MANIFOLD REGULARIZED DISCRIMINATIVE NEURAL NETWORKS

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ABSTRACT

Unregularized deep neural networks (DNNs) can be easily overfit with a limited sample size. We argue that this is mostly due to the discriminative nature of DNNs which directly model the conditional probability (or score) of labels given the input. The ignorance of input distribution makes DNNs difficult to generalize to unseen data. Recent advances in regularization techniques, such as pretraining and dropout, indicate that modeling input data distribution (either explicitly or implicitly) greatly improves the generalization ability of a DNN. In this work, we explore the manifold hypothesis which assumes that instances within the same class lie in a smooth manifold. We accordingly propose two simple regularizers to a standard discriminative DNN. The first one, named Label-Aware Manifold Regularization, assumes the availability of labels and penalizes large norms of the loss function w.r.t. data points. The second one, named Label-Independent Manifold Regularization, does not use label information and instead penalizes the Frobenius norm of the Jacobian matrix of prediction scores w.r.t. data points, which makes semi-supervised learning possible. We perform extensive control experiments on fully supervised and semi-supervised tasks using the MNIST, CIFAR10 and SVHN datasets and achieve excellent results.

1 INTRODUCTION

Discriminative models are widely used for supervised machine learning tasks. In a probabilistic setting, they directly model the conditional probability of labels given the input $P(y|x)$ without considering the data distribution $P(x)$. Feed-forward neural networks are discriminative in nature, with which one can easily parameterize the conditional probability $P(y|x)$. However, it is well known that unregularized DNNs trained in this fashion (with MLE, for instance) suffers from serious overfitting problems with a limited sample size.

In the past decade, we have witnessed several effective regularization techniques that help DNNs better generalize to unobserved data, most noticeably pretraining [Hinton & Salakhutdinov (2006), Bengio et al. (2007)] and dropout [Srivastava et al. (2014)]. In pretraining, several layers of either RBMs or regularized autoencoders are trained on unlabeled data. One then uses the weights of the stacked deep RBM/autoencoder as the initialization weights for a discriminative DNN, which is further trained on labeled dataset by adding an appropriate classifier layer on top. It is shown that pre-trained weights perform very well as an implicit regularization as they prevent the model to get stuck in poor local optimums. The reason for its success is that with the pretrained RBM/autoencoder, the discriminative model gains (implicit) prior knowledge about the data distribution $P(x)$, thus is able to generalize better to unobserved data. Dropout works by randomly masking out part of both the input and hidden units during the discriminative training with SGD. [Konda et al. (2015)] shows that the effectiveness of dropout can be understood by considering it as a kind of data augmentation [Simard et al. (2003)]. From this perspective, dropout can be considered as implicitly modeling the data manifold by sampling from it.

Another motivation of our work is the recent findings of [Szegedy et al. (2014)], where the authors show that the prediction of a trained discriminative DNN could be greatly changed by adding to the
input a certain small perturbation that is indistinguishable by human eyes. This shows that even the state-of-the-art discriminative DNNs fail to generalize to what seems to be trivial examples. As a remedy, Goodfellow et al. (2015) proposes a way to generate adversarial examples (neighbors of sample data points that increase the loss function significantly) as the additional training data.

In this paper, we propose two simple regularizers to the standard discriminative DNNs: Label-Aware Manifold Regularization (LAMR) and Label-Independent Manifold Regularization (LIMR). Our assumption is that data points within each class should lie in a smooth manifold. If we move from a data point $x$ by a tiny step $\epsilon$, our prediction should remain unchanged, as $x + \epsilon$ is very likely to still lie in the same manifold. In the label-aware version, we encourage the loss function to be flat around observations, which amounts to minimizing the norm of the loss function w.r.t. data points. In the label-independent version, we instead encourage the prediction scores to be flat, which can be computed without labels. We then accordingly minimize the Frobenius norm of the Jacobian matrix of the prediction scores w.r.t. inputs. In addition, we propose stochastic approximations of the regularizers, which avoids explicitly computing the gradients and Jacobians. We perform extensive experiments on both fully labeled and semi-supervised versions of the MNIST dataset, and set state-of-the-art results.

