Deforming the Loss Surface

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Abstract

In deep learning, it is usually assumed that the shape of the loss surface is fixed. Differently, a novel concept of deformation operator is first proposed in this paper to deform the loss surface, thereby improving the optimization. Deformation function, as a type of deformation operator, can improve the generalization performance. Moreover, various deformation functions are designed, and their contributions to the loss surface are further provided. Then, the original stochastic gradient descent optimizer is theoretically proved to be a flat minima filter that owns the talent to filter out the sharp minima. Furthermore, the flatter minima could be obtained by exploiting the proposed deformation functions, which is verified on CIFAR-100, with visualizations of loss landscapes near the critical points obtained by both the original optimizer and optimizer enhanced by deformation functions. The experimental results show that deformation functions do find flatter regions. Moreover, on ImageNet, CIFAR-10, and CIFAR-100, popular convolutional neural networks enhanced by deformation functions are compared with the corresponding original models, where significant improvements are observed on all of the involved models equipped with deformation functions. For example, the top-1 test accuracy of ResNet-20 on CIFAR-100 increases by 1.46%, with insignificant additional computational overhead.

1 Introduction

The optimization problem in deep learning is considered to be a non-convex problem with high dimension. Various optimization methods may obtain low training losses, but the testing results are diverse. A promising direction is to link the generalization ability with the flatness near the critical point [1-5]. Some research indicates that although the sharpness alone is not enough to predict the generalization performance accurately, there is still a trend that the flat minima generalize better than that of sharp ones [5-8]. The method of deforming the loss surface proposed in this paper can effectively make the optimizer fall into the flat minima more easily, supported by both theoretical analyses and experiments.

For deep learning models, there are numerous parameters to enable the cost function value to decrease along the negative gradient direction. Even some of the minima are escaped, the optimizer still have the capability to obtain tiny enough cost function value [9]. To provide an intuitive understanding, numerical simulations with two parameters are performed in Fig. 1. Besides, to evaluate the performance of the proposed deformation function, in practice, comparative classification experiments are conducted on ImageNet [10], CIFAR-10 [11], and CIFAR-100 [11] for popular convolutional neural networks (CNNs). Experimental results show that the proposed deformation functions improve the test performances of all the participating models significantly. It is worth mentioning that the proposed deformation functions bring little additional calculation and memory burden. In

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Figure 1: Deformation for a simulated loss surface with two parameters to illustrate that the deformation function has the capability to filter out the sharp minimum.

addition, the deformation method can be applied to various existing first-order optimization methods. Our contributions in this paper are summarized as follows:

- The concept of deforming the loss surface is proposed for the first time, to the best of our knowledge. In order to achieve the purpose of deforming loss surface, deformation operator is proposed, along with conditions it should meet.
- As one kind of deformation operator, deformation function is proposed, along with its deformation characteristics on the loss surface. Specific examples of the deformation functions, i.e., arctan-power-based (AP) deformation function and log-exp-based (LE) deformation function are given, as well as their contributions to loss surfaces.
- The theoretical analyses are provided to prove that the stochastic gradient descent (SGD) optimizer has the ability to filter out sharp minima, while the deformation-function-equipped SGD can find flatter minima. One-dimensional case and high-dimensional case are analyzed theoretically. Specifically, the landscape near the solution obtained by the deformation-function-equipped optimizer has small Lipschitz constant, because all the sharp minima are filtered out during the training process. Besides, visualizing experiments also support that the deformation functions have the capability to filter out the sharp minima.
- Popular CNNs enhanced by deformation functions are compared with the original models on ImageNet, CIFAR-10, and CIFAR-100. The results are surprising—all the involved models get significant improvements, such as, 1.46% top-1 test accuracy improvement for ResNet-20 on CIFAR-100, 0.50% improvement for PreResNet-20 on CIFAR-10, and 1.19% improvement for EfficientNet-B0 on CIFAR-100. These improvements are significant for the involved image classification tasks, especially without introducing additional tricks.

2 Related work

The connection between the flatness of a minimum and generalization is first investigated in [12], with a method of searching the flat minimum. A visualization method is provided by Li et al. to
**Algorithm 1**

**Require:** \( h \): the group of hyperparameters includes learning rate \( h_r \), and other hyperparameters required by the specific first-order optimization method, such as exponential decay rates \( \beta_1 \) and \( \beta_2 \) for ADAM, and momentum \( m \) for SGD with momentum (SGDM).

**Require:** \( \Theta \): a function with respect to \( g^{(1)} \), \( g^{(k-1)} \), \( h \), and step \( k \), represents the increment from \( p^{(k-1)} \) to \( p^{(k)} \). In practice, not all of these independent variables will be explicitly involved in parameter updating. For example, in SGDM, \( \Delta p^{(k-1)} \) contains information from \( g^{(1)} \), \( g^{(k-2)} \) at each step.

