Gradient Regularization Improves Accuracy of Discriminative Models

Dániel Varga, Adrián Csiszárik, Zsolt Zombori
Alfréd Rényi Institute of Mathematics
Hungarian Academy of Sciences
Budapest, Hungary
{daniel,csadrian,zombori}@renyi.hu

ABSTRACT

Regularizing the gradient norm of the output of a neural network with respect to its inputs is a powerful technique, first proposed by Drucker & LeCun (1991), who named it Double Backpropagation. The idea was independently rediscovered several times since then, most often with the goal of making models robust against adversarial sampling. This paper presents evidence that gradient regularization can consistently and significantly improve classification accuracy on vision tasks, especially when the amount of training data is small. We introduce our regularizers as members of a broader class of Jacobian-based regularizers, and compare them theoretically and empirically.

A straightforward objection against minimizing the gradient norm at the training points is that a locally optimal solution, where the model has small gradients at the training points, may possibly contain large changes at other regions. We demonstrate through experiments on real and synthetic tasks that stochastic gradient descent is unable to find these locally optimal but globally unproductive solutions. Instead, it is forced to find solutions that generalize well.

1 INTRODUCTION

Regularizing the gradient norm of a neural network’s output with respect to its inputs is an old idea, going back to Drucker & LeCun (1991), where it was named Double Backpropagation. Variants of this core idea were independently rediscovered several times since 1991 (Sokolic et al., 2017; Ororbia II et al., 2017; Czarnecki et al., 2017; Gulrajani et al., 2017), most recently by the authors of this paper. Outside the domain of artificial neural networks, Sobolev regularization (Rosasco et al., 2013) is essentially the same concept, a special case of the very general, classic method of approximating functions in Sobolev space (Györfi et al., 2002). Smoothing splines (Wahba, 1990) are another important special case.

These regularization techniques work by adding a regularization term to the main loss function. This term is a function of the Jacobian of the outputs with respect to the inputs, calculated at the training points. Depending on the choice of the regularizer function (e.g. Frobenius norm) and the choice of the output (e.g. the loss function of the model, the vector of logits, the vector of class probabilities) we have a broad class of possible regularizers.

Calculating these regularization terms is made easy and fast by modern tensor libraries. Drucker & LeCun (1991) had to tediously calculate the gradients manually. This and performance issues restricted their experiments to 3-layer networks. In contrast, tensor libraries have no issues calculating these terms for networks that are hundreds of layers deep, without excessive increase in computation. Figure 1 shows the full Tensorflow implementation of the two regularizers that we focus on.

Most recent applications of gradient regularization (Sokolic et al., 2017; Gu & Rigazio, 2014; Ororbia II et al., 2017; Slavin Ross & Doshi-Velez, 2017) focused on robustness against adversarial sampling (Szegedy et al., 2013) on classification tasks. This is a very natural application, as gradient regularization means that small perturbations of the input can not lead to large perturbations in predicted class probabilities.
datagrad_loss = tf.reduce_sum(tf.square(tf.gradients(loss, [x])[0]), axis=1)

gradients = tf.gradients(logits * tf.random_normal((OUTPUT_DIM,)), [x])[0]
spectreg_loss = tf.reduce_sum(tf.square(gradients), axis=1)

Figure 1: TensorFlow implementations for the DataGrad and SpectReg regularizers

In this paper we present results on a task arguably more fundamental than robustness against adversarial sampling: classification accuracy itself. Specifically, we present natural visual classification tasks and strong baselines for these tasks where adding gradient regularization leads to significant and consistent accuracy improvements. The effect is most emphasized when the number of training examples is small.

We present comparisons between several gradient regularization terms, and conclude that two of them are the most promising ones on classification tasks. One is classic Double Backpropagation by Drucker & LeCun (1991): the L2 gradient norm of the loss function. We will shorten the term 'Double Backpropagation' to DataGrad after Ororbia II et al. (2017) who discovered and named it independently. The other, which we term SpectReg is the L2 gradient norm of a random projection of the logit vector. In our MNIST experiments, DataGrad outperforms all alternative regularization methods, and both DataGrad and SpectReg significantly outperforms our well tuned baseline. The improvement is most pronounced for smaller training set sizes. In our CIFAR-10 experiments with decreased data set size, SpectReg outperforms all alternatives, and both SpectReg and DataGrad improves on the baseline.

