purpose DNN model (Dogra & Redman, 2020; Tano et al., 2020; Manojlovic et al., 2020). (Dietrich et al., 2020) is generally considered the first work that establishes the connection between KOT and acceleration of numerical computation. Dogra (2020) is also one of the pioneer works but with a focus specifically on neural networks for solving differential equations. Generally speaking, these works take advantage of the predictive power of the KOT framework to directly predict network weights a few epochs later, thus bypassing the time-consuming SGD iterations. However, we show in Fig. 2 that these methods tend to fail for larger network structures as the network size increases.



(a) 2-layer FC (b) 4-layer FC (c) 6-layer FC

Figure 2: Performance comparison on CIFAR-10 using fully connected (FC) networks with varying depths, among SGD (iterative), PDT (predictive-differential), and the non-selective prediction, i.e., Koopman-based predictive training where the predicted weights are applied to *all* parameters without checking the prediction quality (Tano et al., 2020). Batch size=256, lr=0.01. In our setup, for every three epochs of SGD, predictions are performed for the next five steps.

Directly predicting the evolution of neural network weights, by bypassing SGD, is inherently difficult due to the complex and unstable nature of training dynamics. The loss landscape is highly non-convex, filled with local minima, saddle points, and flat regions (Goodfellow et al., 2014), while the effective dynamics is non-stationary (Ghorbani et al., 2019), as both gradients and curvature shift as training progresses (Sagun et al., 2017). In addition, neural systems can exhibit chaotic or highly sensitive regimes, where small perturbations quickly amplify and destabilize predictions (Li & Ravela, 2021; Engelken et al., 2023). This challenge is compounded by the stochastic noise introduced through mini-batch sampling.

Small prediction errors are highly sensitive and cumulative, risking divergence in the absence of continual gradient correction (Andrychowicz et al., 2016). Moreover, predictors trained in one context often fail to generalize across architectures and datasets, highlighting the difficulty of extracting universally valid patterns (Wichrowska et al., 2017; Metz et al., 2019). Together, these factors make weight prediction a fundamentally unstable and error-prone task.

The proposed PDT, largely due to its adaptive attention to different training dynamics from different parameters, is able to sustain network growth and provide a viable solution to the weight prediction challenge. The efficiency of PDT has been validated on several benchmark models (e.g., AlexNet, ResNet, and ViT), datasets (e.g., CIFAR-10 and ImageNet), spanning both supervised and self-supervised tasks.

3 METHODS

Let us first use a toy example to demonstrate the effect of accelerating the learning of a *subset* of variables to motivate the concept of differential learning. Consider the function,

$$f(x, y, z, u, v, w) = x^2 + y^2 + \sin(z) + u^2 - \cos(v) + w^2 + xy + y\sin(z) + uvw,$$

which involves six variables: x, y, z, u, v, w. To find the minimum of this function, we employ a simple GD optimization with a learning rate of 0.01. GD takes 53 steps to reach a loss value below our predefined threshold (0.1).

We then explore an alternative optimization strategy where the variables x, y, z use a learning rate three times faster than that of the standard process, while u, v, w are optimized at the normal rate but employing the updated values of x, y, z. See Fig. 7 in Appendix A.1 for the acceleration trajectory, where the trajectory maintains the same direction for x and y but reaches the threshold in just 25 steps. This example demonstrates by strategically identifying a subset of variables and simply increasing their learning rate, the training can be accelerated by about 53%. We also apply the proposed PDT to the same optimization problem and it reaches the threshold in 27 steps. See Fig. 8 in the Appendix.

This toy example demonstrates the principle behind the idiom, a rising tide lifts all boats!

3.1 PDT Training Framework

The PDT Training Framework addresses three key questions: 1) when to enable prediction, 2) how to integrate predictions with existing optimizers, and 3) which parameters should undergo accelerated updates. The complete PDT workflow and the mechanism involved in a single acceleration step are illustrated in Fig. 3. The "prediction" block (`Pred`) is automatically but strategically placed among the baseline optimization blocks (`OPT`), acting as a plug-in enhancement within the existing optimization framework. Training begins with a "Burn-in stage," where the model is trained using the baseline optimizer for several epochs to accumulate a sufficient history of weight snapshots. Following this stage, a prediction step is performed with an adaptive interval, τ, to achieve accelerated learning.

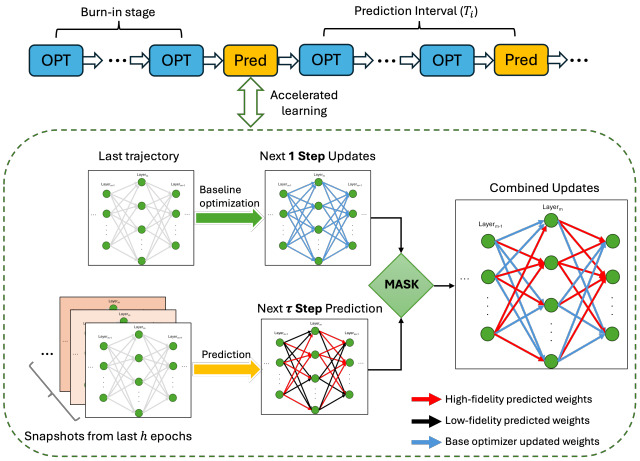


Figure 3: Illustration of the proposed PDT framework and the detailed mechanism for a τ-step prediction, where qualified (or high-fidelity) predicted weights (red) and standard SGD-derived weights (blue) are integrated that accelerate the training of the entire network.

The bottom part of Fig. 3 provides a detailed illustration of how qualified predicted weights and standard SGD-derived weights are integrated together to achieve accelerated learning, as showcased in the toy example. The mask is governed by the dynamic consistency analysis to be elaborated in Sec. 3.2. If no element in the mask satisfies the criteria, then standard SGD-based optimization takes over. The pseudocode of the complete PDT algorithm is presented in Appendix A.2.

The amount of computation required to perform a DMD-based prediction is comparable to that of a GD operation. It is important to note that the prediction operations are much less frequent (once for several epochs) compared to the standard GD operations (multiple times per epoch, depending on the batch size). Considering that PDT requires fewer epochs to reach convergence (see Table 1), it can lead to significant computational savings and efficiency enhancements in the training of large-scale neural networks. A detailed analysis of computational efficiency in terms of FLOPs is provided in Appendix A.3 and the theoretical complexity analysis provided in Appendix A.4.

3.2 DYNAMIC CONSISTENCY ANALYSIS

Our prediction step begins by applying DMD to the weight snapshots $\mathbf{w}$, which yields a finite-dimensional approximation of the Koopman operator. Instead of directly using the operator A for prediction via matrix exponentiation (i.e., A^τ), which can be unstable for large systems as shown in Fig. 2, we perform eigendecomposition of A that yields the DMD modes and their corresponding eigenvalues. To practically implement the spectral prediction from Eq. 2, the predicted weight vector is computed from Eq. 5:

$$\mathbf{w}_{i+\tau}^{\text{pred}} = \mathbf{\Phi}\mathbf{\Lambda}^\tau\mathbf{\Phi}^\dagger\mathbf{w}_i \tag{5}$$

where $\mathbf{\Phi}$ is the matrix whose columns are the DMD modes (approximating the eigenfunctions ϕ_k), and $\mathbf{\Lambda}$ is the diagonal matrix containing the corresponding eigenvalues λ_k. The term $\mathbf{\Phi}^\dagger\mathbf{w}(i)$ projects the current state onto the DMD modes, calculating the Koopman mode amplitudes $\mathbf{c}_k$ in Eq. 2.

Our approach is based on the principle that DMD extracts the dominant patterns of the entire system's dynamics. However, at any given training stage, different parameters may exhibit varying degrees of alignment with these global patterns. Parameters experiencing rapid transitions, or local instabilities, may not conform to the global linear dynamics assumption underlying DMD. The eigendecomposition of A yields the eigenvalues and eigenfunctions. With these components, we can perform a multi-step prediction through a more stable spectral evolution process using Eq. 5, which provides a prediction for the system's global dynamics and also offers a perspective on the prediction for each parameter. The challenge, however, is how to determine whether such a prediction for each parameter has "high-fidelity" or "low-fidelity".

In fact, the correlation between the quality of prediction and training effectiveness has been heavily studied. From a neuroscience perspective, the quality of predictions made by neurons is intricately linked to their learning dynamics (Schultz et al., 1997; Friston, 2010). Accurate predictions lead to more stable and efficient learning, while poor predictions need stronger synaptic adjustments to improve future performance.

Therefore, we design a masking mechanism to identify parameters whose current local dynamics align with the system's global dynamics, based on the following two principles.