**Require:** \( p_0 \): initial value of the parameter \( p \) to be updated.

**Require:** \( \ell \): the loss function.

**Require:** \( \delta \): the deforming function.

\[
\begin{align*}
k & \leftarrow 0 \\
\text{while } \ell \text{ is not small enough do} & \\
& k \leftarrow k + 1 \\
& g^{(k-1)} \leftarrow \nabla \delta(\ell(p^{(k-1)})) \\
& \Delta p^{(k)} \leftarrow \Theta(g^{(1)}, \cdots, g^{(k-1)}, h, k) \\
& p^{(k)} \leftarrow p^{(k-1)} + \Delta p^{(k)} \\
\text{end while} & \\
\text{return } p^{(k)} &
\end{align*}
\]

Illustrate the potential relationship between hyperparameters and generalization ability of CNNs [13]. This visualizing method gives us an intuitive picture of loss surfaces to inspire the studies of deep learning. It is observed in [13] and [14] that the model with smaller batch performs better than that with larger batch in generalization, and the minima obtained by small-batch methods are flatter. In addition, the \( (C, A) \)-sharpness to measure the sharpness at a specified point is defined in [14], and the experimental results support that the generalization performance is highly related to the sharpness. However, research in [7] introduces a re-parametrization method and indicates that the previous measurements of sharpness are not sufficient to predict the generalization capability. Moreover, it is shown in [2] that the generalization ability is affected by the scale of samples, Hessian matrix with its Lipschitz constant of the loss function, and the amount of parameters. Additionally, the flat minimum occupies a larger parameter space than the sharp minimum [15]. Specifically, the possibility that the extreme value is obtained is positively correlated with the volume of the region in the high-dimensional space rather than the width in a single dimension. To eliminate the sharp minima, SmoothOut is proposed in [16]. Both theoretical and practical evidences show that the SmoothOut can find the flat minima. However, SmoothOut still requires the computation of noise injecting and de-noise process. Compared with SmoothOut, the proposed deformation-function-based method in this paper only brings the computation overhead of the deformation function acting on the loss function. In practice, there is no significant time consumption difference between the CNN equipped with deformation function and the original CNN (see supplementary material). Overall, these studies demonstrate the importance of sharpness around the minima.

3 Method

In this section, the method of deforming the loss surface is proposed, followed by theoretical analyses of the flat minima filter.

3.1 Deforming the loss surface

For deforming the loss surface so as to obtain ideal parameters, deformation operator \( \triangledown \) is proposed.
The algorithm for deformation-function-enhanced training process is shown in Algorithm 1. It can be seen from Algorithm 1 that, deforming the loss surface by deformation function can be regarded as a deformation operator if the following conditions are met:

- \( \forall p, \nabla p \ell(p) \ni \exists; \)
- \( \exists \{\ell, p\}, \nabla \{\ell, p\} \neq \{\ell, p\}; \)
- \( \forall n \in [1, n], if p_n^{[i]} < p_n^{[j]}, then \check{p}_n^{[i]} < \check{p}_n^{[j]}; \)
- \( \forall n \in [1, n], if \ell(p_n^{[i]}) < \ell(p_n^{[j]}), then \hat{\ell}(p_n^{[i]}) < \hat{\ell}(\check{p}_n^{[j]}). \)

where \( p_n^{[i]} \) and \( \check{p}_n^{[j]} \) both denote the \( n \)th element of \( p \) and are arbitrary.

As one kind of deformation operator with simple form, the deformation function \( \delta \) is proposed as follows.

**Definition 2.** Suppose that \( \delta : \mathbb{R} \to \mathbb{R} \). For an optimization problem \( \min_p \ell(p) \) with \( p \in \mathbb{R}^n \), \( \delta(\ell) \) is called a deformation function if the following conditions are met:

- \( \delta \) is a deformation operator;
- \( \frac{\partial \delta}{\partial \ell} > 0. \)

**Theorem 1** (Deformation function influences the spectrum of the Hessian matrix). Assuming that \( \ell : \mathbb{R}^n \to \mathbb{R}, \partial^2 \ell / (\partial p_r \partial p_s) \) exists and is continuous for any \( r, s \in [1, n] \), of which \( p_r \) and \( p_s \) denote the \( r \)th and \( s \)th element of \( p \), respectively, and \( \delta \) is the deformation function, then \( \lambda(\mathbf{H}^\ast) = (\partial \delta / \partial \ell) \lambda(\mathbf{H}) \), where \( \lambda(\cdot) \) denotes the spectrum of a matrix, \( \mathbf{H} \) denotes the Hessian matrix of \( \ell \), and \( \mathbf{H}^\ast \) denotes the Hessian matrix of \( \delta \).

Proof is given in the supplementary material. Besides, one can derive that \( \nabla \delta(\ell(p)) = (\partial \delta / \partial \ell) \nabla \ell(p) \). Thus \( \partial \delta / \partial \ell \) can be deemed as a factor that controls the strategy of deformation. If \( \partial \delta / \partial \ell > 1 \), the loss surface is deformed to be sharper; if \( \partial \delta / \partial \ell < 1 \), the surface becomes flatter.

The algorithm for deformation-function-enhanced training process is shown in Algorithm 1. It can be seen from Algorithm 1 that, deforming the loss surface by deformation function can be regarded as acting a function on the loss value, and thus introduces little additional computational overhead—\( O(1) \). The training time comparisons are provided in the supplementary material. Moreover, it is worth noting that although the potential parameters that can give the minimum remain the same after deforming the loss surface, the actual parameters obtained by the optimizers with or without deformation could be diverse. The goal of deforming the loss surface in this paper is to affect the trajectory of the optimizer, and then find the minimum that is flat on the original loss surface. As discussed in Sections 3.2 and 4.1, deforming the loss surface to be sharper when \( \ell \) is small contributes to search the flat minimum instead. Consider that the flatness is more relevant to the landscape near the minimum (i.e., loss value is small), and thus the loss surface where the loss value is smaller is deformed to be sharper in order to filter out the sharp minima.