A possible objection against gradient regularization is that it focuses its attention on the metric of the input space, as opposed to the latent spaces emerging during training. The recent success of techniques with the same limitation weakens this objection significantly in our view. Examples include mixup (Zhang et al., 2017) and Gradient Penalty (Gulrajani et al., 2017). Nevertheless, overcoming this limitation is a promising future research direction, possibly by regularizing gradients with respect to hidden layers.

A more fundamental objection against minimizing the gradient norm at the training points is that this constraint can be satisfied purely locally, without any globally preferred behavior. We demonstrate through experiments on real and synthetic tasks that stochastic gradient descent is unable to find these locally optimal but globally unproductive solutions. Instead, it is enforced to find solutions that generalize well.

2 Notation

Throughout the paper we consider feed-forward networks with a loss function in the following form:

\[ L(x, y, \Theta) = M(f(x, \Theta), y) \]

where \( x \) is the input, \( y \) is the desired output, \( \Theta \) are the parameters of the network represented by the function \( f \), and \( M \) is a metric comparing network output to ground truth. In discriminative models, \( y \) is the one-hot encoding of the output label, and the map \( f \) is often in the following form:

\[ f(x, \Theta) = \text{softmax}(g(x, \Theta)), \]

where the softmax function maps the logit vector output of \( g \) to the vector of predicted label probabilities (denoted with \( p \)). The softmax function is given by:

\[ \text{softmax}(z)_i = \frac{e^{z_i}}{\sum_{k=1}^{m} e^{z_k}} \quad \text{for} \quad i \in \{1 \ldots m\} \]
where \( m \) is the number of class labels and \( z \) is the logit vector. The metric function of classification networks is most commonly the categorical cross-entropy, which leads to the following loss function:

\[
L(x, y, \Theta) = -\langle y, \log(f(x, \Theta)) \rangle = -\langle y, \log(\text{softmax}(g(x, \Theta))) \rangle.
\]

Below \( J_g(x) = \frac{\partial}{\partial x} g(x) \) is the Jacobian of logits and \( J_f(x) = \frac{\partial}{\partial x} f(x) \) is the Jacobian of class probabilities.

3 Our Contributions

The paper presents evidence that gradient regularization can increase classification accuracy in vision tasks. We compare several gradient regularization schemes empirically on small-scale vision tasks, and conclude that two of these outperform strong baselines: Double Backpropagation (which we shorten to DataGrad) and Spectral Regularization:

\[
R_{\text{DataGrad}}(x, y, \Theta) = \| \frac{\partial}{\partial x} L(x, y, \Theta) \|^2_2
\]

\[
R_{\text{SpectReg}}(x, y, \Theta) = E_{r \sim N(0, I_m)} \| J_f r \|^2_2
\]

An objection against minimizing the gradient norm at the training points is that this constraint can be satisfied purely locally, without any globally preferred behavior. We demonstrate through experiments on real and synthetic tasks that stochastic gradient descent is unable to find these locally optimal but globally unproductive solutions. Instead, it is forced to find solutions that generalize well.

4 Related Work

Our original inspiration for using symbolically computed gradient norms to regularize a classifier network came from observing the Gradient Penalty technique by Gulrajani et al. (2017), who employ symbolically computed gradient norms in the context of training Wasserstein GANs. But after obtaining the first, promising implementation of our method, our literature search gradually unearthed a large amount of earlier incarnations of the core idea. This literature search was made harder by the fact that the citation graph between these results is quite sparse, with many independent rediscoveries.

To our current best knowledge, the basic method first appeared in Drucker & LeCun (1991) who called it Double Backpropagation. Due to slow hardware and a missing technical apparatus for symbolic differentiation, they were restricted to evaluate the idea on networks with two hidden layers. The TangentProp variant was introduced in Simard et al. (1991) where instead of taking the gradient norm, which controls magnitude of change in all input space directions, selected invariances are specified by constraining the derivatives in corresponding directions. (E.g. helping the model achieve rotation invariance by using the direction of infinitesimal rotation in pixel space.)

In the last few years, the core idea was rediscovered independently several times, with much variation in implementation details and choice of applications. Below we review the instances that we are aware of and compare our results to each of these.