The acceleration effectiveness criterion. The absolute weight change between the predicted weight, $\mathbf{w}_{i+\tau}^{\text{pred}}$, and the current weight, $\mathbf{w}_i^{\text{opt}}$, at each epoch, i, should be *larger* than the absolute weight change from the one-step optimization, $\mathbf{w}_{i+1}^{\text{opt}} - \mathbf{w}_i^{\text{opt}}$, to enable accelerated learning. That is,

$$\|\mathbf{w}_{i+\tau}^{\text{pred}} - \mathbf{w}_i^{\text{opt}}\| \geq \tau\|\mathbf{w}_{i+1}^{\text{opt}} - \mathbf{w}_i^{\text{opt}}\|, \tag{6}$$

This criterion ensures that the prediction provides a significant advancement beyond what single-step optimization would achieve, making the acceleration worthwhile. See Appendix A.5 for convergence guarantee analysis.

The dynamic consistency criterion. The direction of weight change from prediction should align with the local gradient-based dynamics. That is, the temporal evolution captured by the global DMD analysis should be consistent with the current local optimization trajectory. Specifically:

$$sign(\mathbf{w}_{i+k,j}^{\text{pred}} - \mathbf{w}_{i+k-1,j}^{\text{pred}}) = sign(\mathbf{w}_{i+1,j}^{\text{opt}} - \mathbf{w}_{i,j}^{\text{opt}}), \tag{7}$$

where j is the index for each element in the weight vector and $k = \{1, \cdots, \tau\}$. This criterion ensures that each step of the prediction interval follows the same trend of growth as that of the local optimization.

Based on these two principles, a mask, $\mathbf{m}$ can be constructed with its element equal to 1 if both Eqs. 6 and 7 are satisfied; otherwise, the corresponding element is zero. This dynamic consistency analysis evaluates these two criteria independently for each parameter. Parameters satisfying both criteria are deemed to be in a predictable evolutionary phase, allowing safe application of temporal acceleration through the global dynamic model. Parameters failing these criteria may be experiencing complex local behaviors (such as rapid transitions, oscillations, or instabilities) that deviate from the global linear dynamics assumption, requiring fallback to gradient-based updates. Note that Eq. 7 is a rigid criterion to enforce not only that the final predicted weight changes align with the local optimization direction, but also that every intermediate step in the predicted trajectory maintains direction consistency.

4 EXPERIMENTS

4.1 GENERALIZATION STUDY OF PDT

We evaluate the effectiveness of the proposed PDT framework in accelerating learning across a variety of popular neural network architectures with different scales, including Fully-Convolutional-Network (FCN) (3.9M parameters), AlexNet (57M parameters), ResNet-50 (25.6M parameters), ViT-Base (86.4M parameters), and ViT-Huge (632M parameters). PDT shows a significant advancement over previous prediction-only Koopman-based methods limited to simpler models [e.g., (Tano et al., 2020) with 2.9M trainable parameters]. We also use a range of optimizers, including SGD, SGD with momentum, and AdamW (Loshchilov & Hutter, 2019). Our validation spans multiple benchmark datasets, from CIFAR-10 to the more challenging ImageNet-1K.

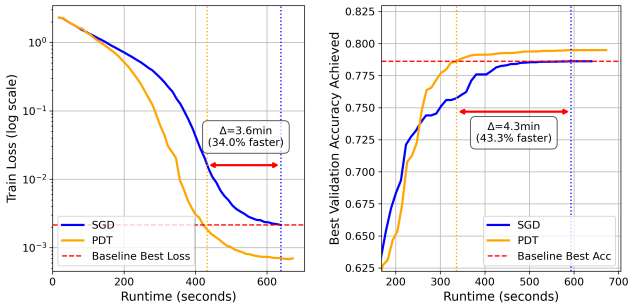


Figure 4: Analysis of PDT's Optimization and Generalization Efficiency. Trained on CIFAR-10 using AlexNet, batch size=256, lr=0.05, with CosineAnnealingLR scheduler.

Fig. 4 illustrates the efficiency of PDT by showing the training curve on CIFAR-10 using AlexNet. We assess PDT's performance from two perspectives: (1) Optimization Efficiency, measured by the **Time to Baseline Best Train Loss** (or **TTB-Loss**), quantifies the speed at which PDT converges on the training objective. (2) Generalization Efficiency, measured by the **Time to Baseline Best Validation Accuracy** (or **TTB-Acc**), reflects the speed at which PDT obtains a useful, well-generalized model. The detailed training curves on various network structures can be found in Fig. 10 in Appendix A.6.

In all experiments, we use the past five epochs to form the snapshot with a one-epoch interval to predict weights in the next five steps. Prediction starts from the 5th epoch. A comprehensive study of PDT's performance under different training configurations (batch sizes, learning rates, and optimizers) and hyperparameters [i.e., prediction steps (τ), prediction interval (T_i), starting epoch (T_0), and past snapshot counts (h)] can be found in Appendix A.9, demonstrating robust performance across various training hyperparameters.

As elaborated in Sec. 3, the computational load of the Koopman-related calculations is comparable to that of batch-level updates. However, since we apply these calculations at the epoch level, the overhead introduced by DMD is effectively compensated by the acceleration in loss reduction. We observe from both Table 1 and Fig. 10 that the proposed PDT consistently achieves the best training loss of the Baseline but in fewer number of epochs without sacrificing performance. All experiments were repeated with five random seeds to ensure reliability. Unless otherwise specified, all results in the tables are reported as mean ± standard deviation over five runs.

The last column in Fig. 10 illustrates a so-called "masked ratio curve" unique to PDT, where it tracks the percentage of predictions accepted according to the masking strategy described in Sec. 3.2. We observe that the masked ratio always starts with higher values in the early stage of the training process, then generally decreases as training progresses. This pattern implies that for large networks on large datasets, the training dynamics is very complex and challenging to predict at the initial training stage, resulting in a rapid reduction of the percentage of weights that can be convincingly predicted (according to the proposed masking strategy). A detailed analysis of how the mask distribution evolves across different layers of the network during training is provided in Appendix A.7.

To further demonstrate the versatility of PDT as a plug-in enhancement, we extended our evaluation to include a broader range of optimizers [SGD, SGD with momentum, Adam, AdamW, RMSprop,

Table 1: Runtime comparison. FCN and AlexNet are trained on a single Nvidia RTX A6000 GPU, while ResNet-50, ViT-Base, and ViT-Huge are trained on three Nvidia H100 (80 GB) GPUs. Using the same experimental setup and hyperparameter configurations as in Fig. 10.

Model	TTB-Loss (s)		TTB-Acc (s)		Runtime Reduction (%)	
	Baseline	PDT	Baseline	PDT	Train Loss	Val. Acc.
FCN	2174.32	1313.52	2088.58	1424.14	**39.59**	**31.81**
AlexNet	683.93	430.91	531.30	347.11	**37.00**	**34.67**
ResNet-50	110063.72	88752.33	121449.60	92133.34	**19.36**	**24.14**
ViT-Base	259241.21	232810.62	296028.36	243097.58	**10.20**	**17.88**
ViT-Huge	725564.86	653854.05	741220.54	660711.80	**9.88**	**10.86**

Shampoo (Gupta et al., 2018), and LAMB (You et al., 2020)] while keeping the network architecture and other configurations fixed. The results in Table 2 show that PDT consistently reduces the time to reach baseline best loss across these optimizers.

Table 2: Impact of baseline optimizers on PDT performance. Trained on CIFAR-10 using AlexNet, batch size=256, momentum=0.9, with CosineAnnealingLR scheduler.