2 Model

Consider a multi-way classification problem with data $\{(x_1, y_1), \ldots , (x_{N^l}, y_{N^l})\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \{1, \ldots, K\}$ are the observation and label for the $i$-th instance, respectively; $N^l$ is the number of labeled instances. We also assume a set of $N^u$ unlabeled instances $\{x_1^u, \ldots , x_{N^u}^u\}$ available. A discriminative model minimizes an objective function in the following form:

$$\frac{1}{N^l} \sum_{i=1}^{N^l} \ell(y_i, f(x_i; \theta)) + R(\theta),$$

where $f(x_i) \in \mathbb{R}^K$ computes the predicted score of $x_i$ belonging to each of the $K$ class; $\ell$ is a loss function indicating the compatibility between the ground truth $y_i$ and the prediction $f(x_i)$; $R(\theta)$ is the regularization term. For example, $f(x; \theta)$ could be the conditional probability $p(y|x; \theta)$ represented by a DNN with a softmax layer, and $\ell(\cdot)$ is accordingly the cross entropy. Alternatively, as in Tang (2013), $f(x; \theta)$ could be the output of a DNN with a linear output layer, and $\ell$ is the one-vs-rest squared hinge loss. We use the later form for all the models in this paper. The focus of this paper is on $R(\theta)$, and we now propose two versions of regularization depending upon the availability of labels.

2.1 Label-Aware Manifold Regularization

In this version, we consider the fully supervised setting where all data points are labeled. According to the manifold assumption, data points within each class lie in a smooth manifold. Without any prior knowledge about the shape of the data manifold, we assume that moving any observation by a tiny step should still keep it in the same manifold. As a result, the loss function to be flat around each observation. In other words, the derivative of the loss function w.r.t. to input $\nabla_x (\ell(y, f(x; \theta)))$ should be small. This directly leads us to a regularization in the form:

$$R^1(\theta) = \frac{\lambda}{N^l} \sum_{i=1}^{N^l} \| \nabla_{x_i} \ell(y_i, f(x_i; \theta)) \|_2^2,$$

where $\lambda > 0$ is the regularization strength factor. We call $R^1(\theta)$ Label-Aware Manifold Regularization (LAMR).

2.2 Label-Independent Manifold Regularization

LAMR assumes the availability of fully labeled data, which prohibits its application to semi-supervised settings where large portions of data are unlabeled. To this end, we propose a slightly
different view on the regularization. The idea is that we can consider \( f(x; \theta) \) as a mapping from the data manifold to the label manifold embedded in \( R^K \). Following a similar reasoning, we then encourage \( f(x; \theta) \), instead of the loss function, to be flat when we move the input along the data manifold. While the very same idea has been proposed in \cite{Gu2014} as deep contractive network (DCN), we further extend it by observing that this regularization also applies to unlabeled data. This makes this view particularly interesting as we are now able to better explore the data distribution with the help of unlabeled data. As a result, we minimize the Frobenius norm of the Jacobian matrix as follows:

\[
R^2(\theta) = \frac{\lambda}{N_l} \sum_{i=1}^{N_l} \| \nabla_{x_i} f(x_i^l; \theta) \|^2_2 + \frac{\beta}{N_u} \sum_{i=1}^{N_u} \| \nabla_{x_i} f(x_i^u; \theta) \|^2_2. \tag{3}
\]

Here we have slightly overloaded the notation by letting \( \nabla_x f(x; \theta) \) denote the Jacobian matrix of \( f(x; \theta) \) w.r.t. \( x \). We also allow different regularization strengths \( \lambda \) and \( \beta \) on labeled and unlabeled data. We call \( R^2(\theta) \) Label-Independent Manifold Regularization (LIMR). Note that LIMR is, different from LAMR, also loss independent. To see this, consider \( f(x; \theta) \) as the output of a DNN with a linear output layer. LIMR would be the same no matter if we use the squared loss or hinge loss, but LAMR would be different for the two cases. This difference is verified in our experiments where we observe that LAMR achieves slightly lower test error on the fully supervised task. On the other hand, LAMR and LIMR are also closely related, simply by noting that minimizing LIMR implicitly minimizes LAMR, as \( R^1(\theta) \rightarrow 0 \) when \( R^2(\theta) \rightarrow 0 \).