4.1 Jacobian Regularization

The Jacobian Regularizer introduced by Sokolic et al. (2017) works by regularizing the Frobenius norm of the Jacobian of the softmax output with respect to the input. For smaller networks the authors symbolically compute the Jacobian. For larger networks they employ a Frobenius-norm based regularization for each layer individually, for performance reasons. Such layer-wise regularization of the Frobenius of the Jacobian was also employed in Gu & Rigazio (2014). The computation of the symbolic Jacobian Regularizer roughly requires \( m \) parallel computations of the forward pass,
where \( m \) is the number of output labels. The alternatives we present are significantly less expensive computationally while their accuracy is higher on our tasks.

One difference between the Jacobian Regularizer and our Spectral Regularizer is that we work with the Jacobian of the logits (the input of the top softmax layer) while Sokolic et al. (2017) work with the Jacobian of the softmax output. We experimentally compare these approaches and conclude that for our tasks the logits are the more appropriate choice. This can be justified theoretically by noting that diminishing gradients (with respect to weights) are more of a concern when a sigmoid (or in our case, softmax) is applied to the output.

4.2 Robustness to Adversarial Examples

The Double Backpropagation formula was rediscovered by Ororbia II et al. (2017) who named it DataGrad. It is introduced with the goal of making classifiers more robust to adversarial sampling. The authors do not actually implement the formula, rather, a finite difference approximation is used. It proceeds by first finding adversarial samples by gradient descent then penalizing large changes in the loss function between the data point and its adversarially perturbed version. This approximation in fact improves robustness to adversarial sampling. Accuracy increases are not reported.

Very recently, Slavin Ross & Doshi-Velez (2017) used symbolically computed Double Backpropagation to improve robustness against adversarial noise. They also report improvements in what they call interpretability of adversarial perturbations: when Double Backpropagation is used, human perceptual differences between originals and adversarial samples increase, making it easier for human observers to understand how the model output depends from the model inputs. Accuracy increases are not reported.

4.3 Sobolev Training

A generalized form of the Double Backpropagation idea is when an oracle gives us information about the gradients (or even the Hessian) of the function to be learned, and we employ a loss term to incorporate this extra information. This variation is investigated by Czarnecki et al. (2017). The paper’s focus is distillation and synthetic gradients, applications where such an oracle is available. In contrast to this approach, we demonstrate the counter-intuitive fact that in the absence of such an oracle, simply pushing gradient norms toward zero at the data points can already have a beneficial regularization effect that improves accuracy on classification tasks.

5 Analysis

Below we will assume that we are dealing with a classifier network with a softmax layer at the top, and a categorical cross-entropy loss. Most of our results and techniques can easily be generalized to other top layers and loss functions. We call the input of the softmax layer the logits and denote them with \( z \), and denote the output of the softmax layer with \( p \). Let \( g \) denote the neural network’s mapping from inputs to logits. We denote the correct label’s one-hot encoded form with \( y \). With this notation, the categorical cross-entropy loss is

\[
L(x, y) = -\langle y, \log(\text{softmax}(g(x))) \rangle = -\langle y, z - \text{lse}(z) \rangle
\]

where \( \text{lse} \) is the logsumexp function

\[
\text{lse}(z) = \log \sum_{i=1}^{m} e^{z_i}.
\]

The central object of our investigation is the Jacobian of the logits with respect to the inputs:

\[
J_g(x) = \frac{\partial}{\partial x} g(x).
\]
5.1 Gradient Regularization Schemes

Gradient regularization schemes act by penalizing large changes in the output of some neural network layer with respect to the input. This general idea can be applied in different variations. One dimension of this variation is whether we compute the gradients on the loss term, on the predicted class probabilities, or even before, at the level of the logits. Since the loss term is scalar, its gradient is a vector, which can be computed effectively. However, both the logits and the probabilities are vectors and their gradients yield Jacobi matrices that are expensive to compute. Consequently, another dimension of the different gradient regularization schemes is whether they compute the full Jacobian matrix or first apply some sort of projection. Such a projection not only speeds up computation, but can also introduce additional useful regularization. We have found that several projections are reasonable. After the projection one applies some loss function $R$ to create an additional loss term. In our investigation, we use the squared $L^2$ norm for $R$, but the $L^1$ norm could also be reasonable. Below we summarize the different approaches that will be discussed throughout our paper.

- **Double Backpropagation** ([Drucker & LeCun, 1991]) or **DataGrad** ([Ororbia II et al., 2017]): take the original loss term and penalize the squared $L^2$ norm of its gradient.
  \[
  L_{\text{DataGrad}}(x, y, \Theta) = L(x, y, \Theta) + \lambda \| \frac{\partial}{\partial x} L(x, y, \Theta) \|_2^2
  \]
  Although not obvious from its definition, DataGrad can be interpreted as applying a particular projection to the Jacobian of the logits and regularizing it. We give a proof for this for the case when the main loss is the categorical cross entropy in Subsection 5.2.

