Numerical Exploration of Training Loss Level-Sets in Deep Neural Networks

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Abstract
We present a computational method for empirically characterizing the training loss level-sets of deep neural networks. Our method numerically constructs a path in parameter space that is constrained to a set with a fixed near-zero training loss. By measuring regularization functions and test loss at different points within this path, we examine how different points in the parameter space with the same fixed training loss compare in terms of generalization ability. We also compare this method for finding regularized points with the more typical method, that uses objective functions which are weighted sums of training loss and regularization terms. We apply dimensionality reduction to the traversed paths in order to visualize the loss level sets in a well-regularized region of parameter space. Our results provide new information about the loss landscape of deep neural networks, as well as a new strategy for reducing test loss.

Introduction
Recent advances in neural networks have led to impressive but often inexplicably high performance. For example, networks trained with local optimization often converge to globally optimal (zero) training loss. Our incomplete theoretical understanding of how neural networks operate (and when they might fail) is often described as an “explainability” or “interpretability” problem in AI.

Inexplicable AI sometimes translates low user adoption in high stakes applications such as self-driving cars, medical diagnosis, or criminal justice. In response, researchers have recently sought to strengthen our mathematical understanding of how and when various neural architectures perform well. For example, [Poole et al. 2016] showed that global curvature of a neural network function increases exponentially with depth but not width, to some extent explaining why deep architectures perform so well (although cf. (Zagoruyko and Komodakis 2016)). Soudry and Carmon (2016) explained performance from a different perspective, proving that when the topmost layers of a network are sufficiently large relative to the training data, then any differentiable local minimum is in fact a global minimum with zero training error. Conversely, Baldi and Vershynin (2019) showed that the number of boolean functions that can be represented exactly by feed-forward networks is a cubic polynomial of the layer sizes. Using different techniques than Soudry and Carmon, Du et al. (2019) also show that gradient descent converges to zero training error for a variety of network architectures.

Related to these theoretical results, various practical techniques can “easily” achieve negligible training error when the hidden layers and weights are set up correctly. For example, reservoir computing (Jaeger and Haas 2004), extreme learning machines (Huang, Zhu, and Siew 2006), and some applications of the neural engineering framework (Eliasmith and Anderson 2004), have all used techniques where weights and/or activity patterns leading up to the penultimate layer are chosen randomly, and then “decoding” or “read-out” by the output weights is achieved by solving a linear system with near-zero residual.

Given that real-world neural networks are mostly smooth functions, and achieve arbitrarily low training loss via over-parameterization relative to the training data, we can expect that the optima are not isolated points in parameter space, but rather, comprise smooth manifolds (perhaps modulo some singular points). In this paper we seek to empirically characterize such manifolds to improve our understanding and engineering of neural networks. For example, are the level-sets for a fixed training loss typically path connected? What is the distribution of various regularization values and test loss within the level-set? For a given regularizer, how does the most regularized point in the level-set compare to those found in the standard way, by optimizing a weighted sum of training loss and regularization term?

To begin answering such questions, we use numerical methods to construct randomly sampled paths within manifolds for fixed near-zero levels of training loss. We focus on near-zero, rather than exactly zero, training loss for two reasons: (1) in practice numerical optimization will not reach true zero loss, and (2) the gradient is non-zero at near-zero loss, which enables level set traversal with first-order methods. The approach can be described in terms of two phases. First, we use standard optimization from random initial weights to minimize the training loss, thereby locating a starting point in the manifold corresponding to a near-zero fixed training loss. Second, we use mathematical principles from gradient projection and numerical path following [Rosen 1960; Allgower and Georg 1997] to enumerate a sequence of points within the manifold along a path of interest (for example, one that minimizes a regularization function).
These two phases are repeated many times with random initial conditions to form a random sample of paths within level sets of fixed training loss. In addition, we collect an empirical distribution of test loss and regularization scores, among other metrics, along these paths to better characterize these level sets. This experimental setup is used on an illustrative toy example as well as multiple real-world datasets including MNIST (LeCun et al. 1998), CIFAR10 (Krizhevsky 2009), Iris (Fisher 1936), and Auto-MPG (Quinlan 1993) datasets. We also compare our method against the more typical approach where the objective is a weighted sum of training loss and a regularization term. Our results show that our method effectively locates regularized points within the training loss level-sets that better generalize to test data. All of the code needed to reproduce our results and figures is open source and freely available online.