### 2.3 Stochastic Approximation

Although it is possible to express \( R^1(\theta) \) and \( R^2(\theta) \) in a closed form for feed-forward neural networks, the resulting objective function could be complicated for DNNs and structured architectures such as CNNs. This makes computing the gradient w.r.t. model parameters inefficient. To address this issue, we take a simple stochastic approximation of the regularization terms. Let \( g : R^d 
\rightarrow R \) be a differentiable function, and \( \epsilon \in N(0, \sigma^2) \) be a draw from an isotropic Gaussian distribution with variance \( \sigma^2 \); then

\[
g(x + \epsilon) \approx g(x) + \epsilon^T \nabla_x g(x), \tag{4}
\]

according to first order Taylor expansion. As a result, we have:

\[
E_\epsilon[g(x + \epsilon) - g(x)]^2 \approx E_\epsilon[\epsilon^T \nabla_x g(x)]^2 = \sigma^2 \| \nabla_x g(x) \|_2^2, \tag{5}
\]

where in the last step we have marginalized out the isotropic Gaussian random variable. With this trick, we approximate the regularisation terms for LAMR and LIMR as follows:

\[
\tilde{R}^1(\theta) = \frac{\lambda}{N_l} \sum_{i=1}^{N_l} E_\epsilon[\ell(y_i, f(x_i^l + \epsilon; \theta)) - \ell(y_i, f(x_i^l; \theta))]^2
\]

\[
\tilde{R}^2(\theta) = \frac{\lambda}{N_l} \sum_{i=1}^{N_l} E_\epsilon[f(x_i^l + \epsilon; \theta) - f(x_i^l; \theta)]^2 + \frac{\beta}{N_u} \sum_{i=1}^{N_u} E_\epsilon[f(x_i^u + \epsilon; \theta) - f(x_i^u; \theta)]^2. \tag{6}
\]

where we have absorbed the scaling factor \( \sigma^2 \). In practice, we simulate the expectations in \( \tilde{R}^1 \) and \( \tilde{R}^2 \) by randomly sampling the Gaussian noise \( \epsilon \) at each iteration of stochastic gradient descent (SGD), in the same way as \cite{Vincent2010}.

In theory, the stochastic approximation is more accurate when using a small \( \sigma \). However, we find that it is beneficial to use a relatively large \( \sigma \) in practice, which actually allows the regularization to explore points from the data manifold that are relatively far from the observations.

### 2.4 Connection With Existing Regularizers

**Feature Noising** \cite{Bishop1995}: One long existing trick for training neural networks is randomly adding noise to data during training. Marginally, its objective function can be expressed as

\[
\frac{1}{N} \sum_{i=1}^{N_l} E_{\epsilon \in P_{\text{noise}}} \ell(y_i, f(x_i^l + \epsilon; \theta)),
\]

where \( P_{\text{noise}} \) is the additive noise distribution to generate samples around \( x_i^l \). Feature noising thus implicitly explores the data manifold with \( P_{\text{noise}}(x_i^l) \).
in a way that is similar to LAMR. However, it does not stress the flatness of the loss function as LAMR does. To see this, consider the simplest case where $P_{\text{noise}} = N(0, \sigma^2_{\text{noise}} I)$, we can then marginalize the noise by using the second order Taylor expansion as:

$$
\frac{1}{N_l} \sum_{i=1}^{N_l} \ell(y_i, f(x'_i; \theta)) + \frac{\sigma^2_{\text{noise}}}{N_l} \sum_{i=1}^{N_l} tr(H_i(\theta)),
$$

(7)

where $H_i(\theta) = \nabla^2_y \ell(y_i, f(x'_i; \theta))$ is the Hessian matrix of the loss function at $x'_i$. We see that the regularization term now encourages the trace of Hessian matrix to be small around the observations, which corresponds to functions with low curvature. This is different from LAMR, as it is that the gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small. Also, note that one variant of Dropout [Srivastava et al. (2014)] when mask out noise is only applied to the input layer gradient is large under even though the trace of the Hessian matrix is small.