Optimizer	lr	Final Accuracy	Best Train Loss	TTB-Loss (s)	Runtime Reduction (%)
SGD	0.1	0.7930 ± 0.0023	0.0002 ± 0.0000	665.27 ± 9.08	**19.67**
PDT		0.7978 ± 0.0032	0.0002 ± 0.0000	534.41 ± 12.64	
Momentum	0.001	0.6672 ± 0.0068	0.8609 ± 0.0166	752.74 ± 9.62	**41.06**
PDT		0.7298 ± 0.0051	0.5358 ± 0.0165	443.68 ± 8.75	
Adam	0.0005	0.7952 ± 0.0063	0.0001 ± 0.0000	779.13 ± 11.81	**14.87**
PDT		0.8050 ± 0.0050	0.0002 ± 0.0000	663.28 ± 15.30	
AdamW	5e-5	0.8031 ± 0.0021	0.0077 ± 0.0002	652.92 ± 5.26	**28.36**
PDT		0.8149 ± 0.0037	0.0013 ± 0.0002	467.76 ± 6.05	
RMSprop	0.0001	0.7996 ± 0.0032	4.1e-5 $\pm$ 1.6e-5	661.08 ± 0.42	**15.35**
PDT		0.8108 ± 0.0026	2.4e-5 $\pm$ 0.6e-5	559.61 ± 0.00	
Shampoo	0.001	0.8012 ± 0.0071	0.0040 ± 0.0005	736.56 ± 10.58	**16.03**
PDT		0.8101 ± 0.0043	0.0033 ± 0.0003	618.49 ± 12.72	
LAMB	0.001	0.8034 ± 0.0025	0.1215 ± 0.0085	663.25 ± 5.44	**44.24**
PDT		0.8140 ± 0.0027	0.0036 ± 0.0006	369.82 ± 10.59	

We also extend our evaluation to the domain of self-supervised learning (SSL). We select SimSiam (Chen & He, 2021), a prominent non-contrastive method, as our testbed. SimSiam's training dynamics, which are driven by a stop-gradient mechanism and a negative cosine similarity objective, are fundamentally different from those of supervised learning. The results, summarized in Table 3, demonstrate that PDT's advantages generalize effectively to SSL.

Table 3: Performance comparison of SimSiam pre-training on CIFAR-10 with a ResNet-18 backbone, trained for 200 epochs, lr=0.03, batch size=256, momentum=0.9, with CosineAnnealingLR scheduler.

Optimizer	Final Accuracy	TTB-Loss (s)	TTB-Acc (s)	Runtime Reduction (%)	
				Train Loss	Val. Acc.
SGD Momentum	0.7285 ± 0.0166	9611.35 ± 837.98	7353.12 ± 1063.96	**48.78**	**16.10**
PDT	0.7685 ± 0.0144	4922.92 ± 712.55	6169.04 ± 1142.97		

In addition, further analysis of PDT's performance under non-i.i.d. training conditions is presented in Appendix A.8.

4.2 Masking Strategy: Random Selection and Validation Loss?

In this experiment, we study the effectiveness of the proposed masking strategy by comparing it with randomly selecting a subset of predicted weights. We perform a series of runs where subsets of Koopman predicted weights are randomly selected. The regions highlighted in green in Fig. 5 show the outcomes of these trials. Quite frequently, these runs result in gradient explosions, leading to non-recoverable errors (NaN values) in subsequent epochs. This experiment underscores the importance of a principled masking strategy in Koopman Training. Random masking, without considering the training dynamics can lead to severe divergence and training failure. Our findings highlight that strategic selection based on "high-fidelity" predictions is crucial to the success of PDT.

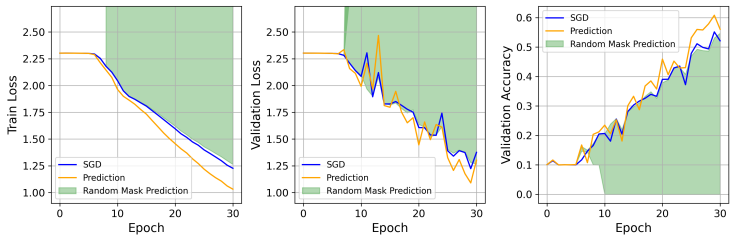


Figure 5: PDT vs. random mask prediction (with the same mask ratio). Trained on CIFAR-10 using AlexNet, batch size=256, lr = 0.01.

We implement another baseline scheduling scheme that switches between prediction and SGD based on the validation loss trend: apply prediction when validation loss decreases and roll back to SGD updates when validation loss starts to increase. Fig. 6 illustrates the training dynamics under this strategy. Initially, DMD is engaged due to its slight advantage in reducing validation loss. However, as training progresses, a significant surge in loss is observed, suggesting a misalignment between the DMD-predicted weights and the optimal trajectory for the network. Even after reverting to SGD, the model failed to recover, indicating that relying solely on validation loss as a trigger for switching between PDT and SGD is inadequate.

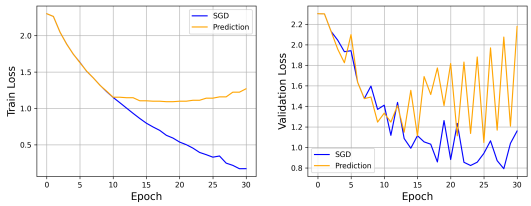


Figure 6: Performance comparison on CIFAR-10 using AlexNet: SGD vs. Koopman-based prediction (switching between prediction and SGD based on validation loss). L: Train loss. R: Validation loss.

5 Conclusion

This paper proposed a novel predictive differential training (PDT) framework based on the study of training dynamics. PDT incorporate the idea of "differential learning" into the predictive training framework for accelerated learning even for complex network structures. The key contribution is the design of an effective masking strategy based on a dynamic consistency analysis, which selects only those predicted weights of high-fidelity whose local training dynamics align with the global dynamics. Analogous to the saying *a rising tide lifts all boats*, in our setting, a subset of high-fidelity predicted weights facilitates more efficient training across the entire network!

The training process of a deep network with millions to billions of parameters indeed presents an intriguing dynamical system that the control community has not faced before. This would stimulate further investigation into the development of better data-driven dynamical system analysis algorithms in addition to DMD.

REFERENCES

Marcin Andrychowicz, Misha Denil, Sergio Gomez, Matthew W Hoffman, David Pfau, Tom Schaul, Brendan Shillingford, and Nando De Freitas. Learning to learn by gradient descent by gradient descent. *Advances in neural information processing systems*, 29, 2016.

Xinlei Chen and Kaiming He. Exploring simple siamese representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 15750–15758, 2021.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv:1810.04805*, 2019.

F. Dietrich, T. N. Thiem, and I. G. Kevrekidis. On the koopman operator of algorithms. *SIAM Journal on Applied Dynamical Systems*, 19(2):860–885, 2020.

Akshunna S Dogra. Dynamical systems and neural networks. *arXiv preprint arXiv:2004.11826*, 2020.

Akshunna S Dogra and William Redman. Optimizing neural networks via koopman operator theory. *Advances in Neural Information Processing Systems*, 33:2087–2097, 2020.

John Duchi, Elad Hazan, and Yoram Singer. Adagrad: Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12:2121–2159, 2011a.

John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. *Journal of machine learning research*, 12(7), 2011b.

Rainer Engelken, Fred Wolf, and Larry F Abbott. Lyapunov spectra of chaotic recurrent neural networks. *Physical Review Research*, 5(4):043044, 2023.

K. Friston. The free-energy principle: a unified brain theory? *Nature Reviews Neuroscience*, 11(2): 127–138, 2010.

Behrooz Ghorbani, Shankar Krishnan, and Ying Xiao. An investigation into neural net optimization via hessian eigenvalue density. In *International Conference on Machine Learning*, pp. 2232–2241. PMLR, 2019.

Ian J Goodfellow, Oriol Vinyals, and Andrew M Saxe. Qualitatively characterizing neural network optimization problems. *arXiv preprint arXiv:1412.6544*, 2014.

Vineet Gupta, Tomer Koren, and Yoram Singer. Shampoo: Preconditioned stochastic tensor optimization. In *International Conference on Machine Learning*, pp. 1842–1850. PMLR, 2018.

Tong He, Zhi Zhang, Hang Zhang, Zhongyue Zhang, Junyuan Xie, and Mu Li. Bag of tricks for image classification with convolutional neural networks. *arXiv:1812.01187*, 2019.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

J. Nathan Kutz, Steven L. Brunton, Bingni W. Brunton, and Joshua L. Proctor. *Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems*. SIAM-Society for Industrial and Applied Mathematics, 2016. ISBN 978-1-61197-449-2.

Mu Li, David G Andersen, Jun Woo Park, Alexander J Smola, Amr Ahmed, Vanja Josifovski, James Long, Eugene J Shekita, and Bor-Yiing Su. Scaling distributed machine learning with the parameter server. In *11th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 14)*, pp. 583–598, 2014.

Shen Li, Yanli Zhao, Rohan Varma, Omkar Salpekar, Pieter Noordhuis, Teng Li, Adam Paszke, Jeff Smith, Brian Vaughan, Pritam Damania, et al. Pytorch distributed: Experiences on accelerating data parallel training. *arXiv preprint arXiv:2006.15704*, 2020.

Ziwei Li and Sai Ravela. Neural networks as geometric chaotic maps. *IEEE Transactions on Neural Networks and Learning Systems*, 34(1):527–533, 2021.

Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=Bkg6RiCqY7.