Related Work

The connectedness, or lack thereof, of the training loss landscape has been an interesting theme of exploration in recent studies on deep neural networks. Large (deep and wide) networks embody a certain redundancy which has been argued to cause lowered energy (i.e., loss) barriers and increased connectivity in the loss landscape (Sagun et al. 2018; Venturi, Bandeira, and Bruna 2019; Nguyen 2019; Draxler et al. 2018). More generally, a similar adapting procedure can be used to find new, and perhaps neighboring, points in the loss landscape with comparable performance. Recently, Garipov et al. (2018) and Draxler et al. (2018) independently showed that for multi-layer neural networks it is possible to path-connect a pair of distinct minima in the parameter space. The former show that a pair of distinct sets of weights obtained, for example, by training two randomly initialized instances of the same network can be connected through polygonal curves along which the training loss remains nearly the same as that on the distinct end-points. The latter show that the same connection can also be established using the Nudged Elastic Band method (Jonsson 1998), a method used to discover reaction pathways in chemical reactions. Similarly, Nguyen (2019) showed that every sublevel-set of an over-parametrized feed-forward network is connected under mild assumptions on the topology of the network. Our work complements and extends these works in several ways. First, we propose a numerical method which provides for an architecture-agnostic way of traversing loss level-set with respect to a given curve or path of interest. Such a traversal requires a single starting point and does not require any of the consecutive points on the level-set to be known beforehand (as is the case in (Garipov et al. 2018) and in (Draxler et al. 2018)). Second, the numerical nature of the method allows it to sidestep some of the assumptions (such as those on the layer width and topology of the network deduced by Nguyen (2019) and Venturi, Bandeira, and Bruna (2019)) as the traversal is carried out.

Approach

We consider smooth neural network models with trainable parameters \(\theta \in \mathbb{R}^N\), where \(N\) is the number of parameters, along with a non-negative training loss function \(L : \mathbb{R}^N \rightarrow \mathbb{R}\) and a regularization function \(R : \mathbb{R}^N \rightarrow \mathbb{R}\). Here \(\theta\) can be interpreted as a vector obtained by concatenating the flattened weight matrices and bias vectors that span multiple layers in a network. We are interested in characterizing a level set with a fixed near-zero training loss \(\epsilon > 0\). We denote this level set by \(\mathcal{M}\), defined as:

\[
\mathcal{M} = \{\theta \in \mathbb{R}^N : L(\theta) = \epsilon\}. 
\]

In particular, we are interested in how \(\mathcal{R}(\theta)\) varies within this set. We focus on the case where \(\epsilon > 0\) is near, but not exactly, a minimum value of \(L\). In this case, \(\nabla_\theta L \neq 0\), and \(\mathcal{M}\) is a smooth manifold, with implicit equation \(L(\theta) = \epsilon\). An initial point \(\theta_0 \in \mathcal{M}\) can be found with standard gradient-descent-based optimization. Then we can use a numerical procedure to generate a sequence of discrete steps \(\theta_0, \theta_1, \ldots, \theta_n, \ldots\) in this manifold. Expanding around the base point \(\theta_n \in \mathcal{M}\), a second-order Taylor approximation of \(\mathcal{M}\)'s implicit equation is

\[
L(\theta_n + \delta) \approx L(\theta_n) + \delta^\top \nabla_\theta L(\theta_n) + \delta^\top H(\theta_n)\delta / 2 
\]

where \(H(\theta)\) is the Hessian of \(L(\theta)\). We seek a numerical step \(\theta_{n+1} = \theta_n + \delta\) that remains in \(\mathcal{M}\), i.e., \(L(\theta_{n+1}) = L(\theta_n) = \epsilon\). From (2) it is apparent that such a \(\delta\) should satisfy

\[
0 \approx \delta^\top \nabla_\theta L(\theta_n) + \delta^\top H(\theta_n)\delta / 2 
\]