In the following, the method to obtain deformation functions is given, and several well-performed deformation functions in practice are analysed. Theorem 1 shows that \( \partial \delta / \partial \ell \) directly contributes to the spectrum of the Hessian matrix. With this in mind, one can construct \( \phi(\ell) = \partial \delta / \partial \ell \) firstly, and
The deformation functions can also be constructed directly rather than by antiderivative. Table 1: Comparisons among learning-rate-scheduler-equipped PreResNet-20 and loss-surface-deformed PreResNet-20 on CIFAR-10.

| $1h_\tau$ | $3h_\tau$ | $10h_\tau$ | Cosine | HTD | LE (1, 1) | LE (1, 0.99) | LE (1, 0.95) |
|-----------|-----------|-----------|-------|-----|-----------|-------------|-------------|
| Acc. (%)  | 91.88     | 92.35     | 91.52 | 92.13 | 92.44     | 92.64       | 92.09       |

then use $\int \varphi(\ell)\,d\ell + C$ to obtain the antiderivative of $\varphi(\ell)$, where $C$ is the constant of integration. The deformation functions can also be constructed directly rather than by antiderivative.

In what follows, several well-performed deformation functions designed by following the rule discussed previously are given. The AP deformation function is defined as $\delta(\ell) = a_1 \arctan(a_2 \ell) + a_4 \ell$, where $a_1, a_2, a_3, a_4 > 0$ are the coefficients that control the shape of the AP $(a_1, a_2, a_3, a_4)$. Another well-performed deformation function is LE deformation function: $\delta(\ell) = e_1 \ln(\exp(\ell) - e_2)$, where $e_1, e_2$ are the coefficients that control the shape of the LE $(e_1, e_2)$ with $e_1 > 0$ and $1 \geq e_2 > 0$. Figure 2 illustrates the derivatives of the AP and LE deformation functions with different coefficients. For example, for LE deformation functions with $e_1 = 1$, the deformed surface remains similar to the original one (i.e., $\delta \ell / \delta \ell = 1$) if $\ell$ is large enough, and the deformed surface becomes sharper if $\ell$ approaches zero. Note that one of the differences between learning rate scheduler and deformation function is that the learning rate scheduler is a function of epoch, while deformation function is a function of loss. To compare the performance between learning rate schedulers and deformation functions, Table 1 are provided (see supplementary material for more comparisons on CIFAR-100).

In addition to the proposed deformation function acting on $\ell$, some transformations on the parameters can also be regarded as cases of deformation operators. For example, reparameterization. Specifically, suppose that $\sigma : \mathbb{R}^n \to \mathbb{R}^n$ is bijective, then the parameter is transformed by $\varphi = \sigma(p)$. This approach can be described intuitively as scaling the loss surface along the coordinate axes corresponding to parameters. Due to space limitations, this approach is only presented as an example of deformation operator, and its details will not be investigated in this paper.

3.2 Flattening filter

It is worth noting that, if the deformed model gives the same parameters with the original one, although the shape of the loss surface is changed to be flatter, the accuracy remains the same. However, the trajectories on the deformed loss surface and the original loss surface are diverse, so that the parameters obtained finally are diverse as well, as shown in Section 4.1. With this in mind, the focus is deforming the loss surface to obtain the well-generalizable minima, while the sharp minima are filtered out. For illustrations, the trajectories of SGDM on simulated loss surfaces are given to demonstrate that the deformation function can play a role as a flattening filter, which makes the optimizer to escape from sharp minimum, as depicted in Fig. 1.

In the following, the minima obtained by deformation function are investigated theoretically. Assume that for SGD equipped with the deformation function which follows $p^{(k+1)} = p^{(k)} - h_x \nabla \delta(\ell(p^{(k)}))$, total step $k$ is large enough to drive the model to converge. Firstly, one-dimensional case is discussed, and then the results are extended to high-dimensional case.

Definition 3. Assume that within an interval $(x^{[a]}, x^{[b]})$, $f(x) : \mathbb{R} \to \mathbb{R}$ is differentiable, there are only three extreme points $(x^{[\text{min}]}, f(x^{[\text{min}]})$, $(x^{[\text{max}]}, f(x^{[\text{max}]})$, and $(x^{[\text{max}]}, f(x^{[\text{max}]})$ with $(\partial f(x) / \partial(x)^2)_{\text{[min]}} > 0$, $(\partial f(x) / \partial(x)^2)_{\text{[max]}} < 0$, $(\partial f(x) / \partial(x)^2)_{\text{[max]}} < 0$, and $x^{[\text{max}]}, x^{[\text{max}]}$, and then $(x^{[a]}, x^{[b]})$ is called local concave region (or “local M region” in the sight of geometrical shape) for $f(x)$.