Iva Manojlovic, Maria Fonoberova, Ryan Mohr, Aleksandr Andrejcuk, Zlatko Drmac, Yannis Kevrekidis, and Igor Mezić. Applications of koopman mode analysis to neural networks. *arXiv preprint arXiv:2006.11765*, 2020.

James Martens. Deep learning via hessian-free optimization. In *ICML*, pp. 735–742, 08 2010.

Luke Metz, Niru Maheswaranathan, Jeremy Nixon, Daniel Freeman, and Jascha Sohl-Dickstein. Understanding and correcting pathologies in the training of learned optimizers. In *International Conference on Machine Learning*, pp. 4556–4565. PMLR, 2019.

I. Mezić. Spectrum of the Koopman operator, spectral expansions in functional spaces, and state-space geometry. *Journal of Nonlinear Science*, 30(5):2091–2145, 2020.

I. Mezić and A. Banaszuk. Comparison of systems with complex behavior. *Physica D: Nonlinear Phenomena*, 197(1-2):101–133, 2004.

Igor Mezić. Spectral properties of dynamical systems, model reduction and decompositions. *Nonlinear Dynamics*, 41:309–325, 2005.

Igor Mezić. Koopman operator, geometry, and learning of dynamical systems. *Notices of the American Mathematical Society*, 68(7):1087–1105, 2021.

William Redman, Maria Fonoberova, Ryan Mohr, Ioannis G Kevrekidis, and Igor Mezić. An operator theoretic view on pruning deep neural networks. *International Conference on Learning Representations (ICLR)*, 2022.

William Redman, Juan Bello-Rivas, Maria Fonoberova, Ryan Mohr, Yannis Kevrekidis, and Igor Mezic. Identifying equivalent training dynamics. *Advances in Neural Information Processing Systems*, 37:23603–23629, 2024.

Herbert Robbins and Sutton Monro. A stochastic approximation method. *The Annals of Mathematical Statistics*, 22(3):400 – 407, 1951. doi: 10.1214/aoms/1177729586. URL https://doi.org/10.1214/aoms/1177729586.

David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning representations by back-propagating errors. *nature*, 323(6088):533–536, 1986.

Levent Sagun, Utku Evci, V Ugur Guney, Yann Dauphin, and Leon Bottou. Empirical analysis of the hessian of over-parametrized neural networks. *arXiv preprint arXiv:1706.04454*, 2017.

Peter J. Schmid. Dynamic mode decomposition of numerical and experimental data. *Journal of Fluid Mechanics*, 656:5–28, 2010. doi: 10.1017/S0022112010001217.

W. Schultz, P. Dayan, and P.R. Montague. A neural substrate of prediction and reward. *Science*, 275 (5306):1593–1599, 1997.

Ilya Sutskever, James Martens, George Dahl, and Geoffrey Hinton. On the importance of initialization and momentum in deep learning. In *International Conference on Machine Learning (ICML)*, pp. 1139–1147. PMLR, 2013.

Mauricio E Tano, Gavin D Portwood, and Jean C Ragusa. Accelerating training in artificial neural networks with dynamic mode decomposition. *arXiv preprint arXiv:2006.14371*, 2020.

Tijmen Tieleman and Geoffrey Hinton. Rmsprop: Divide the gradient by a running average of its recent magnitude. coursera: Neural networks for machine learning. *COURSERA Neural Networks Mach. Learn*, 17, 2012.

Olga Wichrowska, Niru Maheswaranathan, Matthew W Hoffman, Sergio Gomez Colmenarejo, Misha Denil, Nando Freitas, and Jascha Sohl-Dickstein. Learned optimizers that scale and generalize. In *International conference on machine learning*, pp. 3751–3760. PMLR, 2017.

Yang You, Jing Li, Sashank Reddi, Jonathan Hseu, Sanjiv Kumar, Srinadh Bhojanapalli, Xiaodan Song, James Demmel, Kurt Keutzer, and Cho-Jui Hsieh. Large batch optimization for deep learning: Training bert in 76 minutes. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=Syx4wnEtvH.

A Appendix

A.1 Convergence Path of the Toy Example

To better illustrate the effectiveness of differential learning strategies, we designed a toy optimization problem with six variables. See Sec. 3.1 for the description of the problem. Starting from the initial point $[2.0, 2.0, 1.0, 0.5, -0.5, 1.5]$ with a learning rate of 0.01. Fig. 7 shows the optimization trajectories in the x-y plane, where the background color represents the function value at each point. The blue line with dots represents the GD trajectory, while the red dashed line shows the path of accelerated GD where x, y, z variables use 3x learning rate. All points on the trajectories represent the state after each optimization step. The arrows indicate where each method reaches the threshold value (0.1). Building upon this observation, we apply our proposed PDT method to the same optimization problem. Fig. 8 presents the comparison between standard GD and our proposed PDT method on the same toy optimization problem. Fig. 8(a) uses the same visualization scheme as Fig. 7, showing how PDT follows a similar path but reaches the threshold faster (PDT reaches the threshold in 27 steps). Fig. 8(b) clearly demonstrates the acceleration effect, where PDT's loss decreases more rapidly than GD. The horizontal dashed line indicates the threshold value used as the stopping criterion.

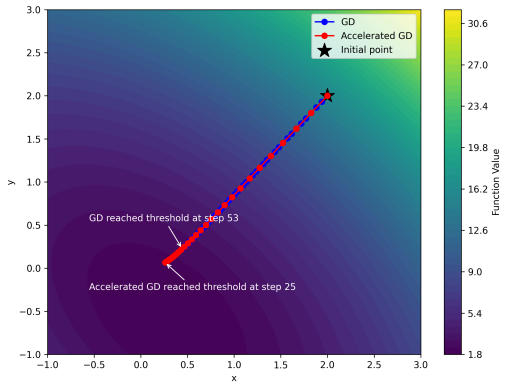
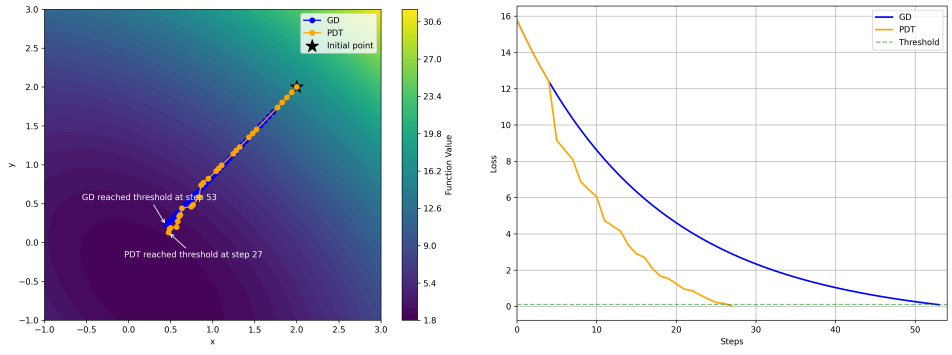


Figure 7: The differential learning trajectory of the toy example provided in Sec. 3.1. Only the x and y dimensions are shown.



(a) (b)

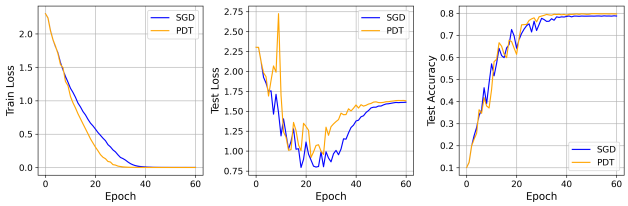
Figure 8: Performance comparison between GD (53 steps) and PDT (27 steps) on the toy optimization problem. (a) Optimization trajectories in the x-y plane. (b) Loss values during optimization.