We consider the case when \(\mathcal{M}\) is a level set of training loss near, but not at, a local minimum. In this case, the first-order Taylor term dominates, and we seek a \(\delta\) satisfying

\[
\delta^\top \nabla_\theta L(\theta_n) = 0. 
\]

An infinitesimal step in direction \(\delta\) satisfying the condition above will remain in \(\mathcal{M}\). More interestingly, there is some freedom in choosing \(\delta\) as long as it satisfies Eq. (1). Let \(r\) denote some direction of interest that may or may not be confined to \(\mathcal{M}\). For example, \(r\) could be \(-\nabla_\theta R(\theta_n)\), in which case we seek to minimize the regularization term, or it could be sampled from a multidimensional normal distribution, in which case we will proceed on a random walk.

Given \(\nabla_\theta L\) and some such \(r\), we therefore seek a \(\delta\) with a non-zero component along \(r\) that also satisfies Eq. (1). Let \(r\) denote some direction of interest that may or may not be confined to \(\mathcal{M}\). For example, \(r\) could be \(-\nabla_\theta R(\theta_n)\), in which case we seek to minimize the regularization term, or it could be sampled from a multidimensional normal distribution, in which case we will proceed on a random walk.

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steps are then used to return to $M$. More formally, the loss deviation $D$ for the $n^\text{th}$ iteration of phase 2 is defined below:

$$D(\theta_n) = (\mathcal{L}(\theta_n) - \mathcal{L}(\theta_0))^2$$  

(5)

where $\theta_0$ is the traversal starting point in $M$ found by the first phase. In a predictor step, while the training loss deviation is below a pre-specified small threshold, the network weights will be updated according to the following relations:

$$\delta_p = \nabla_\theta R - \text{proj}_{\nabla_\theta \mathcal{L}} \nabla_\theta R$$

$$\theta_{n+1} = \theta_n - \eta \delta_p$$

(6)

where $\delta_p$ is the unit vector along the prediction direction $\hat{\delta}_p$, $\eta$ is the learning rate, and $\text{proj}_{\theta,a}$ is the projection of a vector $a$ onto another vector $b$, defined as:

$$\text{proj}_{\theta,a} = (a^\top \hat{b}) \hat{b}$$

(7)

A practical choice of $R$ is the squared norm function defined as:

$$R(\theta) = \theta^\top \theta$$

(8)

Note that equation (6) differs from standard gradient descent-based weight update equations in the sense that we project away the component of the regularization gradient $\nabla_\theta R(\theta_n)$ along the training loss gradient $\nabla_\theta \mathcal{L}(\theta_n)$. Since the resulting $\delta_p$ has no components along $\nabla_\theta \mathcal{L}(\theta_n)$, taking an infinitesimal step along this direction will not change $\mathcal{L}(\theta)$ but will change (reduce) $R(\theta)$. However, in practice, numerical steps are not infinitesimal and small errors would accumulate without a corrector step.

In the corrector step, which sets in if the training loss deviation $D$ is above the aforementioned threshold, the deviation is minimized using gradient descent. In order to avoid undoing the work in the predictor step, we constrain the corrector steps to move orthogonally to $\delta_p$. This is done by computing a descent direction $-\nabla D$ that reduces the loss deviation, and then projecting away its component along $\delta_p$. The resulting weight update equations for a corrector step, therefore, are:

$$\delta_c = \nabla_\theta D - \text{proj}_{\delta_p} \nabla_\theta D$$

$$\theta_{n+1} = \theta_n - \eta \delta_c$$

(9)

The predictor/corrector procedure described here has to stop gracefully. Two reasonable stopping criteria include the number of total predictor/corrector steps allowed and the vectors $\nabla_\theta \mathcal{L}$ and $\nabla_\theta R$ being anti-parallel. While the total number of steps criterion is a simple resort in case of limited available compute, the anti-parallel criterion is informed by the method of Lagrange multipliers (Boyd, Boyd, and Vandenberghe 2004) using which the problem of manifold traversal can also be described as a constrained optimization problem. More precisely, for a given $\mathcal{L}$, $\epsilon$ and $R$, we are interested in traversing $M$ along a path that minimizes $R$. Mathematically,

$$\begin{align*}
\text{minimize} & \quad R(\theta) \\
\text{subject to} & \quad \mathcal{L}(\theta) = \epsilon
\end{align*}$$