Theorem 2. [Deformation function contributes to the Lipschitz constant] Assume that an interval $(p^{[a]}, p^{[b]})$ is a local M region for $\ell(p)$ with extreme points $(p^{[\text{min}]}, \ell(p^{[\text{min}]})$, $(p^{[\text{max}]}, \ell(p^{[\text{max}]})$, and $(p^{[\text{max}]}, f(p^{[\text{max}]})$, where $p^{[\text{max}]} < p^{[\text{max}]}$, $\ell(p) : \mathbb{R} \to \mathbb{R}$ is differentiable, and that SGD is taken as the optimizer. Let $\Delta p^{[\text{max}]} = p^{[\text{max}]} - p^{[\text{max}]}$ represent the projection of the distance between the adjacent maximum values on $p$. For a sufficiently large $k$, if $p^{(k+1)}$ remains in $(p^{[a]}, p^{[b]})$,
\[ \frac{\partial \ell(p^{(k)})}{\partial p^{(k)}} \text{ is bounded by} \]
\[
\left| \frac{\partial \ell(p^{(k)})}{\partial p^{(k)}} \right| \leq \frac{\Delta p^{[\text{max}]} h_r}{\Delta s \Delta t}.
\]  
(1)

Proof is given in the supplementary material.

**Lemma 1.** Under assumptions of Theorem\(^2\) Lipschitz condition is met:
\[
\|\ell(p^{(k)}) - \ell(\hat{p}^{(k)})\| \leq \frac{\Delta p^{[\text{max}]} \|p^{(k)} - \hat{p}^{(k)}\|}{h_r \Delta s \Delta t},
\]
where \( \hat{p}^{(k)} \in \mathbb{R} \) is arbitrary one-dimensional parameter \( p \) on step \( k \).

**Remark 1.** Note that, if \( \forall k \leq \hat{k}, p^{(k)} \in (p^{[a]}, p^{[b]}) \), and then the model converges within the interval. Moreover, \( \hat{p}^{(k)} \) can be deemed as a set sampled from a subspace of the loss surface where \( \hat{k} = \{ k | p^{(k)} \in (p^{[a]}, p^{[b]}) \} \). The samples contain some information about the nature of the region where the model converges to. From inequality (2), one can deduce that the original SGD have the capability to filter out sharp minima. For SGD equipped with deformation function, if \( \delta s / \delta t \) is increased, the Lipschitz constant of \( \ell(p^{(k)}) \) decreases. This result demonstrates that the deformation method with larger \( \delta s / \delta t \) tend to give flatter minimum.

**Remark 2.** For the high-dimensional case, assume that \( \Delta p^{(k)} = p^{(k+1)} - p^{(k)} = -h_r(\delta \delta / \delta t)\nabla \ell(p^{(k)}) \) and \( \Delta p^{(k+1)} = p^{(k+1)} - p^{(k)} = -h_r(\delta \delta / \delta t)\nabla \ell(p^{(k)}) \) are arbitrary, and then
\[
\Delta p^{(k)} = \frac{(\delta \delta / \delta t)}{(\delta \delta / \delta t)} \Delta p^{(k+1)}.
\]

This result means that the points \( (p^{(k)}, p^{(k)}, \ldots, p^{(k)}) \), \( (p^{(k+1)}, p^{(k+1)}, \ldots, p^{(k+1)}) \), and \( (\hat{p}^{(k+1)}, \hat{p}^{(k+1)}, \ldots, \hat{p}^{(k+1)}) \) are collinear. Denote this line as \( \zeta = \{ (1 - \alpha) p^{(k)}, p^{(k)}, \ldots, p^{(k)} \} \) for \( \alpha \in \mathbb{R} \). Consider another line \( \eta = \{ (1 - \beta) p^{(k)}, p^{(k)}, \ldots, p^{(k)} \} \) for \( \beta \in \mathbb{R} \), then \( \zeta \) and \( \eta \) belong to the same plane (denoted by \( \chi \)). Denote the loss surface as \( \gamma \), then \( \omega = \chi \cap \xi \) is a curve. As can be derived that, even in the high-dimensional space, \( (p^{(k)}, p^{(k)}, \ldots, p^{(k)}, \ell(p^{(k)})), (\hat{p}^{(k+1)}, \hat{p}^{(k+1)}, \ldots, \hat{p}^{(k+1)}, \ell(\hat{p}^{(k+1)})) \) are in the same plane \( \chi \). Consider a Cartesian coordinate system in \( \chi \) with axes \( \xi \) and \( \zeta \), and then Theorem\(^2\) and Lemma\(^4\) can be applied for high-dimensional case.

**Definition 4.** Assume that \( \ell \) is \( \varepsilon \)-Hessian Lipschitz continuous and \( \ell(p) \) is convex in the neighborhood of \( p^* \), a metric named pacGen can be applied to evaluate the generalization\(^2\):
\[
G_{\mu, \nu}(\ell, p^*) = \sum_{n=1}^{\tilde{n}} \ln((|p^*_n| + 1 + \mu) + \nu) \max(\sqrt{\nabla^2 \ell(p^*) + \varepsilon \sqrt{\tilde{n}(\mu|p^*_n| + \nu)}}),
\]
(3)
where \( \mu, \nu \) are positive constants, \( \nabla^2 \ell(p^*) \) denotes the \( n \)-th diagonal element in the Hessian matrix of \( \ell(p^*) \), \( \varepsilon \) is the Lipschitz constant of the Hessian matrix.