Manifold Tangent Classifier (MTC) [Rifai et al. (2011a)]: MTC is a semi-supervised classifier that considers the data manifold, which builds upon the Contractive Autoencoders (CAE) [Rifai et al. (2011a)]. The idea is that one first trains a stacked CAE on all the data (with or without label) as in pretraining, from which the tangent bundles $B_x$ around each observation is then computed and stored. The corresponding regularization takes the form:

$$
R_{\text{mtc}}(\theta) = \frac{\lambda}{N_l} \sum_{i=1}^{N_l} \sum_{u_i \in B_x} \langle u_i^T \nabla_x \ell(y_i, x'_i; \theta) \rangle^2.
$$

(8)

In Equation(8) the gradient of loss function is encouraged to be orthogonal to the tangent vectors $u_i$. The connection with LAMR can be observed if we replace $u_i$ with a random vector drawn from a Gaussian distribution $N(0, \sigma^2 I)$, and replace the inner sum with expectation over the random vector:

$$
\frac{\lambda}{N_l} \sum_{i=1}^{N_l} \mathbb{E}_{u_i} \langle u_i^T \nabla_x \ell(y_i, x'_i; \theta) \rangle^2 = \frac{\lambda \sigma^4}{N_l} \sum_{i=1}^{N_l} \|\nabla_x \ell(y_i, x'_i; \theta)\|_2^2 \propto R^1(\theta).
$$

(9)

We see that forcing the gradient to be orthogonal to any random direction instead of the tangent vectors reduces MTC to LAMR. This highlights our assumption about the data manifold: if an observation is moved by a small random step, it is very likely to still fall into the same manifold. MTC on the other hand, explicitly characterizes the shape of the manifold with a dedicated model (CAE). As a result, LAMR puts a stronger regularization by enforcing $\nabla_x \ell(y_i, x'_i; \theta)$ to be small, which also implicitly minimizes Equation(8). MTC is also able to perform semi-supervised learning, as unlabeled data could help better characterize the data manifold. LIMR takes a similar idea, but instead encourages the flatness of the prediction score function on the unlabeled data points. This also enables one to directly incorporate the regularization with the supervised objective, which makes the two-step pretraining fashion unnecessary.

Deep Contractive Network (MTC) [Gu & Rigazio (2014)]: In the purely supervised setting, DCN is marginally equivalent to LIMR. However, there are two notable differences. First, we extend LIMR to the semi-supervised learning setting. Second, our stochastic approximation allows LIRM to be applied to deep neural networks with complicated structures (with convolutional layers, for example) easily. Moreover, as shown in the experiments, the stochastic approximation with a large noise allows us to explore a larger area of the input space, which puts more regularization on the flatness of the target function.

Adversarial Training [Goodfellow et al. (2015)]: Recently in [Szegedy et al. (2014)], the authors point out that the state-of-the-art DNNs can misclassify examples that are generated by adding to the training examples with certain small perturbations (adversarial examples). To address this issue, [Goodfellow et al. (2015)] propose a strategy to generate adversarial examples and add them to the training set along training. LAMR and LIMR are able to alleviate the very same problem from a different angle: reducing the chance that adversarial examples occur by restricting the loss function to be flat around the observations.
3 Experiments

3.1 Supervised Learning

In the first set of experiments, we use the MNIST dataset to validate the regularization effects in the supervised learning setting. MNIST consists of 50000 training, 10000 validation and 10000 testing images of handwritten digits, each with shape 28x28. We train a three layer feed-forward neural network with size $500 \times 500 \times 500 \times 10$, where 10 is the size of outputs. We use ReLU as the nonlinear activation function for each of the three hidden layers, and a linear output layer (whose output corresponds to $f(x; \theta)$) together with the one-vs-rest squared hinge loss as in Tang (2013). Parameters are initialized following Glorot & Bengio (2010) and optimized with Adadelta Zeiler (2012) using a batch size of 100. We set the standard deviation $\sigma$ as 0.5, and vary the regularization strength $\lambda$ in Equation 6 for both LAMR and LIMR ($\beta = 0$ in the fully supervised task), respectively. We show the results in Table 1. We see that without regularization ($\lambda = 0$), this three layer network achieves a test error rate of 1.64. For both LAMR and LIMR, the error rate is significantly reduced and gradually changes as we vary the regularization strength. Overall, we see that the two regularizers achieve similar best results and are both pretty robust w.r.t. $\lambda$ within a certain range.