(10)

Using the method of Lagrange multipliers, we have

$$F(\theta, \lambda) = R(\theta) + \lambda \mathcal{L}(\theta) - \epsilon$$

(11)

where $\lambda \geq 0$, $F$ is usually called the Lagrangian. The solution to Eq. (11) involves finding the critical points of $F$, i.e., points where $\nabla_\theta F = \nabla_\theta R - \lambda \nabla_\theta \mathcal{L} = 0$. At a point minimizing $R$, where the constraint is also satisfied, the gradients $\nabla_\theta \mathcal{L}$ and $\nabla_\theta R$ will be anti-parallel. This is because a decrease in the regularizer $R$ translates into an increase in $\mathcal{L}$ and vice versa.

**Small illustrative Example**

We demonstrate an application of the procedure described in the section above with a simple optimization problem of the following form:

$$\begin{align*}
\text{minimize} & \quad x + y \\
\text{subject to} & \quad x^2 + y^2 = 1
\end{align*}$$

(12)

A visual depiction of this problem is given in Fig. 1. For a given $(x, y)$ initialized randomly on the unit circle corresponding to the constraint $x^2 + y^2 = 1$, a series of predictor/corrector steps, informed by the directions specified by the objective gradient and the constraint gradient, drives the solver towards the point at which the constrained objective $x + y$ is at its minimum. The exact number of steps taken by the procedure varies and is determined by hyper-parameters such as the predictor/corrector step size. However, the overall progress of the procedure can be assessed by tracking metrics such as the angle between the objective gradient and the constraint gradient. The progress of the predictor/corrector procedure, when applied to the constrained optimization problem above, is also visualized in Fig. 1. Note that the two gradients are anti-parallel at the final point.

**Experimental Methods**

In order to assess the generality of the method across multiple datasets and architectures, we used it on the MNIST (LeCun et al. 1998), CIFAR10 (Krizhevsky 2009), Iris (Fisher 1936), and Auto-MPG (Quinlan 1993) datasets. On each of
these, we used the two-phase method described earlier to carry out near-zero-loss level-set traversal of the training loss function using the training split of the dataset. All experiments described below were carried out using an Asus ROG Strix Nvidia GTX 1080 Ti GPU with TensorFlow v2.3.0 on Ubuntu 18.04. The system had an Intel i5 9600k CPU and 32 GB of DDR4 2400 MHz RAM.

**MNIST**

The MNIST dataset corresponds to a 10-class classification problem and has 60k training examples and 10k test examples of size 28x28 pixels containing images of handwritten digits from 0 to 9. The pixel values for all examples were standardized to be in the [0, 1] interval. In order to accommodate the maximum number of experiments on large networks within the available computational capacity, all MNIST experiments used different random subsamples of 1000 examples from the full training set. The whole test set was used. The predictor/corrector scheme described earlier was used as the loss level-set traversal method.

For feed-forward experiments, we used a network with 3 hidden feedforward layers with 100 neurons each. For convolutional experiments, the network again had 3 hidden layers in total: two 2D convolutional layers followed by a feedforward layer. Each convolutional layer had 20 convolutional filters of dimensions 3 × 3 and was followed by a 2D average pooling layer with pool size 2 × 2. The final feedforward layer had 10 outputs, one per class. All hidden layers used \( \tanh \) activation and the output layer used \( \text{softmax} \). A fully-differentiable activation such as \( \tanh \) was a convenient choice since it guaranteed smoothness of the loss function.

In phase 1 of the predictor/corrector scheme, the weights of a network were initialized using Glorot normal initialization \cite{Glorot2010} and the network was trained using minibatch-gradient descent with a categorical cross-entropy loss \( \mathcal{L} \) using the Adam \cite{Kingma2015} optimizer. More specifically, the network was trained with a batch size of 32 for 100 epochs to achieve a near-zero loss on the training set of 1000 examples.