The second partial derivative of \( \ell(p) \) in a critical point can be written as
\[
\frac{\partial^2 \ell}{\partial p_r \partial p_s} = \lim_{\Delta p_r \rightarrow 0} \frac{\ell_{p_r}(p_1, \ldots, p_r + \Delta p_r, \ldots, p_n) - \ell_{p_r}(p_1, \ldots, p_r, \ldots, p_n)}{\Delta p_r},
\]
(4)
where \( \ell_{p_r} = \partial \ell / \partial p_s, r \in [1, \tilde{n}], s \in [1, \tilde{n}] \). In practice, the gradient usually does not change sharply. With this in mind, together with Equation (4), it can be seen that deformation functions with \( \delta s / \delta t > 1 \) tend to make \( \partial \ell / \partial p_s \) smaller, which further leads to smaller \( \partial^2 \ell / (\partial p_r \partial p_s) \) and smaller \( \nabla^2 \ell(p^*) \). If \( \nabla^2 \ell(p^*) \) becomes smaller, \( G_{\mu, \nu}(\ell, p^*) \) becomes smaller, which implies better generalization capability.

According to the above analyses, the AP deformation function and LE deformation function are conducive to search the well-generalizable minimum. From Lemma\(^1\) it can be seen that the deformation function is also beneficial for reducing the value of the \( (C_r, A) \)-sharpness defined in [14]. The filtering for minima is usually not performed when the loss value is large, since it is difficult.
to determine the landscape around the final minimum. If the search is performed in this case, some flat areas may be ignored by mistake. Beyond that, if the flat extreme value is accompanied by a high cost function value, it may still bring poor performance. Therefore, there is a trade-off between the extreme value flatness and the cost function value. A suggestion is to filter only when the loss value is not large. To give some empirical illustrations, loss curves of both the original ResNet-20 and the deformation-function-equipped ResNet-20 are presented. As shown in Fig. 3, AP deformation functions can make the loss curve flatter, and the larger \( a_4 \) is, the flatter the curve could be. These results demonstrate that the involved deformation functions play a role as the flat minimum filter.

4 Experiments

In this section, experiments for various CNNs on ImageNet, CIFAR-10, and CIFAR-100 are conducted [11, 10]. Settings of hyperparameters are provided in the supplementary material.

4.1 Deformation-function-equipped SGDM can find flat minima

![Loss curves around the minimum obtained by deformation functions for ResNet-20 on CIFAR-100 with caption of each subfigure denoting the deformation function acting on the loss.](image)

The loss surface in the deep learning is a high-dimensional hypersurface, which is difficult to draw on 2D plane directly. Literature [13] provides the filter normalization method for visualizing the loss landscape. Besides, [13] also shows that the loss curves visualized using different random directions are very similar. In addition, the computational cost required to visualize the loss surface in 3D view is much more than that to depict the loss curve. With this in mind, the conducted experiments visualize loss curves instead of loss surfaces by using the method proposed in [13], and it is sufficient to illustrate the nature of the deformed loss surface. Figure 3 gives the loss curves for different deformation settings on CIFAR-100. As can be seen from Fig. 3(a) and 3(b), the model deformed by \( \delta(\ell) = 0.5\ell^2 \) falls into the sharp minimum, and performs worse than the original model (see supplementary material for results). However, models deformed by APs with \( a_4 \geq 1 \) obtain flat minima. In Fig. 3(c) to 3(f), for AP deformation function with larger \( a_4 \), the minima obtained by the SGDM are flatter. These observations support that the deformation-function-equipped optimizer filters out some sharp minima, and then finds flat minima.

4.2 Comparison experiments

In this subsection, comparisons among learning-rate-scheduler-equipped CNNs and loss-surface-deformed CNNs, and comparisons among loss-surface-deformed CNNs and the original CNNs are performed. In order to achieve maximum fairness, the comparison models in the experiment are all trained from scratch with the same hyperparameters (except the one that is evaluating). For all of
Table 2: Top-1 test accuracies on CIFAR-10 and CIFAR-100 with deformation functions.

| Model       | CIFAR-10 | CIFAR-100 |
|-------------|----------|-----------|
|             | Original | Deformed  | Original | Deformed |
| PreResNet-20| 91.88    | 92.64 [LE (1, 0.8)] | 67.03    | 68.49 [AP (2, 1, 2, 1)] |
| ResNet-20   | 92.04    | 92.29 [LE (1, 0.9)] | 69.76    | 70.67 [AP (18/π, 1, 2, 1)] |
| PreResNet-110| 94.24   | 94.43 [LE (1, 0.9)] | 72.96    | 73.63 [AP (2, 1, 2, 1)] |
| ResNet-110  | 93.73    | 94.19 [LE (1, 0.8)] | 73.93    | 74.14 [AP (2, 1, 2, 1)] |
| DenseNet-BC-100| 94.99  | 95.13 [LE (1, 0.99)] | 77.38    | 77.40 [AP (2, 1, 2, 1)] |
| EfficientNet-B0| 94.89   | 94.91 [AP (10, 1, 1, 1)] | 77.34    | 78.53 [AP (18/π, 1, 2, 1)] |
| EfficientNet-B1| 94.49   | 94.87 [AP (1.5, 0.7, 1, 0)] | 78.33    | 79.36 [AP (1.5, 0.7, 1, 0)] |
| SE-ResNeXt-29| 96.15    | 96.39 [AP (10, 1, 1, 1)] | 83.65    | 83.83 [LE (1, 0, 3)] |

Table 3: Comparisons of classification performance (%, 1-crop testing) on ImageNet validation set.