A.2 Algorithm Descriptions

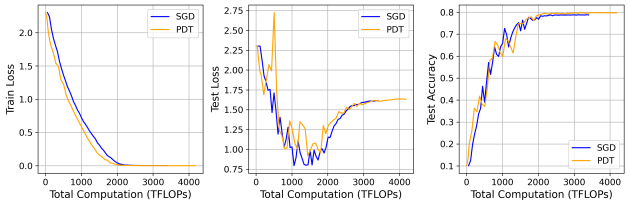
Algorithm 1 PDT algorithm

Require: baseline optimizer O_{base}, past snapshot counts h, start epoch for prediction T_0, predicted steps τ, prediction interval T_i
Ensure: Trained model parameters $\mathbf{w}$

Initialize weight history matrix $\mathbf{W}_{N\times h}$, counter $c_e = 0$
for epoch $t = 0$ to T **do**
  if $t \geq T_0$ **and** $c_e \geq T_i$ **then**
    Obtain $\mathbf{w}^{opt}(t-1)$ from $\mathbf{W}_{N\times h}$
    Train model for one epoch using O_{base}, save weights after training as $\mathbf{w}^{opt}(t)$
    Calculate DMD from $\mathbf{W}_{N\times h}$ to obtain modes $\mathbf{\Phi}$ and eigenvalues $\mathbf{\Lambda}$
    Predict future weights from $\mathbf{w}^{pred}(t)$ to $\mathbf{w}^{pred}(t+\tau-1)$
      1) Decompose: $\mathbf{c} \leftarrow \mathbf{\Phi}^{\dagger}\mathbf{w}(t-1)$ {Project state onto modes}
      2) Evolve: $\mathbf{c}_{\text{evolved}} \leftarrow \mathbf{\Lambda}^{\tau}\mathbf{c}$ {Evolve amplitudes in spectral domain}
      3) Reconstruct: $\mathbf{w}^{pred}(t+\tau-1) \leftarrow \text{real}(\mathbf{\Phi}\mathbf{c}_{\text{evolved}})$ {Synthesize future state}
    {Intermediate predictions for $k \in \{1, ..., \tau-1\}$ are computed similarly for the mask}
    Create mask M based on $\mathbf{w}^{opt}(t-1)$, $\mathbf{w}^{opt}(t)$, $\mathbf{w}^{pred}(t)$ ... $\mathbf{w}^{pred}(t+\tau-1)$ (Eqs. 6 and 7)
    Assemble new weights $\mathbf{w}(t)$ using mask M to combine $\mathbf{w}^{opt}(t)$ and $\mathbf{w}^{pred}(t)$
    Update model parameters with updated $\mathbf{w}(t)$
    $c_e \leftarrow 0$
  else
    Train model for one epoch using O_{base}
    $c_e \leftarrow c_e + 1$
  end if
  Update weight history matrix $\mathbf{W}_{N\times h}$
end for



(a)



(b)

Figure 9: Performance comparison between baseline optimization and PDT, with (a) epochs and (b) TFLOPs as x-axis. Trained on CIFAR-10 using AlexNet, batch size=256, lr=0.05, with Cosine Annealing scheduler.

A.3 Analysis of Computational Efficiency

To provide a detailed analysis of PDT's computational efficiency, we compare the computational cost in terms of FLOPs (Floating-point operations per second) between the baseline optimizer and PDT. Fig. 9 shows the training dynamics with respect to both epochs and total computation cost (measured in TFLOPs). The experiments in Fig. 9 are conducted on AlexNet with CIFAR-10 using batch size of 256, learning rate of 0.05, with Cosine annealing scheduler. While the per-epoch computation of PDT is slightly higher (69.71 TFLOPs) than that of SGD (56.74 TFLOPs) due to the additional DMD

calculations and prediction operations, it achieves faster convergence in terms of total computation. Specifically, PDT requires 2596.30 TFLOPs to reach the baseline's best loss, compared to SGD's 3404.32 TFLOPs, representing a 23.74% reduction in computational cost. Moreover, PDT achieves better final accuracy (79.70% vs 78.75%) despite using fewer FLOPs to reach convergence.

The results also validate our design choice of keeping the past snapshot count (h) small (set to 5 in our experiments). Even with this small h value, which minimizes the computational cost of DMD calculations, PDT achieves substantial acceleration in terms of FLOPs.

A.4 Computational Complexity Analysis

To facilitate our discussion, we consider a DNN with N parameters. The computational load for processing each batch is directly proportional to both the batch size (B) and the number of parameters (N), resulting in a complexity of $\mathcal{O}(B \times N)$ per batch. When extended to the entire dataset with S samples across one epoch, the complexity scales to $\mathcal{O}(S \times N)$.

Integrating Koopman operator predictions into the DNN training process entails constructing a data matrix from h past epochs of the parameter trajectories, with the matrix dimension being $N \times h$. The primary computational burden arises from performing SVD on this matrix with a complexity of $\mathcal{O}(N \times h^2)$. Given that N significantly exceeds h — with h usually being a small number (e.g., 5), and N potentially reaching the millions or even billions—the quadratic impact of h remains manageable relative to N.

A.5 Convergence Analysis

We establish the convergence properties of our hybrid training methodology, which integrates DMD-based predictions with traditional gradient descent updates.

A.5.1 Upper Bound Constraint

Let $\mathbf{w}_i^{\text{opt}}$ denote the optimal weights at iteration i using traditional gradient descent, and $\mathbf{w}_{i+\tau}^{\text{pred}}$ represent the predicted weights using DMD τ steps ahead. We impose the following constraint:

$$\|\mathbf{w}_{i+\tau}^{\text{pred}} - \mathbf{w}_i^{\text{opt}}\| \leq \tau \cdot \|\mathbf{w}_{i+1}^{\text{opt}} - \mathbf{w}_i^{\text{opt}}\| \tag{8}$$

This ensures that the magnitude of any τ-step prediction is bounded by τ times the magnitude of a single gradient step.

A.5.2 Convergence Proof

Let $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ be the loss function with L-Lipschitz continuous gradients. Consider the weight update rule:

$$\mathbf{w}_{i+1} = \mathbf{w}_i - \eta \cdot \mathbf{m}_i \odot \mathbf{u}_i \tag{9}$$

where $\mathbf{m}_i \in \{0, 1\}^d$ is a binary mask, $\odot$ denotes element-wise multiplication, and $\mathbf{u}_i$ is either the gradient $\nabla\mathcal{L}(\mathbf{w}_i)$ or the bounded DMD prediction.

Theorem 1 *Given the update rule above with learning rate $\eta < \frac{2}{L}$ and the constraint in (1), the sequence $\{\mathbf{w}_i\}$ converges to a stationary point of $\mathcal{L}$ as $i \to \infty$.*

[Proof Sketch] For iterations where $\mathbf{u}_i = \nabla\mathcal{L}(\mathbf{w}_i)$, standard convergence results for gradient descent apply. For iterations using DMD predictions, the upper bound constraint ensures:

$$\mathcal{L}(\mathbf{w}_{i+1}) \leq \mathcal{L}(\mathbf{w}_i) - \eta \left(\frac{\eta L}{2} - 1 \right) \|\nabla\mathcal{L}(\mathbf{w}_i)\|^2 \tag{10}$$

Therefore, the sequence $\{\mathcal{L}(\mathbf{w}_i)\}$ is monotonically decreasing and bounded below, guaranteeing convergence to a stationary point.

Proof Outline: Consider the sequence of weight updates given by:

$$w_{t+1} = w_t - \eta \times \text{mask}(t) \times \text{update}(t),$$

where update(t) is selected based on the masking strategy that either applies the gradient of the loss function or the bounded DMD prediction. Given that each update is capped by the gradient's scaling factor, and assuming standard conditions such as Lipschitz continuity of the gradients and a small enough learning rate, the sequence $\{w_t\}$ is guaranteed to make consistent progress towards minimizing the loss function, thereby ensuring convergence.

This bounded predictive approach introduces a robust framework for integrating non-traditional updates into the training of neural networks, offering a safeguard against the instability that unbounded predictions might introduce. Future studies will explore the potential for adjusting the bounding factor dynamically based on the training stage or observed performance metrics, potentially enhancing the adaptability and efficiency of the training process.

A.6 Detailed training curves on various Network Structures

Fig. 10 presents the detailed training curves and performance comparison of PDT and baseline optimizer across various network structures.

A.7 Analysis of Mask Distribution

We further analyze the mask distribution and dynamics in AlexNet. Fig. 11 shows how the ratio of the predicted weights evolves over training epochs. The analysis is conducted using the same experimental setup as in Fig. 10(b), where AlexNet is trained on CIFAR-10.

Fig. 11(a) presents the layer-wise evolution of the ratio of the predicted weights throughout the training process. We observe a pattern here: the masked ratio of each layer starts relatively high, maintaining a stable period, and then gradually declining. The decline phase at the later epochs suggests that as the network approaches convergence, it relies more on gradient-based updates rather than predictions. This aligns with the intuition that predictive updates can be beneficial in the early phases for accelerating convergence but become less necessary as the model stabilizes. The early convolutional layers (e.g., Conv0) exhibit more fluctuations in the percentage of predictive updates, suggesting a higher sensitivity to training dynamics.