- **Jacobian Regularizer (JacReg)** ([Sokolic et al., 2017]): use the squared Frobenius norm of the Jacobian of the softmax output (probabilities) with respect to the input.
  \[
  L_{\text{JacReg}}(x, y, \Theta) = L(x, y, \Theta) + \lambda \| J_f \|_F^2
  \]
  Symbolically computing the Jacobian is expensive as computation scales linearly with the number of output labels. To alleviate this, a layer-wise approximation is employed in [Gu & Rigazio, 2014] and Sokolic et al., [2017].

- **Frobenius Regularizer (FrobReg)**: use the squared Frobenius norm of the Jacobian of the logits with respect to the input.
  \[
  L_{\text{FrobReg}}(x, y, \Theta) = L(x, y, \Theta) + \lambda \| J_g \|_F^2
  \]
  FrobReg only differs from JacReg in that the Jacobian is computed on the logits instead of the probabilities. Computation is equally expensive, however, diminishing gradients due to the softmax transformation are less of a concern.

- **Spectral Regularization (SpectReg)**: apply a random projection to the Jacobian of the logits, and take the $L^2$ norm of the result:
  \[
  L_{\text{SpectReg}}(x, y, \Theta) = L(x, y, \Theta) + \lambda \| P_{\text{rand}}(J_g) \|
  \]
  where $P_{\text{rand}}(J_g) = J_g^T \frac{1}{\sqrt{m}} r$ and $r \in \mathcal{N}(0, I^m)$.
  When the random normal projector is normalized onto the unit sphere, the norm of the random projection can be interpreted as a lower bound to the (hard to compute) spectral norm of the Jacobian, which is equal to the Lipschitz constant of the input-logit mapping at the given point. We show in Subsection 5.2 that SpectReg is an unbiased estimator of the Frobenius norm of the Jacobian, with a constant scaling. The same is true for the normalized variant. We have not observed any empirical differences between the behavior of the normalized (spherical) and the un-normalized variants. SpectReg is significantly faster to compute than FrobReg, as the random projection of the Jacobian of the logits can be calculated as the gradient of the random projection of the logits (see Subsection 5.2).
• True label one-hot projection (OneHot): compute the Jacobian of the logits and apply the projection:

\[ P_{\text{True}}(J_g) = J_g^T y \]

where \( y \) is the one-hot encoding of the true label of the data point. This approach penalizes sudden changes in the true label’s logit at the data points, but does not consider sudden changes in the other labels’ logits. We have found that OneHot’s classification accuracy is similar to SpectReg’s, but slightly below it, so in this paper we focus on SpectReg instead.

• Random one-hot projection (RandomOneHot): compute the Jacobian of the logits and apply the projection

\[ P_{\text{OneRnd}} = J_g^T \sqrt{m} r \]

where \( r \) is a uniformly chosen random basis vector of the logit space. (The scaling factor \( \sqrt{m} \) makes the covariance matrix the identity.) Similar to OneHot, this approach brings improvements compared to our baselines, but it lags behind SpectReg, so we do not deal with it in the rest of the paper.

5.2 Computationally efficient regularization of the Jacobian

Subsection 5.1 presents a wide range of options for turning the Jacobian matrix into a regularizer. Some of these options have the important advantage that when computing them, we can avoid the intermediate step of computing the full Jacobian. The trick that achieves this is based on the linearity of the gradient. If our regularizer is of the form \( \|J_g^T w\|_2^2 \), where \( w \) is a vector from the logit space, then

\[ \|\nabla_{x} g(x)^T w\| = \| \nabla_{x} \langle g(x), w \rangle \| . \]

This means that the expensive Jacobian calculation can be replaced with a gradient calculation. SpectReg, OneHot and RandomOneHot are examples of this simplification. The following Claim is an easy consequence of the linearity of expectation:

\textbf{Claim 1.} If \( R \) is a distribution of row vectors with covariance matrix \( I_m \), then \( E_{r \sim R}[\|r J\|_2^2] = \|J\|_F^2 \).

\textbf{Proof.}

\[ E[\|r J\|_2^2] = E[\text{Tr}(J^T r^T J)] = \text{Tr}(J^T E[r^T r] J) = \text{Tr}(J^T J) = \|J\|_F^2 \]

It follows that the SpectReg, normalized SpectReg and RandomOneHot regularizers are unbiased estimators of the Frobenius norm of the Jacobian.