| Model       | Top-1 acc. (%) | Deformation function | Epoch | Batch size |
|-------------|----------------|----------------------|-------|------------|
|             | Original | Deformed  |                   |       |            |
| ResNet-18   | 70.19    | 70.43 [LE (1, 0.5)] | 120   | 256        |
| PreResNet-18| 69.61    | 69.64 [LE (1, 0.5)] | 90    | 256        |
| ResNet-34   | 73.51    | 73.61 [LE (1, 0.6)] | 120   | 256        |
| DenseNet-121| 74.09    | 74.11 [AP (1, 0.5, 2, 0.3)] | 90    | 64         |

the experiments, SGDM is chosen as the optimizer, with no dropout. The data augmentations are random crop and random horizontal flip for both CIFAR (32 × 32) and ImageNet (224 × 224). The comparison experiments are conducted on CIFAR-10, CIFAR-100, and ImageNet [11][10]. Firstly, the comparisons among the state-of-the-art (SOTA) learning rate scheduler (such as hyperbolic-tangent decay which is abbreviated as HTD [17]) and deformation functions are conducted. The step decay scheduler is used for models equipped with deformation functions, while other hyperparameters remain the same. The results are shown in Table 1. Besides, original DenseNet-BC-100 [18], EfficientNet-B0 [19], EfficientNet-B1 [19], PreResNet-110 [20], PreResNet-20 [20], ResNet-110 [21], ResNet-20 [21] and SE-ResNeXt-29 (16 × 64d) [22] with their deformed versions are compared on CIFAR-10 and CIFAR-100, with the same hyperparameters. The comparisons are also conducted on ImageNet, and only the lightweight models such as ResNet-18 are involved, due to the limitation of computing power. On ImageNet, PreResNet-18 and DenseNet-121 are trained only for 90 epochs, and ResNet-18, and ResNet-34 are trained for 120 epochs. As indicated in Table 2 and 3 all of the models with deformation functions performs better than the original models. Under the same settings of training, the accuracy improvements between the original models and the deformed ones are significant for CNNs, especially without introducing additional tricks.

5 Conclusions

In this paper, the novel concept of deforming the loss surface has been proposed with its mathematical form given. Several deformation functions have been investigated for their contributions to deforming the loss surface. Theoretical analyses demonstrate that the proposed deformation functions have the capability to filter out the sharp minima. Moreover, relevant numerical experiments have been organized to visually illustrate the superiority of the proposed deformation functions. Besides, the performance of finding the flat minima for the original SGDM and deformation-function-enhanced SGDM have been evaluated on CIFAR-100 with the actual loss curve visualization. On CIFAR-10 and CIFAR-100, popular deep learning models enhanced by the proposed method in our experiments have shown superior test performance than the original model with up to 1.46% improvement. Overall, the theoretical analyses, simulations, and the related comparative experiments have illustrated the effectiveness and potential of the proposed deformation method in improving the generalization performance. In addition to deformation function which aims at filtering sharp minima, more forms of deformation operators will be studied in the future to address other problems in deep learning, such as the saddle point problem and gradient explosion problem.
6 Broader impact

In recent years, the SOTA models in deep learning often involve high computing resource overheads, which means that training these models may bring a lot of energy consumption or carbon emissions. Unlike structure-based approaches, using deformation functions to improve performance does not introduce significant additional computational overhead, which means the same result can be obtained by fewer power consumption. Besides, deforming the loss surface is a novel perspective for better performance. The method of deformation is not only the deformation-function-based method, and the effect of deformation is not only to promote the optimizer to find a flat solution. However, like most methods of promoting computers to replace part of human labor, this work may increase unemployment slightly, until finding a living art that can cope with the automation course.

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Deforming the Loss Surface
(Supplementary Material)

In the supplementary material, illustration of the deformation method are provided, proofs of Theorems are given, and details of simulations and experiments are presented. Besides, additional experiments are conducted.

A Sketch of the deformation method

Sketches of the flat minimum filter are shown in Fig. 4. In this figure, the blue solid line denotes the original training loss; the orange dashed line denotes the original test loss; the yellow solid line denotes the deformed training loss; the purple dashed line denotes the deformed test loss. From Fig. 4(a), it can be seen that the sharp minimum leads to higher test loss than the flat one, and the sharp minimum is obtained finally for the original loss curve. However, if the loss curve is deformed as Fig. 4(b) shows, the sharp minimum is escaped with the same initial parameter.

Figure 4: Sketches of the flat minimum filter. (a) The original loss curve. (b) The deformed loss curve.

B Proofs

In the following subsections, Theorem 1 and Theorem 2 are proved.

B.1 Proof of Theorem 1

Proof. The \((r, s)\)th element of \(H^*\) can be written as
\[
H^*_{rs} = \frac{\partial^2 \delta(\ell)}{\partial p_r \partial p_s} = \frac{\partial \delta}{\partial \ell} \frac{\partial^2 \ell}{\partial p_r \partial p_s} = \frac{\partial \delta}{\partial \ell} H_{rs}.
\]
Thus,
\[
H^* = \frac{\partial \delta}{\partial \ell} H.
\]
Considering the definition of eigenvalues, the following equation is obtained:
\[
\lambda(H^*) = \frac{\partial \delta}{\partial \ell} \lambda(H).
\]
The proof is thus completed.