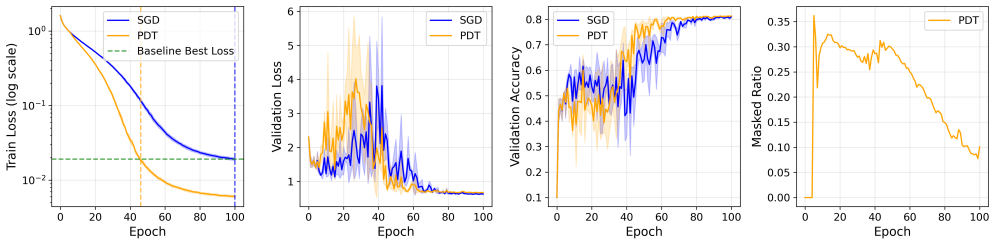
Fig. 11(b) tracks the evolution of predicted weights ratios by layer type. The overall percentage of predictively updated weights is also included. Interestingly, convolutional layers consistently maintain a higher prediction ratio compared to fully connected layers throughout the training process. Due to the majority of the weights in the AlexNet network belonging to the fully connected layers (54.6 million vs. 2.5 million), the overall masked ratio closely follows the trend of fully connected layers.

To provide a finer-grained visualization of the mask distribution, Fig. 12 depicts the mask heatmap for different layers at epoch 20. Each horizontal band represents a layer, where blue regions indicate weights updated by SGD, and red regions correspond to weights updated by prediction results. We can observe that the distribution of predictive updates is not uniform across layers, with some layers showing clustered regions of predictive updates, potentially indicating structured weight adaptations.

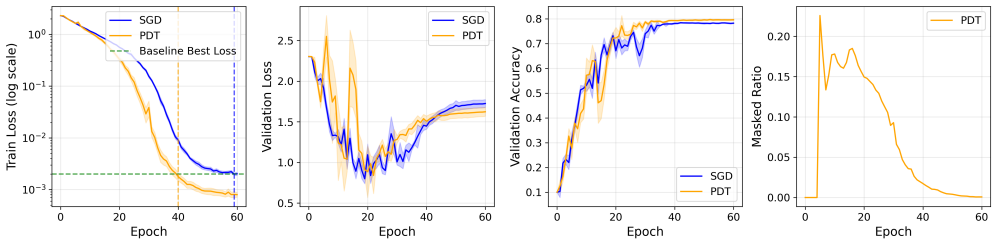
A.8 Effect of Non-i.i.d. Training Data

We further investigate the robustness of PDT under some challenging training conditions. For example, when the batch is too small for a diverse dataset like ImageNet, the weight updates could be chaotic since each consecutive batch is no longer an identical distribution. There are two experimental designs that can test this: 1) test PDT on a very large dataset like ImageNet-22K and 2) design a batching scheme to intentionally violate the i.i.d. assumption of mini-batches using a smaller dataset such as CIFAR-10. In the second design, we maintain the normal batch size, but only put samples of the same class in the batch. We also randomize the batch sequence instead of using any fixed order so that there is no regular training set dynamics that DMD might pick up on.

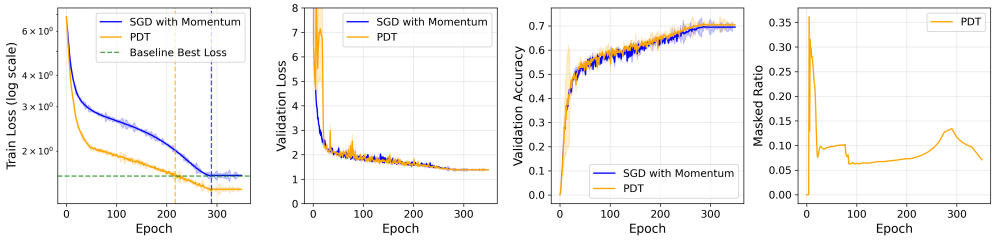
Fig. 13 and Table 4 show the performance and runtime comparison between SGD and PDT under the non-i.i.d. setting using the second experimental design since non-i.i.d. is guaranteed. We preserve



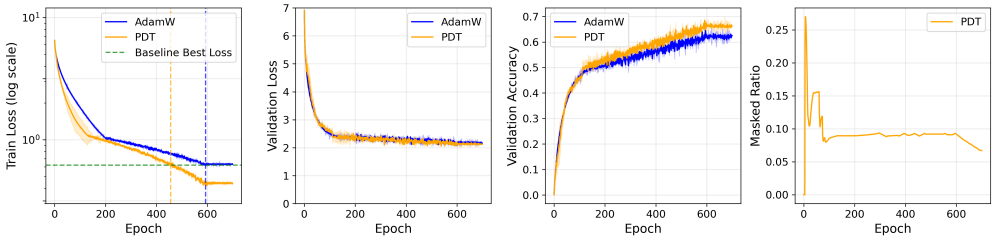
(a) Trained on CIFAR-10 using FCN, batch size=256, lr=0.01, with CosineAnnealingLR scheduler.



(b) Trained on CIFAR-10 using AlexNet, batch size=256, lr=0.05, with CosineAnnealingLR scheduler.



(c) Trained on ImageNet-1K using ResNet-50, batch size=600, lr=0.1, momentum=0.9, with CosineAnnealingLR scheduler.



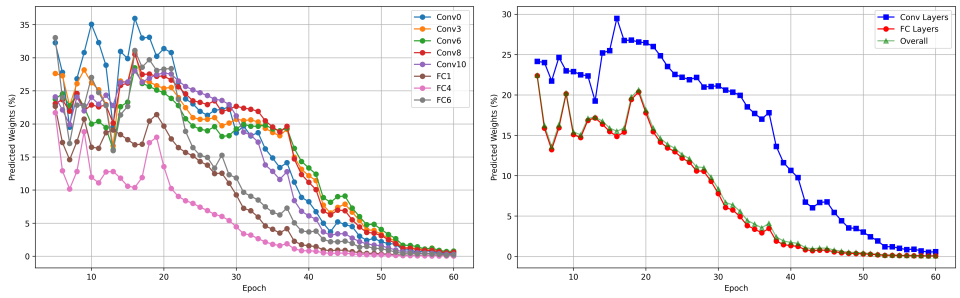
(d) Trained on ImageNet-1K using ViT-Base, batch size=600, lr=0.003, momentum=0.9, with CosineAnnealingLR scheduler.

Figure 10: Performance comparison between baseline optimization and PDT.

the original i.i.d. sampling of the validation set. All experiments are repeated with five random seeds (0, 100, 200, 300, 400) to ensure statistical significance.

We make some interesting observations. First, despite the challenging non-i.i.d. setup, PDT still achieves better performance than SGD in terms of faster convergence without sacrificing accuracy. However, we also observe that in the non-i.i.d. case, learning starts out much more slowly for both SGD and PDT and both take longer to converge. Second, in the non-i.i.d. case, the variance of each of the performance curves is generally larger than those of the i.i.d. case. This is because the model needs to handle more abrupt transitions between different class distributions.

Fig. 13 and Table 4 further demonstrate that PDT's advantage extends beyond standard i.i.d. training conditions, showing its robustness to challenging data sets where traditional assumptions about data distribution are violated.



(a) (b)

Figure 11: Analysis of mask distribution in AlexNet. (a) Layer-wise mask evolution over training epochs. (b) Comparison of prediction ratios between convolutional and fully connected layers.