In the following, we show that DataGrad (Double Backpropagation) can also be interpreted as a projection of the Jacobian, if we allow \( w \) to depend on the output of the network.

\textbf{Claim 2.} With a cross-entropy loss function, the DataGrad regularizer is equivalent to applying the projection

\[ P_{\text{DataGrad}}(J_g) = J_g^T (f(x) - y) \]

and then L2 regularizing the obtained vector. Here \( J_g \) is the Jacobian of the logits, \( y \) is the one-hot encoding of the expected output and \( f(x) = \text{softmax}(g(x)) \) is the output of the network.

\textbf{Proof.} The DataGrad regularization term is

\[ \| \nabla_{x} L(x, y, \Theta) \|_2 \]

\[ L(x, y, \Theta) = - \sum_{i=1}^{m} y_i \log(\text{softmax}(g(x))_i) = - \sum_{i=1}^{m} y_i \log(\text{softmax}(z)_i) \]
\[ L(x, y, \Theta) = -\sum_{i=1}^{m} y_i (z_i - \log(\sum_{j=1}^{m} e^{z_j})) \]

\[ \frac{\partial}{\partial z_k} L(x, y, \Theta) = -y_k + \sum_{i=1}^{m} y_i \frac{e^{z_k}}{\sum_{j=1}^{m} e^{z_j}} = -y_k + \text{softmax}(z)_k \]

\[ \frac{\partial}{\partial z} L(x, y, \Theta) = -y + \text{softmax}(z) \]

\[ \frac{\partial}{\partial g(x)} L(x, y, \Theta) = \text{softmax}(g(x)) - y \]

In the above derivation we have exploited that \( y \) sums to 1. Using the chain rule, we obtain that

\[ \frac{\partial}{\partial x} L(x, y, \Theta) = \frac{\partial}{\partial g(x)} L(x, y, \Theta) \frac{\partial}{\partial x} g(x) = J_g^T (\text{softmax}(g(x)) - y) \]

\[ \| (\frac{\partial}{\partial x} L(x, y, \Theta)) \|_2 = \| J_g^T (\text{softmax}(g(x)) - y) \|_2 \]

This concludes our proof.

It is instructive to consider the toy edge case when the neural network consists of a single dense linear layer. Here the weight matrix and the Jacobian coincide. Thus, for this network, the Frobenius Regularizer is identical to L2 weight decay and SpectReg is an estimator for weight decay.

The Frobenius norm is submultiplicative, and the gradient of the ReLU is upper bounded by 1. Thus, for a dense ReLU network the product of layer-wise weight norms is an upper bound for the Frobenius Regularizer loss term. Applying the inequality of arithmetic and geometric means, we can see that the total weight norm can be used to upper bound the Frobenius Regularizer loss term.

The Lipschitz constant of the function \( g(x) \) at a smooth neighborhood of \( x \) is equal to the spectral norm \( \| J_g \|_2 \). For multi-valued functions, directly calculating, or even approximating the spectral norm is infeasible. The Frobenius norm is within a constant factor of the spectral norm, so it can be interpreted as a proxy when our goal is to enforce a Lipschitz property locally. However, the example of L1 and L2 weight regularization reminds us that optimizing different regularization terms can lead to very different behavior even when they are within a constant factor of each other.

5.3 Continuity violated

It is worth noting that for the important class of piecewise linear activation functions, gradient-based regularizers violate an important standard assumption: that the loss is a continuous function of the network parameters. \( J_g(x) \) is a piecewise constant function of the inputs. It is also a piecewise constant function of the biases, implying that the biases of the network do not get a gradient update from the gradient-based loss terms. More importantly, loss is a non-continuous, piecewise multilinear function of the weights. Nevertheless, we have not observed optimization issues that could be attributed to non-continuity.

Let us now assume using ReLU activations for simplicity. For a fixed input \( x \) and a fixed \( \Theta \), let us call the set of neurons with positive output the network’s firing pattern for the given \( x \) and \( \Theta \). Gradient regularization terms are continuous on subsets of the parameter space where the firing pattern is constant. We speculate that the reason non-continuous gradient regularization loss terms can successfully be optimized using gradient descent is that they are “close to continuous”, in the sense that a single gradient update does not cause a drastic change in the firing pattern for a given input.