| $\lambda$ for LAMR | 0   | 0.01 | 0.05 | 0.1 | 0.2 | 0.3 | 0.5 |
|-------------------|-----|------|------|-----|-----|-----|-----|
| validation error rate | 1.64 | 1.41 | 1.13 | **1.01** | 1.11 | 1.04 | 1.08 |
| test error rate    | 1.64 | 1.64 | 1.15 | **0.95** | 1.11 | 0.99 | 1.2  |

| $\lambda$ for LIMR | 0.01 | 0.05 | 0.1  | 0.3  | 0.7  | 1   | 1.5 |
|-------------------|------|------|------|------|------|-----|-----|
| validation error rate | 1.39 | 1.22 | 0.95 | 0.97 | **0.94** | 0.94 | 0.98 |
| test error rate    | 1.45 | 1.13 | 0.96 | 1.03 | **0.96** | 0.99 | 1.01 |

Table 1: The effect of varying regularization strength $\lambda$ for LAMR (top tabular) and LIMR (bottom tabular), no regularization is used when $\lambda = 0$. We see that both regularizers achieve significant better test errors (0.95 and 0.96) than the plain neural net without regularization (1.64).

We additionally visualize the filters of the first layer learned by two models in Figure 1. The left panel corresponds to $\lambda = 0$ where no regularization is used; the right panel corresponds to LIMR with $\sigma = 0.5$ and $\lambda = 0.7$. LIMR learns sharp filters that mostly correspond to pen strokes, which are very similar to those learned by a regularized autoencoder (eg., Rifai et al. (2011c)).

To investigate the property of the stochastic approximation, we have also tried using different values for $\sigma$ from the set $\{0, 0.1, 0.5, 1\}$ to demonstrate its effect on the regularization quality. Here we
denote $\rightarrow 0$ as using the explicit expression of gradients [Gu & Rigazio (2014)] as regularization, as it corresponds to the case where the variance of noise approximates zero. We show the test error rate for different $\sigma$s for LAMR in Figure 2. We see that all the three values of $\sigma$ are able to help reduce the error rate by varying the regularization strength $\lambda$, and $\sigma = 0.5$ achieves the lowest test error rate among the three. In particular, note that taking $\sigma = 0.5$ actually outperforms directly using the gradients as regularization explicitly. This confirms our speculation that a relatively large $\sigma$ allows the stochastic approximation to explore areas that are further from the observed data points; and by minimizing the difference between the loss of the clean input and the noisy input, the curvature of the target function is further encouraged to be flat.

To compare with the existing methods, we also train this three layer neural network with LAMR and LIMR on 60000 examples by combining the training and validation set and report the test error rate in Table 2. LAMR sets the state-of-the-art result of 0.74 on this permutation invariant data set (which does not consider the 2D structure of image); LIMR also achieves a result that is close to the previous state-of-the-art. As a direct comparison, we also try applying feature noising with the same type of noise as used in LAMR and LIMR, which is outperformed by both. Note that we did not try to optimize the architecture of the network at all. In fact, our models have the fewest number of parameters among all the competitors, so it is still possible to reduce the error rate by trying different model sizes.

| Method | Test error rate |
|--------|-----------------|
| $8192 \times 8192$ NN + Dropout [Srivastava et al. (2014)] | 0.95 |
| $500 \times 500 \times 2000$ DBN + Dropout finetuning [Srivastava et al. (2014)] | 0.92 |
| $500 \times 500 \times 2000$ DBM + Dropout finetuning [Srivastava et al. (2014)] | 0.79 |
| $2000 \times 2000$ Contractive Autoenconder [Rifai et al. (2011b)] | 1.04 |
| $2000 \times 2000$ Manifold Tangent Classifier [Rifai et al. (2011a)] | 0.81 |
| $1600 \times 1600$ Maxout NN + Adversarial Training [Goodfellow et al. (2015)] | 0.782 |
| $500 \times 500 \times 500$ NN + Feature Noising ($\sigma = 0.5$) | 1.06 |
| $500 \times 500 \times 500$ NN + LAMR ($\sigma = 0.5, \lambda = 0.1$) | **0.74** |
| $500 \times 500 \times 500$ NN + LIMR ($\sigma = 0.5, \lambda = 0.7$) | 0.83 |

Table 2: When trained on 60000 labeled data with the parameters selected from the validation set, LAMR achieves the state-of-the-art test error rate on this permutation invariant version of MNIST; LIMR also achieves a result close to the state-of-the-art.