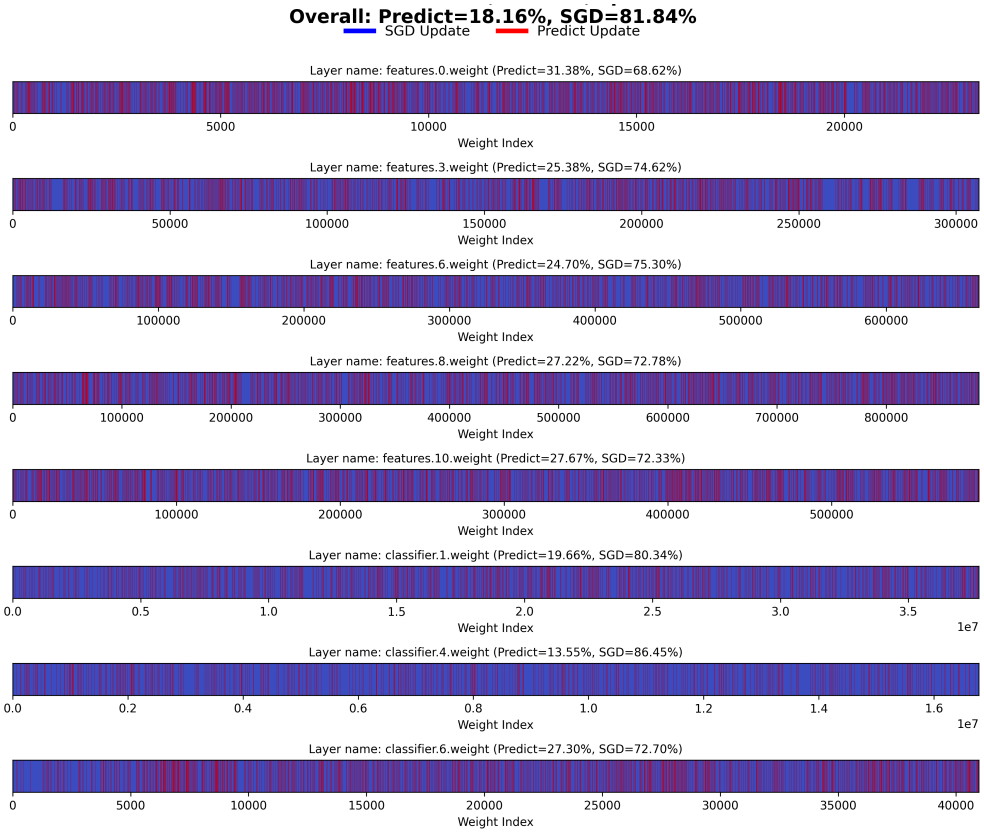


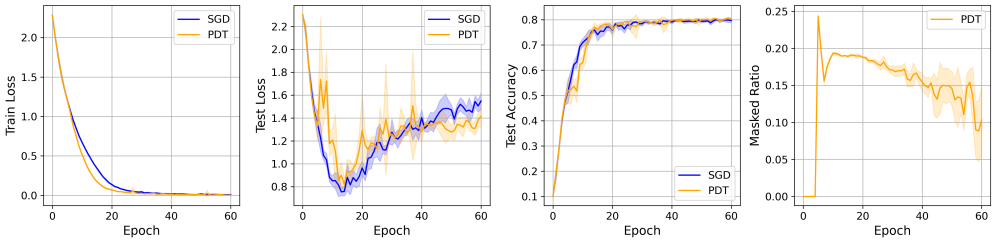
Figure 12: A snapshot at epoch 20 with the mask heatmap for different layers.

A.9 Effect of Training Hyperparameters

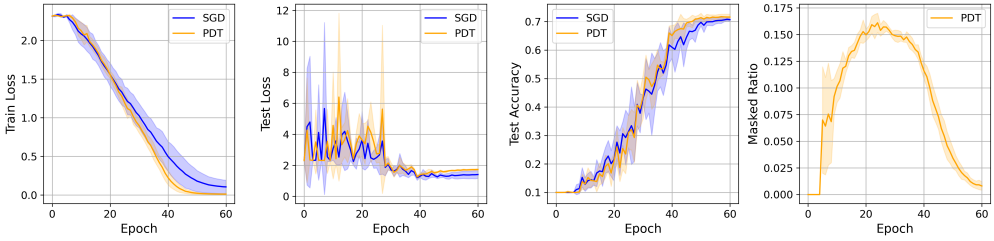
Several primary hyperparameters require careful consideration in PDT:

Prediction Steps (τ): Derived from DMD, the number of prediction steps significantly influences the training speed. As shown in Fig. 14(a) in Appendix Sec. A.9, training accelerates within a certain range of prediction steps. However, extending beyond a critical threshold, such as nine steps in our study, can introduce large errors and potentially cause gradient explosion.

Prediction Interval (T_i): The interval between Prediction blocks impacts the effectiveness of acceleration, as depicted in Fig. 14(b). A shorter interval can enhance training speed if the predictions



(a) Under normal i.i.d. training data distribution.



(b) Under non-i.i.d. training data distribution.

Figure 13: Performance comparison between SGD and PDT under i.i.d. and non-i.i.d. training data distributions, with the same hyperparameters configuration. Trained on CIFAR-10 using AlexNet, batch size=128, lr=0.05, with CosineAnnelingLR scheduler. The shaded areas represent the standard deviation across 5 runs with different random seeds (0, 100, 200, 300, 400).

Table 4: Performance and runtime comparison between SGD and PDT under i.i.d. and non-i.i.d. training data distributions, with the same hyperparameters configuration. Trained on CIFAR-10 using AlexNet, batch size=128, lr=0.05, with CosineAnnelingLR scheduler.

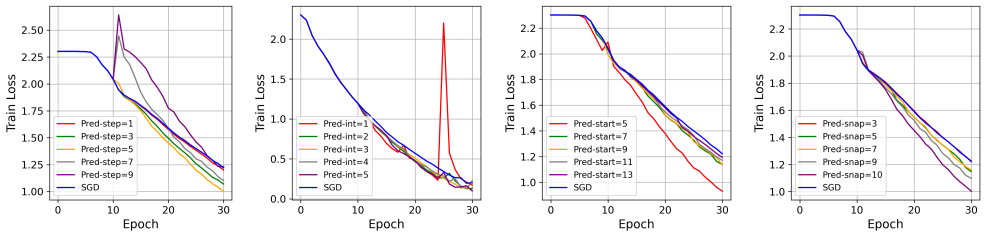
Training Data Distribution	Method	Final Accuracy (mean ± std)	Best Train Loss (mean ± std)	Time to Baseline Best Loss (s) (mean ± std)	Runtime Reduction (%)
i.i.d.	SGD	0.7969 ± 0.0093	0.0039 ± 0.0017	662.48 ± 7.73	9.15
	PDT	0.8011 ± 0.0067	0.0016 ± 0.0017	601.86 ± 17.78	
non-i.i.d.	SGD	0.7067 ± 0.0062	0.1053 ± 0.0874	806.83 ± 13.15	27.90
	PDT	0.7159 ± 0.0103	0.0119 ± 0.0057	581.73 ± 19.34	

are accurate. Nevertheless, the quality of predictions may decline as the training progresses, rendering the network more sensitive to errors, particularly as it nears convergence.

Starting Epoch (T_0): The starting epoch for acceleration must be greater than or equal to the number of epochs used to build the snapshot, as illustrated in Fig. 14(c). The initiation of acceleration is influenced by factors such as initialization, learning rate, and model architecture.

Past Snapshot Counts (h): Fig. 14(d) indicates that the number of epochs needed to construct the snapshot matrix for prediction also influences the train loss. This value cannot be too small or too large. If it is too small, the snapshot will not have sufficient measurements to precisely estimate the dynamics of the training process. If it is too large, DMD would have missed the local dynamics with only a coarser grasp of the general training dynamics.

To thoroughly evaluate the effectiveness and robustness of PDT under different training configurations, we conduct comprehensive experiments across different learning rates from 0.001 to 0.1 (0.001, 0.01, 0.05, 0.1) and batch sizes from 32 to 512 (32, 64, 128, 256, 512). All experiments were repeated with five random seeds (0, 100, 200, 300, 400) to ensure statistical significance. All experiments are performed on AlexNet with the CIFAR-10 dataset, using SGD as the baseline optimizer and trained for 60 epochs. The PDT-related hyperparameters mentioned in Sec. **??** were set to prediction step=5, prediction interval=1, start epoch=5, and past snapshot counts=5.



(a) lr=0.01, int=1, start=10, snap=10.

(b) lr=0.05, step=9, start=10, snap=10.

(c) lr-=0.01, int=1, step=5, snap=5.

(d) lr=0.01, step=5, int=1, start=10.

Figure 14: The influence of different parameters. (a) prediction steps, (b) prediction interval, (c) starting epoch, (d) past snapshot counts. Trained on CIFAR-10 using AlexNet, batch size=256.

The results in Table 5 show the impact of different batch sizes and learning rates on the performance of PDT. At lower learning rates (0.001, 0.01, and 0.05), PDT consistently outperforms SGD in terms of convergence speed across different batch sizes. PDT shows a significant reduction in the runtime to reach baseline best loss, with an average runtime reduction of 22.76% compared to SGD. For higher learning rates (0.1), both SGD and PDT struggled to achieve stable training, and PDT's advantage over SGD became less pronounced. Sometimes PDT can significantly reduce the convergence time (for example, when batch size = 64), but other times the accuracy will drop significantly after reaching a high point, or even result in gradient explosion. This suggests that the high learning rate introduced significant stochasticity, reducing the effectiveness of PDT's prediction mechanism. Smaller batch sizes (32, 64) generally achieve more significant runtime reductions.