6 Experiments

We conduct experiments to compare gradient-based regularization with various other regularization methods in order to position this technique on the landscape.
Besides experiments on the full training set, we also experiment with greatly reduced training sets to increase the importance of regularization and thus provide a better insight into the effects of the different approaches. At each experiment we indicate the size of the training set that is used (in most cases the reduced set size is 2000). Final evaluation is performed on a test set of 10000 points.

6.1 Implementation details

We report classification results on the MNIST and CIFAR-10 datasets. Below we detail the network architectures that we use for each dataset. All reported hyperparameters (batch size, learning rate, learning rate decay, weight decay, dropout rate, minibatch count) are carefully tuned for the baseline model, but our experiments suggest that they are good choices for the regularized models as well.

We also use a small synthetic dataset $\sin$ generated from the function $f : \mathbb{R} \to \mathbb{R}, f(x) = \sin(5x)$ which allows for visualizing the function learned by the neural network.

For each regularizer, dataset and training set size, the optimal weight is selected based on a grid search from the following fixed sets:

- DataGrad: 0.0003, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, 2, 5, 10, 20, 50, 100
- SpectReg: 0.0001, 0.0003, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1
- JacReg: 0.0001, 0.0003, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1
- CP: 0.0001, 0.003, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1

We find that these regularizers are not particularly sensitive to their weight parameter, except for DataGrad, which requires more careful tuning. This is probably related to the fact that DataGrad vanishes as the network achieves a good fit on the training set. One needs to strike a careful balance to ensure that DataGrad vanishes neither too quickly nor too slowly.

6.1.1 MNIST

For the MNIST handwritten digits recognition task, we implement a standard modern incarnation of the classic LeNet-5 architecture [LeCun et al., 1998], with maxpooling, ReLU activations and dropout after the dense hidden layer. The total parameter count of the used baseline model is 61706. On the full MNIST dataset, this model achieves 99.1% test accuracy without data augmentation.

We train our models using Adam optimizer with $\beta_1 = 0.9$, $\beta_2 = 0.999$ parameter settings and a batch size of 50. We use an initial learning rate of 0.1, and employ learning rate decay dividing by a factor of 10 at 50% and 75% of the training iterations. We use a weight decay of 0.0005, unless otherwise stated. When employing dropout, we use dropout rate 0.5. Our training runs are stopped after 10000 minibatches in all of our MNIST experiments. We have verified that this is enough to achieve convergence for all of our scenarios. Moreover, early stopping does not provide measurable improvements, as the test accuracy curve plateaus without later accuracy degradation.

In all of the experiments on MNIST, 10000 points from the training set is set aside as a held-out development set for hyperparameter tuning.

6.1.2 CIFAR-10

The CIFAR-10 dataset [Krizhevsky & Hinton, 2009] consists of 60000 32×32 color images in 10 classes, with 6000 images per class. There are 50000 training images and 10000 test images.

We use a residual network (ResNet) architecture [He et al., 2015] for the CIFAR-10 classification task. This architecture consists of three levels, each containing stacked residual blocks. The structure of a residual block is conv-batchnorm-ReLU-conv-batchnorm, followed by elementwise addition and a ReLU nonlinearity. The three levels differ only in the number of convolutional filters and feature map sizes. The number of filters are 48, 96 and 192, respectively. The network has around 2.5 million parameters. On the full CIFAR-10 training set, this model achieves 93.71% test accuracy.

The models are trained for 50000 iterations with SGD, with a mini-batch size of 128. The initial learning rate is 0.1, and we employ learning rate decay dividing by a factor of 10 at 50% and 75% of
Dataset: MNIST, training set size 2000

|                         | NoGR | SpectReg | DataGrad |
|-------------------------|------|----------|----------|
| LeNet unregularized     | 96.99% (0.15) | 97.59% (0.13) | 97.56% (0.24) |
| LeNet Batchnorm         | 96.89% (0.23) | 96.94% (0.27) | 96.89% (0.22) |
| LeNet Dropout           | 97.29% (0.19) | 97.65% (0.14) | **97.98% (0.12)** |

Table 1: Comparison of Dropout, Batch Normalization and two variants of gradient regularization: symbolic DataGrad and SpectReg, using the MNIST dataset. Train size is set to 2000. DataGrad and SpectReg weights for the different base normalizers are as follows: Batchnorm (0.001, 0.001), Dropout (50, 0.01), unregularized (50, 0.01). We can see that both DataGrad and SpecReg achieve higher accuracy than either Dropout or Batchnorm in itself. We obtain the best result by combining Dropout and DataGrad.

the training iterations. We use a momentum of 0.9 and Nesterov momentum with dampening of 0. The weight decay is set to 0.003.