We also consider applying our regularizer to CNNs. CNNs are particularly suitable for modeling image data due to the sharing of convolutional filters across different locations within an image. We use an architecture consisting of a convolutional layer of shape $200 \times 9 \times 9$, a max pooling layer of shape $2 \times 2$, another convolutional layer of shape $200 \times 3 \times 3$, another max pooling layer of shape

![Figure 2: Test error rate of using different $\sigma$ values for LAMR under different regularization strengths. X axis is $\log \lambda$, Y axis is test error rate.](image-url)
Figure 3: Filters learned with different numbers of labels. Number of labels from top left to bottom right: 100, 600, 1000, 3000. We observe a strong correlation between the filter qualities and the number of labels, hence test error rates.

We now consider the semi-supervised learning setting where we only use a small portion of the labels from the training set. We use the same fully connected three layer network as in Section 3.1. We follow the experiment settings as in Rifai et al. (2011a), Kingma et al. (2014), where the 50000 training set is further split into one labeled set and one unlabeled set. We use the validation set to select $\lambda$ and $\beta$, and found that $\lambda = \beta = 15$ works well for all the four settings.

We report the results in Table 4. We see that LIMR consistently boosts the performance of the classifier with the aid of unlabeled data. Compared with the state-of-the-art models, except for the case with only 100 labels, LIMR is comparable or better than pretraining based semi-supervised learning CAE and MTC. The deep generative model proposed by Kingma et al. (2014) works the best with very few labels in general, but it is beat by LIMR in the case of 3000 labels. An error rate of 1.88 also sets the new state-of-the-art result on this sub-task.
| # labels | NN     | NN + LIMR | CAE   | MTC   | Kingma et al. (2014) |
|----------|--------|-----------|-------|-------|---------------------|
| 100      | 32.61  | 26.04     | 13.47 | 12.03 | 3.35                |
| 600      | 13.14  | 5.16      | 6.3   | 5.13  | 2.59                |
| 1000     | 11.15  | 3.03      | 4.77  | 3.64  | 2.40                |
| 3000     | 6.91   | 1.88      | 3.22  | 2.57  | 2.18                |

Table 4: Test error rates with different label numbers. Note that with LIMR we are consistently able to improve the performance of the neural net with unlabeled data. We also achieve the state-of-the-art result on the 3000-labels subtask.

As a qualitative justification, we also visualize the first layer filters learned with different label numbers in Figure 3. We see that even with a few labels, LIMR is still able to learn sharp filters. There is also a clear correlation between the visual quality of the filters and the number of labels. Especially, the filters learned with 3000 labels are almost indistinguishable from those learned with all the 50000 labels in Figure 1. This strongly indicates the power of semi-supervised learning, as
well as that LIMR is able to take advantage of both labels and unlabeled data simultaneously and learn meaningful representations and classifiers at the same time.

We also consider two more challenging benchmarks, CIFAR10 and SVHN. CIFAR10 consists of 60000 $32 \times 32 \times 3$ images in 10 object categories, with 50000 examples as training set and 10000 as testing set. The subset of the SVHN dataset we use consists of images of the size also $32 \times 32 \times 3$, with 70000 for training, 26000 for testing and 100000 unlabeled examples. As CIFAR10 does not come with an unlabeled set, we use the entire CIFAR100 dataset for this purpose. Note that although CIFAR10 and CIFAR100 have input images of the same size, they have two different label sets. For both the two benchmarks, we use a CNN with architecture $64 \times 5 \times 5 64 \times 3 \times 3 64 \times 3$, with $2 \times 2$ max pooling following each convolution layer. We plot the training and testing error curves in Figure 4 under three settings: no regularization, supervised LIMR regularization and semi-supervised LIMR regularization. We see that for both the two datasets, applying LIMR significantly reduces overfitting (larger training error and lower testing error). When incorporated with unlabeled data, LIMR is able to further reduce the testing error. Interestingly, this works despite that CIFAR10 and CIFAR100 have different label sets.

4 CONCLUSION

We have proposed two regularizers that make use of the data manifold to guide the learning of a discriminative neural network. By encouraging the flatness of either the loss function or the prediction scores along the data manifold, we are able to significantly improve a DNN’s generalization ability. Moreover, our label independent manifold regularization allows one to incorporate unlabeled data directly with the supervised learning task and effectively performs semi-supervised learning. We have validated our proposed regularizers on the MNIST, CIFAR10 and SVHN datasets and demonstrated their effectiveness.

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