To address the stability issues observed at higher learning rates and larger batch sizes, different from the previous fixed learning rate, we investigated the effectiveness of the learning rate scheduler. We tested the Cosine Annealing learning rate scheduler with a minimum learning rate of 1e-3. Taking batch size 256 as an example, we observe significantly improved stability and performance. The results are shown in Table 6. The results are particularly noteworthy at higher learning rates (lr=0.1), where the previous experiments in Table 5 show considerable variance. With the cosine annealing scheduler, PDT achieves consistent accuracy improvements across all learning rates while maintaining substantial runtime reductions.

To further investigate PDT's compatibility with different optimization methods, we compare its performance when integrated with different optimizers (SGD, SGD with momentum, and Adam) while keeping the network architecture and other configurations fixed. For SGD with momentum, we set the momentum factor to 0.9. All experiments are conducted on AlexNet with CIFAR-10 using batch size 256, maintaining the same PDT hyperparameters as in previous experiments. The learning

Table 5: Impact of learning rates and batch sizes on PDT performance. Trained on CIFAR-10 using AlexNet. Note: bold numbers indicate the best performance and underlined numbers indicate the second best performance for each column.

Batch Size	lr	Method	Final Accuracy (mean ± std)	Best Train Loss (mean ± std)	Time to Baseline Best Loss (s) (mean ± std)	Runtime Reduction (%)
32	0.001	SGD	0.6981 ± 0.0458	0.6376 ± 0.0127	1232.29 ± 4.45	40.64
		PDT	0.6903 ± 0.0885	0.2724 ± 0.0166	731.52 ± 12.84	
	0.01	SGD	0.8118 ± 0.0041	0.0046 ± 0.0008	1194.89 ± 21.09	24.25
		PDT	**0.8146 ± 0.0048**	0.0021 ± 0.0012	905.07 ± 120.51	
	0.05	SGD	0.8049 ± 0.0053	0.0156 ± 0.0029	1180.72 ± 12.31	**64.57**
		PDT	0.8020 ± 0.0052	0.0149 ± 0.0073	<u>418.38 ± 0.00</u>	
	0.1	SGD	0.1000 ± 0.0000	0.3346 ± 0.0098	1172.49 ± 39.08	-
		PDT	0.1000 ± 0.0000	0.3364 ± 0.0132	-	
64	0.001	SGD	0.5384 ± 0.0173	1.2295 ± 0.0261	902.16 ± 19.68	35.82
		PDT	0.5329 ± 0.1152	0.8798 ± 0.0257	578.99 ± 55.74	
	0.01	SGD	0.7850 ± 0.0226	0.0087 ± 0.0030	800.35 ± 5.39	23.32
		PDT	<u>0.8140 ± 0.0021</u>	<u>0.0015 ± 0.0010</u>	613.70 ± 8.80	
	0.05	SGD	0.8067 ± 0.0035	0.0051 ± 0.0016	798.20 ± 3.50	27.54
		PDT	0.8029 ± 0.0029	0.0045 ± 0.0006	578.36 ± 16.48	
	0.1	SGD	0.6442 ± 0.2733	0.0484 ± 0.0522	910.37 ± 18.03	<u>56.23</u>
		PDT	0.7976 ± 0.0033	0.0218 ± 0.0011	**398.48 ± 21.34**	
128	0.001	SGD	0.2882 ± 0.0212	1.8456 ± 0.0300	812.42 ± 21.20	17.48
		PDT	0.2951 ± 0.0440	1.6972 ± 0.0272	670.37 ± 23.93	
	0.01	SGD	0.7825 ± 0.0065	0.0675 ± 0.0052	661.09 ± 6.35	14.68
		PDT	0.8009 ± 0.0062	0.0058 ± 0.0008	564.02 ± 16.35	
	0.05	SGD	0.7969 ± 0.0093	0.0039 ± 0.0017	662.48 ± 7.73	9.15
		PDT	0.8011 ± 0.0067	0.0016 ± 0.0017	601.86 ± 17.78	
	0.1	SGD	0.7916 ± 0.0027	0.0083 ± 0.0014	803.93 ± 3.07	8.20
		PDT	0.7863 ± 0.0087	0.0096 ± 0.0016	737.97 ± 0.00	
256	0.001	SGD	0.1171 ± 0.0092	2.2991 ± 0.0011	747.83 ± 20.30	7.08
		PDT	0.1453 ± 0.0213	2.2979 ± 0.0026	694.91 ± 14.63	
	0.01	SGD	0.6989 ± 0.0301	0.5814 ± 0.0147	660.37 ± 0.71	19.98
		PDT	0.7450 ± 0.0236	0.1855 ± 0.0172	528.41 ± 7.26	
	0.05	SGD	0.7931 ± 0.0034	**0.0004 ± 0.0003**	648.39 ± 8.57	21.71
		PDT	0.7916 ± 0.0016	<u>0.0015 ± 0.0014</u>	507.62 ± 11.36	
	0.1	SGD	0.3742 ± 0.3359	0.0508 ± 0.0576	771.77 ± 3.06	-
		PDT	0.3796 ± 0.3425	0.0012 ± 0.0011	-	
512	0.001	SGD	0.1170 ± 0.0251	2.3017 ± 0.0005	748.44 ± 42.46	6.23
		PDT	0.1377 ± 0.0288	2.3020 ± 0.0001	701.82 ± 23.31	
	0.01	SGD	0.5710 ± 0.0203	1.1920 ± 0.0238	671.28 ± 9.03	18.89
		PDT	0.5985 ± 0.0078	0.8311 ± 0.0252	544.46 ± 12.10	
	0.05	SGD	0.7717 ± 0.0038	0.0311 ± 0.0174	668.59 ± 7.30	10.11
		PDT	0.7669 ± 0.0237	0.0034 ± 0.0014	601.01 ± 44.11	
	0.1	SGD	0.3721 ± 0.3332	0.0648 ± 0.0735	768.97 ± 3.12	-
		PDT	0.4420 ± 0.3420	0.0373 ± 0.0155	-	

Table 6: Impact of learning rates on PDT performance. Trained on CIFAR-10 using AlexNet, batch size=256, with CosineAnnealingLR scheduler, minimum learning rate 1e-3. Note: bold numbers indicate the best performance and underlined numbers indicate the second best performance for each column.

Batch Size	lr	Method	Final Accuracy (mean ± std)	Best Train Loss (mean ± std)	Time to Baseline Best Loss (s) (mean ± std)	Runtime Reduction (%)
256	0.001	SGD	0.1217 ± 0.0126	2.2991 ± 0.0011	757.66 ± 26.54	9.88
		PDT	0.1461 ± 0.0213	2.2980 ± 0.0025	682.79 ± 2.13	
	0.01	SGD	0.6451 ± 0.0102	0.9276 ± 0.0212	745.97 ± 47.19	**41.54**
		PDT	0.6974 ± 0.0073	0.5853 ± 0.0159	<u>436.07 ± 16.09</u>	
	0.05	SGD	0.7852 ± 0.0016	0.0020 ± 0.0001	675.04 ± 27.56	<u>37.13</u>
		PDT	<u>0.7936 ± 0.0030</u>	<u>0.0006 ± 0.0001</u>	**424.39 ± 20.40**	
	0.1	SGD	0.7930 ± 0.0023	**0.0002 ± 0.0000**	665.27 ± 9.08	19.67
		PDT	**0.7978 ± 0.0032**	**0.0002 ± 0.0000**	534.41 ± 12.64	

rate is 0.1 for SGD, 0.001 for SGD with Momentum, 0.0005 for Adam. The results are shown in Table 7.

Table 7: Impact of baseline optimizers (SGD, SGD with Momentum, and Adam) on PDT performance. Trained on CIFAR-10 using AlexNet, batch size=256, momentum=0.9, with CosineAnnealingLR scheduler. Note: bold numbers indicate the best performance and underlined numbers indicate the second best performance for each column.

lr	Method	Final Accuracy (mean ± std)	Best Train Loss (mean ± std)	Time to Baseline Best Loss (s) (mean ± std)	Runtime Reduction (%)
0.1	SGD	0.7930 ± 0.0023	<u>0.0002 ± 0.0000</u>	665.27 ± 9.08	<u>19.67</u>
	PDT	<u>0.7978 ± 0.0032</u>	<u>0.0002 ± 0.0000</u>	<u>534.41 ± 12.64</u>	
0.001	Momentum	0.6672 ± 0.0068	0.8609 ± 0.0166	752.74 ± 9.62	**41.06**
	PDT	0.7298 ± 0.0051	0.5358 ± 0.0165	**443.68 ± 8.75**	
0.0005	Adam	0.7952 ± 0.0063	**0.0001 ± 0.0000**	779.13 ± 11.81	14.87
	PDT	**0.8050 ± 0.0050**	<u>0.0002 ± 0.0000</u>	663.28 ± 15.30	