In phase 2, the network underwent a number of predictor/corrector steps depending on whether the squared change in training loss along \( \mathcal{R} \) was above or below the loss deviation threshold. \( \mathcal{R} \) was set to be the squared norm function described earlier and the loss change threshold was set to \( 10^{-10} \) for both full-connected and convolutional experiments with MNIST. The predictor or corrector step each had a separate full-batch optimizer the learning rate of which was adjusted heuristically based on the geometry of the landscape being traversed. More precisely, the learning rate for each optimizer was increased or decreased by a multiplicative factor depending on whether the angular change in the associated (predictor or corrector) direction in any consecutive steps was above or below a pre-specified threshold of 0.1 degrees. The multiplicative factor was set to 0.1 and 1.1 for angular changes greater than or less than the 0.1 degrees threshold respectively. We believe the angular change heuristic takes into account the ruggedness of the loss landscape and using it yields a less chaotic traversal of the loss landscape.

Finally, at the beginning every predictor step (after a series of corrector steps had finished), we measured different metrics such as training set loss, test set loss, test set accuracy, sum of squared norms for network weights and the angle between the loss gradient \( \nabla_{\theta} \mathcal{L} \) and the regularization gradient \( \nabla_{\theta} \mathcal{R} \). In theory, phase 2 would stop when the angle between the two is 180° or 0°, at which point there is no direction in which to decrease \( \mathcal{R} \) without changing \( \mathcal{L} \). But in the numerical approximation, we observed that it was difficult to reach those exact angles in practice. For practical reasons, the number of total predictor steps taken in phase 2 was set to 10000 for MNIST feed-forward experiments and 5000 for MNIST convolutional experiments.

**CIFAR10**

The CIFAR10 dataset corresponds to a 10-class classification problem and has 60k training examples and 10k test examples which are RGB images of size 32x32. For CIFAR10 experiments too, the pixel values for all images were standardized to be in the [0, 1] interval. Similarly to the reasons described for the MNIST dataset, all CIFAR10 experiments also used different subsamples of 1000 examples from the training set. The whole test set was used.

We only report convolutional neural network experiments for CIFAR10. In our experiments with feedforward networks, the level-set traversal was not very stable. This is perhaps because the learning problem underlying CIFAR10 is complex and arguably more suited for convolutional neural networks. The convolutional network used for different experiment runs had the same configuration as that for MNIST experiments: 3 hidden layers with two 2D convolutional layers preceding a feedforward layer. However, the number of units in each hidden layer was thrice that in the MNIST case. Specifically, the convolutional layers had 60 2D convolutional filters each and the feedforward layer following them had 300 units. The dimensions for convolutional filters here were the same as those for MNIST, as were the activations and other hyper-parameters such as weight initialization method, batch-size and number of iterations for phase 1 training. The total number of predictor/corrector steps was set to 20000 for CIFAR10 experiments.

**Other Datasets**

We also carried out level-set traversal experiments with Iris and Auto-MPG datasets. The Iris dataset corresponds to a 3-class classification problem and includes 150 examples. Of these examples, 120 were used as the training split and the other 30 as the test split. The Auto-MPG dataset corresponds to a regression problem and has 398 examples in total. Six of these had missing values in one of the variables and were excluded. Of the remaining 392, 314 were used as the training set and the remaining 74 were used as the test set.

For both Iris and Auto-MPG, we used a feed-forward network with 3 hidden layers with 100 neurons each. Various hyper-parameters such as weight initialization method, activations in the hidden layers etc. were the same as those in the MNIST and CIFAR10 experiments. The total number of predictor/corrector steps in phase 2 were set to 20000 and 30000 for Iris and Auto-MPG respectively. Lastly, we
Figure 2: Phase 2-learning curves for MNIST feed-forward experiments. Blue curves are averages over 5 randomly-initialized runs and the bands indicate the standard deviation. From top to bottom: 1) Angle between $\nabla L$ and $\nabla R$ approaches $90^\circ$. 2) Squared norm of network weights decreases. 3) Training set loss remains almost constant. 4) Test set loss decreases. 5) Test set accuracy increases.

weight decay experiments. In our weight decay experiments, its value was taken to be in the log$_{10}$space over the interval $[10^{-6}, 10^6]$.