B.2 Proof of Theorem 2

Proof. The parameter \(p^{(k+1)}\) in step \(k\) can be obtained by the following iterative rule:
\[
\Delta p^{(k+1)} := -h_r \nabla \delta(\ell(p^{(k)})),
\]
(5)
and
\[ p^{(k+1)} := p^{(k)} + \Delta p^{(k+1)}, \]
where \( h_r \) is the learning rate. Assume that there are only three extreme points \((p_{[\min]}, \ell_{[\min]})\), \((p_{[\max]_1}, \ell_{[\max]_1})\), and \((p_{[\max]_2}, \ell_{[\max]_2})\), with \( \partial^2 \ell_{[\min]} / \partial p_{[\min]}^2 > 0 \), \( \partial \ell_{[\max]_1} / \partial p_{[\max]_1}^2 < 0 \), \( \partial \ell_{[\max]_2} / \partial p_{[\max]_2}^2 < 0 \), \( p_{[\max]_1} < p_{[\max]_2} \), and the total number of the steps is sufficiently large, the following results are achieved:

- For the case of \( p^{(k)} \in [p_{[\max]_1}, p_{[\min]}] \), if \( \exists \delta(p^{(k)}) \) such that
  \[ \partial \ell(p^{(k)}) / \partial p^{(k)} < p_{[\min]} - p_{[\max]_1} / h_r \partial \ell / \partial \ell, \]
  and then \( p^{(k+1)} > p_{[\max]_2} \), which means that the parameter will escape from \((p_{[\min]}, p_{[\max]_1})\) if \( k \) is sufficiently large. One can derive that if \( p^{(k+1)} \in [p_{[\max]_1}, p_{[\max]_2}] \), and then \( \forall \delta(p^{(k)}) \),
  \[ 0 \geq \partial \ell(p^{(k)}) / \partial p^{(k)} \geq p_{[\max]_1} - p_{[\max]_2} / h_r \partial \ell / \partial \ell. \]

- For the case of \( p^{(k)} \in [p_{[\min]}, p_{[\max]_2}] \), if \( \exists \delta(p^{(k)}) \) such that
  \[ \partial \ell(p^{(k)}) / \partial p^{(k)} > p_{[\max]_1} - p_{[\max]_2} / h_r \partial \ell / \partial \ell, \]
  and then \( p^{(k+1)} < p_{[\max]_1} \), which means that the parameter will escape from \((p_{[\max]_1}, p_{[\max]_2})\) if \( k \) is sufficiently large. One can derive that if \( p^{(k+1)} \in [p_{[\max]_1}, p_{[\max]_2}] \), then \( \forall \delta(p^{(k)}) \),
  \[ 0 \leq \partial \ell(p^{(k)}) / \partial p^{(k)} \leq p_{[\max]_1} - p_{[\max]_2} / h_r \partial \ell / \partial \ell. \]

Let \( \Delta p_{[\max]} = p_{[\max]_2} - p_{[\max]_1} \) represents the projection of the distance between adjacent maximum values on \( p \). Based on this consideration, \( \Delta p_{[\max]} \) can be regarded as an independent variable that does not depend on \( p \) or \( \partial \ell(p^{(k)}) / \partial p^{(k)} \). For a sufficiently large \( k \), if \( p^{(k+1)} \) remains in \((p_{[\min]}, p_{[\max]_1})\), together with inequalities (8) and (11), \( \partial \ell(p^{(k)}) / \partial p^{(k)} \) is bounded by
\[ \left| \partial \ell(p^{(k)}) / \partial p^{(k)} \right| \leq \Delta p_{[\max]} / h_r \partial \ell / \partial \ell. \]

The proof is thus completed. \( \square \)

### C Additional simulations

First, the details of simulation in Fig. 1 is given: the function of the loss surface is \( \ell(p_1, p_2) = 0.2(0.01(p_1 + 0.5)^2 + 1.32 \arctan(0.5p_1 - 2)^2 + \arctan(10(p_1 + 5))^2 - 0.5232)((0.02(p_2 + 0.5)^2 + 2.64 \arctan(0.5p_2 - 2)^2 + 2 \arctan(10(p_2 + 5))^2) - 5.232) \); the deformation function is \( \text{AP}(10, 1, 1, 1) \); the initial parameters are \( p_1 = -9.5 \) and \( p_2 = -10 \); SGDM is taken as the optimizer and is trained for 400 epochs; the learning rate is 0.02, and the momentum is 0.9.

Moreover, simulations on complex situation is also performed and presented in Fig. 3. The initial parameters are taken as \( p_1 = -6 \) and \( p_2 = 11 \). The minimum obtained by the original optimizer is sharp in one direction with final loss value 0.005, as shown in Fig. 3(a) and 3(c). However, after deforming the loss surface, the minimum obtained by the optimizer is flat in all directions with the loss value \( 1.19 \times 10^{-5} \), as shown in Fig. 3(b) and 3(d). The function of the loss surface is taken as \( \ell(p_1, p_2) = 0.12((0.1p_1)^2 + \cos(p_2) + \sin(3p_1)/3 + \cos(5p_1)/5 + \sin(7p_1)/7 + 1.331)((0.15p_2)^2 + \cos(p_2) + \sin(3p_2)/3 + \cos(5p_2)/5 + \sin(7p_2)/7 + 1.25) \); and the deformation function is \( \delta(\ell) = \ln(\exp(\ell - 0.9)) \). The SGDM is taken as the optimizer and trained for 100 epochs with the learning rate 0.02 and the momentum 0.9. The results from Fig. 3 demonstrate the superiorities of the proposed deformation function: the deformation-function-equipped optimizer escapes from the sharp minimum and finds the flat region.
Figure 5: Deformation on a simulated loss surface in a complex case with two parameters.