6.1.3 SIN

Our synthetic dataset is sampled from function $f: \mathbb{R} \to \mathbb{R}, f(x) = \sin(5x)$. We use a small training set of 100 points sampled uniformly from $[-1, 1]$ and add some Gaussian noise ($\sigma = 0.1$) to the output. For evaluation, we use a fixed grid of 900 points from the same $[-1, 1]$ domain with uncorrupted outputs. The added noise highlights the need for regularization since overfitting on the training set can severely damage performance on the test set.

As a baseline model, we use an MLP network with 5 dense layers of 64 neurons and ReLU nonlinearity, followed by a single linear neuron that produces the output of the network.

6.2 RESULTS

An individual experiment consists of 10 runs of the same setup, each time with a different randomly chosen training set of the given size. All reported numbers are the mean of these 10 runs evaluated on the test set, accompanied with the standard deviation in parentheses.

Consistent with our notation in Section 5, $\lambda$ denotes the weight of the loss term associated with a particular regularizer.

6.2.1 Gradient Regularization Compared with Dropout and Batch Normalization

On the training data limited MNIST task, we examine how the best gradient regularization variants compare with more established techniques, namely Dropout (Srivastava et al., 2014) and Batch Normalization (Ioffe & Szegedy, 2015) on MNIST. Table 1 summarizes our results. Both symbolic DataGrad and SpectReg outperform both Dropout and Batchnorm. We note that on this particular problem Batchnorm does not prove to be useful and does not work well with gradient regularization. All other regularizations are effective and the best result is obtained when combining Dropout with DataGrad.

Since Batch Normalization is a crucial ingredient of large modern neural networks and its weakness is particular to the training data limited MNIST task, it is important to see how Gradient Regularization fares on large networks using Batch Normalization. We demonstrate in Subsection 6.2.2 the usefulness of our methods on CIFAR-10, using a large residual network.

6.2.2 Gradient Regularization versus Confidence Penalty

One recently introduced regularization technique is Confidence Penalty (CP) (Pereyra et al., 2017). It directly penalizes the negentropy of the softmax output, thus preventing model overconfidence at the training points. It is closely related to the technique of label smoothing (Szegedy et al., 2016), and just like label smoothing, it brings small but consistent accuracy improvements on many tasks. Computationally, it is significantly cheaper than our methods.

We compare DataGrad and SpectReg with CP regularization. As Table 2 shows, all the three methods improve the accuracy of the baseline model on MNIST, and in itself DataGrad performs best.
Table 2: Confidence Penalty versus SpectReg and DataGrad on MNIST, using 2000 training points. We note that when using DataGrad and CP in conjunction, we have to re-tune the weight of the DataGrad loss term. All tuning is performed on the held-out development set while the presented numbers are measured on the test set. Optimal weights for DataGrad, SpectReg and CP are 50, 0.03 and 0.01, respectively, and when CP and DataGrad and used in conjunction, the optimal DataGrad weight is 10. We can see that while all regularizers improve the test accuracy of the baseline model, DataGrad performs best. Furthermore, the benefits of gradient regularization and confidence penalty add up when we use them in conjunction.

| Weight decay | No GR | SpectReg | DataGrad |
|--------------|-------|----------|----------|
| No CP        | 97.39% (0.11) | 97.79% (0.12) | 97.89% (0.12) |
| CP           | 97.57% (0.15) | 97.89% (0.12) | 98.07% (0.09) |

Table 3: Comparing SpectReg, DataGrad and Confidence Penalty on CIFAR-10, using 2000 training points. Optimal weights for CP, SpectReg and DataGrad are 0.003, 0.003 and 1, respectively. All regularizers improve the test accuracy of the baseline model, and SpectReg performs best.

| Baseline           | SpectReg    | DataGrad   | CP          |
|--------------------|-------------|------------|-------------|
| 55.63% (2.06)      | 59.24% (1.48) | 57.45% (1.79) | 58.30% (1.79) |

The best result is achieved by combining DataGrad and CP, which indicates that the two methods perform orthogonal tasks.