**Weight Decay Experiments**

We also compared the predictor/corrector approach with the more typical “weight decay” approach: namely, unconstrained optimization of an objective that is a weighted sum of training loss and L2-regularization. To this end, for each of the datasets described earlier, we also trained randomly-initialized instances of the networks described earlier such that the training objective now also included an L2 or squared sum of weights term scaled with a weight-decay parameter. Note that there was no two-phase training or numerical traversal in these experiments; just one phase of standard unconstrained stochastic gradient descent with an additive regularization term in the objective. The weight decay parameter, $\lambda$, is usually set through trial and error in such experiments. In our weight decay experiments, its value was taken to be in the log$_{10}$space over the interval $[10^{-6}, 10^6]$.

For each value of $\lambda$, 15 randomly-initialized networks were trained using mini-batches of 32 for an appropriate number of epochs. The total number of training epochs in these experiments was 200 for MNIST and CIFAR10. For Iris Auto-MPG datasets, the number of epochs was set to 500. The networks for MNIST and CIFAR10 were trained with random subsamples of size 1000 as described earlier.

For a more geometrical comparison between the two methods, we also used dimensionality reduction methods to obtain low-dimensional visualizations for the level-set trajectories. More specifically, we used Principal Component Analysis (PCA) [Pearson 1901] to obtain projections of these trajectories along the top 6 principal components with the most explained variance ratio. PCA was carried out on the set of weight vectors obtained by subsampling every 50th point of every phase 2 traversal. The trajectories, when plotted alongside the points obtained at the end of training with weight decay, provided for a visual confirmation of both methods converging to the same highly-regularized neighborhood in the parameter space.

| Experiment | Our Method | Weight-Decay Experiments | Best $\lambda$ |
|------------|------------|---------------------------|----------------|
| MNIST-FF   | 88.85 ± 0.41% | 65.80 ± 33.74% | $10^{-2}$ |
| MNIST-CONV | 94.79 ± 0.32% | 70.28 ± 34.87% | $10^{-2}$ |
| CIFAR10-CONV | 96.90 ± 0.49% | 80.20 ± 8.94% | $10^{-2}$ |
| IRIS-FF    | 96.67 ± 0.07% | 79.94 ± 30.25% | $10^{-2}$ |
| MPG-FF     | 68.86 ± 0.63% | 73.81 ± 144.30 | $10^{-1}$ |

Table 1: A comparison of average accuracy values (MSE for Auto-MPG) obtained at the end of level-set traversals vs. that obtained from weight decay experiments corresponding to best $\lambda$. Bold values are the best of the two methods.
Results

In visualizing the progress of the proposed near-zero-loss level-set traversal procedure, we focused exclusively on phase 2 of the approach described earlier. Figs. 2 and 3 visualize the phase 2 progress over 5 random runs of MNIST feed-forward and convolutional experiments described earlier. The angle plots for these experiments show low variance over a major fraction of the traversal. This indicates relative smoothness of the landscape, which is also confirmed by the quick drop in squared norm as indicated by the following plots. Similarly, Fig. 6 shows results for 5 random runs of the CIFAR 10 convolutional experiment. Results for 5 random runs of Iris and Auto-MPG feed-forward experiments are shown in Figs. 4 and 5 respectively. Note that different runs of the same experiment for level-set traversal used a different random subsample of the MNIST or CIFAR10 training dataset as described in the sections above. The weights of all the networks trained were also initialized randomly.

The figures show that the training loss for all new points explored during the traversal was at the same level (loss deviation being \( \leq 10^{-5} \) for the set squared deviation of \( 10^{-10} \), to be precise) as that reached at the end of phase 1 training. This confirmed that the proposed numerical procedure almost always successfully navigates a constant near-zero-loss manifold \( M \) along a regularizing \( R \). The traversal of the near-zero-training loss level-set using the predictor/corrector procedure revealed a set of additional near-minima which displayed a generalization ability superior to that exhibited by the point in parameter space reached at the end of conventional training in phase 1. Compared to the point at the end of conventional training in phase 1, the newly-discovered minima almost always had lower values of the test set loss, which naturally translates to a better test set accuracy.