Table 4: Settings of the experiments on CIFAR-10 and CIFAR-100.

| Model             | Epoch | Batch size | Initial learning rate | Milestones | Weight decay | Distributed training |
|-------------------|-------|------------|------------------------|------------|--------------|----------------------|
| PreResNet-20      | 250   | 128        | 0.1                    | {100, 150, 200} | 0.0001        | No                   |
| ResNet-20         | 250   | 128        | 0.1                    | {150, 225}  | 0.0005        | No                   |
| PreResNet-110     | 250   | 128        | 0.1                    | {100, 150, 200} | 0.0001        | No                   |
| ResNet-110        | 250   | 128        | 0.1                    | {150, 225}  | 0.0005        | No                   |
| DenseNet-BC-100   | 300   | 64         | 0.1                    | {150, 225}  | 0.0001        | No                   |
| EfficientNet-B0   | 250   | 128        | 0.1                    | {150, 225}  | 0.0001        | No                   |
| EfficientNet-B1   | 250   | 128        | 0.1                    | {150, 225}  | 0.0001        | No                   |
| SE-ResNeXt-29     | 300   | 128        | 0.1                    | {150, 225}  | 0.0005        | No                   |

Table 5: Settings of the experiments on ImageNet.

| Model             | Epoch | Batch size | Initial learning rate | Milestones | Weight decay | Distributed training | Number of GPUs |
|-------------------|-------|------------|------------------------|------------|--------------|----------------------|----------------|
| ResNet-18         | 120   | 256        | 0.2                    | {30, 60, 90} | 0.0001       | Yes                  | 2              |
| PreResNet-18      | 90    | 256        | 0.2                    | {30, 60}    | 0.0001       | Yes                  | 2              |
| ResNet-34         | 120   | 256        | 0.2                    | {30, 60, 90} | 0.0001       | Yes                  | 2              |
| DenseNet-121      | 90    | 64         | 0.1                    | {30, 60}    | 0.0001       | Yes                  | 2              |
D Details of the Experiments

In this section, settings of experiments are provided, including descriptions of datasets, hyperparameters, and computation hardware information.

Both CIFAR-10 and CIFAR-100 contain 60000 images (32 × 32), where 50000 for training and 10000 for testing. The splitting of the training set and the test set follows the original settings of the Python version of CIFAR (downloading link: [http://www.cs.toronto.edu/~kriz/cifar.html](http://www.cs.toronto.edu/~kriz/cifar.html)). The ImageNet dataset used in this paper contains 1000 classes, with 1281167 training images and 50000 validation images (downloading link: [http://image-net.org/download](http://image-net.org/download)). The splitting of the training set and the test set for ImageNet follows the original settings. The ImageNet images are randomly cropped into 224 × 224. In the validation set of ImageNet, the single 224 × 224 center crop is carried out for testing. All models in this paper are trained by SGDM with momentum 0.9, equipped with Nesterov method, and the loss function in all the experiments is cross entropy. Table 4 and 5 show the experimental settings of ImageNet, CIFAR-10, and CIFAR-100, respectively. In these tables, the set of some specific epochs are denoted as milestones, and the learning rate is multiplied by 0.1 when these epochs are reached. The number of GPUs in distributed training may affect the accuracy, thus the number of GPUs are also listed in Table 5. Our computing infrastructure contains two servers, one with 10 GeForce RTX 2080 Ti GPUs (with 11GB RAM per GPU), and the other with 2 Quadro RTX 8000 GPUs (with 48GB RAM per GPU). However, since not all computing resources can be accessed at all times, some experiments are conducted on 2 or 4 GPUs. The experiments are performed by using PyTorch 1.4.0 and CUDA 10.0 within Python 3.7.6.

E Additional experiments

In this section, additional experiments are conducted. Specifically, comparison of top-1 test accuracies ResNet-20 with wide range learning rates and loss-surface-deformed ResNet-20 on CIFAR-100 are described in Table 6. Although the learning rates are taken from a wide range, ResNet-20 based on AP (18/π, 1, 2, 1) or AP (6, 1, 2, 1) performs better.

Table 6: Top-1 test accuracies of learning rate schedulers and deformation functions on CIFAR-100 for ResNet-20.

| Method           | Top-1 acc. (%) |
|------------------|----------------|
| 0.5h_τ           | 69.31          |
| h_τ              | 69.76          |
| 2h_τ             | 69.10          |
| 3h_τ             | 67.67          |
| 4h_τ             | 66.65          |
| 5h_τ             | 63.97          |
| 6h_τ             | 62.95          |
| 10h_τ            | 53.08          |
| δ(ℓ) = 0.5ℓ²     | 69.60          |
| AP (2, 1, 2, 1)  | 69.53          |
| AP (5, 1, 2, 1)  | 69.60          |
| AP (18/π, 1, 2, 1)| **70.67**      |
| AP (6, 1, 2, 1)  | 69.82          |
| AP (10, 1, 2, 1) | 69.19          |

F Training time consumption

The runtime differences among each deformed models and the original models are insignificant. For example, on ImageNet, the average training time costs of each epoch for the original ResNet-34 and the ResNet-34 equipped with LE (1, 0.6) deformation function are 1202.71 s and 1192.77 s,
respectively. The average validation time costs of each epoch for the original ResNet-34 and the ResNet-34 equipped with LE (1, 0.6) deformation function are 36.22 s and 36.29 s, respectively.