As discussed in the previous sections, the weight decay experiments provided for a comparison between the proposed method and the one where the network loss has an added regularization term. The average test set accuracy values for 5 randomly-initialized runs of each of the MNIST feed-forward, MNIST convolutional, CIFAR10 convolutional, Iris feed-forward, and Auto-MPG feed-forward experiments at the end of level-set traversal are included in Table 1. Compared to the best average test set accuracy values obtained at the end of weight decay experiments runs corresponding to best-performing (\( \lambda \)) and which are given in the same table, these are clearly better. Note that in the Auto-MPG dataset, which corresponds to a regression problem, the loss and the accuracy were both taken as mean squared error (MSE). The results from our method show less variance than those from weight decay experiments. From these results, we can argue that the proposed method does a better job than training on loss with added regularized term at finding well-regularized points in the loss landscape.

Fig. 7 visualizes the whole level-set trajectories for 5 random runs of MNIST feed-forward experiments along with the arithmetic mean of the weight vectors obtained at the end of 15 runs of weight decay experiments corresponding to the best-performing \( \lambda \). The average of the end-points of the trajectories, which occurs very close to the average end-point for training with weight decay, is also visualized in the same plots. Note that the two plots in Fig. 7 visualize the trajectories and points along the directions corresponding to top 6 distinct principal components. A few observations can be made from the plots. All the level-set traversals seem to be converging to the same neighborhood. This indicates the presence of a global heavily-regularized neighborhood in the parameter-space. Based on intuition from stochastic weight averaging (Izmailov et al. 2018), we hypothesized that better test performance might be achieved by collecting the fi-
Figure 6: Phase 2-learning curves for CIFAR10 convolutional experiments.

Figure 7: Visualizing randomly-initialized level-set traversals for MNIST feed-forward experiments. The traversed points have been color-coded from first to last as visualized in the appended colorbar. The mean of endpoints for the traversals as well as the mean of points obtained at the end of training with weight decay for best-performing $\lambda$ is given as blue cross and black star respectively. Note that the latter two points are almost collocated (in the top-6 PCA subspace).

Discussion
We have presented a novel two-phased numerical method for locating almost optimally regularized weights within the manifold of near-zero training loss in deep neural networks. We demonstrate applications of the method on various multivariate datasets corresponding to supervised classification and regression tasks and on different network architectures. Empirically, we find that the traversal method, when applied to the specific problem of minimizing a regularizer at a constant loss level, performs better than the more typical weight decay approach where the objective is a weighted sum of training loss and regularization term. Furthermore, we use dimensionality-reduction methods to visualize the regularization dynamics in constant near-zero loss manifolds.

Since the method uses only first-order information about the loss and constraint functions, it can arguably be used on medium to large datasets and networks. Even though we worked with subsamples of the MNIST and CIFAR10 datasets in order to conduct maximum number of experiments within available compute, the calculations of full-batch update, as utilized in the predictor/corrector steps, can be readily distributed over multiple GPUs. In fact, modern numerical computing libraries such as Google’s TensorFlow (Agrawal et al. 2019) include such provisions (Nilsen et al. 2019). We also include distributed version of the code for a subset of our experiments in the GitHub repository.

While we have reported results for numerical exploration of constant, near-zero loss manifolds along a regularizing path only, the method presented here can possibly be generalized to explore constant-loss manifolds along differentiable paths of interest in deep neural networks. This is akin to multi-objective optimization where optimizing successive objectives improves the overall quality of solutions found. For our future works, we aim to extend the method to such multi-objective problems in the context of machine learning and deep neural networks. We also seek to investigate the scenarios where loss is ‘exactly’ zero, rendering first-order methods insufficient. While second-order methods are expensive and borderline impractical for large networks, some recent works exploring the possible existence of a structure in the Hessian of large networks (Sagun et al. 2018) provide for an interesting starting point in this regard.

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