Table 3 shows how the regularizers perform on CIFAR-10, using a large residual network. While all three methods significantly improve on the baseline, DataGrad performs worse than its peers. We speculate that this might be due to the high sensitivity to the DataGrad coefficient. On large tasks, tuning the coefficient is a significant undertaking, and more precise tuning could potentially increase DataGrad’s performance. SpectReg on the other hand performs robustly, and yields significant accuracy increase for a large range of weight values.

6.2.3 WEIGHT DECAY VERSUS GRADIENT REGULARIZATION

Probably the most widespread regularization method is weight decay. In this subsection we examine how SpectReg and DataGrad perform with respect to weight decay. The results are summarized in Table 4. Both SpectReg and DataGrad improve on the test accuracy of the baseline model more than weight decay. DataGrad performs best.

| Dataset: MNIST, train set size 2000 | Weight decay | NoGR | SpectReg | DataGrad |
|-----------------------------------|--------------|------|----------|----------|
| No WD                             | 97.25 (0.22) |      | 97.69 (0.11) | \(\lambda = 0.03\) | 97.95 (0.15) | \(\lambda = 50\) |
| WD=0.00055                        | 97.40 (0.15) | 97.73 (0.13) | \(\lambda = 0.05\) | 97.92 (0.16) | \(\lambda = 50\) |

Table 4: Comparing SpectReg, DataGrad and the baseline model with and without weight decay on MNIST, using 2000 training points. All regularizers improve the test accuracy of the baseline model, and DataGrad performs best.
Figure 2: Comparison of various regularization methods on MNIST. The x axis shows train set size while the y axis shows test accuracy. The variants are DataGrad, CP, SpectReg, JacReg and Baseline (using only weight decay). We can see that DataGrad performs best consistently for all training set sizes. Note that each measurement in the figure uses the corresponding optimal hyperparameters (tuned on the development set).

Dataset: CIFAR-10, full training set with data augmentation

| λ    |  0  | 0.0001 | 0.0003 | 0.001 | 0.003 | 0.01  | 0.03  | 0.1  |
|------|-----|--------|--------|-------|-------|-------|-------|------|
| SpectReg | 93.71% | 93.74% | 93.66% | 93.55% | 93.54% | 93.01% | 92.49% | 93.14% |
| DataGrad  | 93.71% | 93.98% | 94.08% | 93.94% | 94.04% | 94.14% | 93.80% | 93.46% |

Table 5: Comparing test accuracy for different SpectReg and DataGrad λ values trained on CIFAR-10 with full training set and data augmentation for 200000 iterations (1 run in each cell).

6.2.5 Gradient Regularization and Data Augmentation

Data augmentation is a crucial ingredient for building models with good generalization properties. The role of standard regularization methods to prevent overfitting often diminishes when used alongside data augmentation as reported by Pereyra et al. (2017) in their CIFAR-10 experiments regarding Confidence Penalty regularization.

Our experiments show that gradient regularization improves accuracy even when employed alongside data augmentation. Table 5 shows a comparison of DataGrad, SpectReg with different λ weights and a baseline ResNet model trained on the full CIFAR-10 training set with standard data augmentation applied (using horizontal flip and random translations with at most 4 pixels along both coordinates). DataGrad improves generalization performance, which is in notable contrast with e.g. the Confidence Penalty regularization, which does not help in this case, as reported by Pereyra et al. (2017). Figure 3 shows the learning curves of DataGrad (with the best performing λ = 0.01) and the baseline model. The model with DataGrad gains advantage in the early stages and maintains this over the course of the training.

6.2.6 Approximating the Frobenius of the Jacobian does not lead to loss in accuracy

Directly minimizing the Frobenius of the Jacobian is an expensive operation. We demonstrate that first applying a random projection on the Jacobian and minimizing the obtained vector does not reduce the efficiency of the regularization while reducing the computational burden by a factor of $m$ where $m$ is the number of output labels.
Learning curves on CIFAR-10 with ResNet baseline

![Learning curves on CIFAR-10 with ResNet baseline](image)

**Figure 3:** Learning curves of DataGrad and the baseline ResNet model trained on full CIFAR-10 training set with standard data augmentation applied.

| Dataset: MNIST, training set size 2000 |
|----------------------------------------|
| SpectReg | JacReg | FrobReg |
| 97.79% (0.12) | 97.63% (0.15) | 97.76% (0.13) |

**Table 6:** Comparing SpectReg, FrobReg and JacReg on MNIST, using 2000 randomly chosen training points. SpectReg performs best, but the differences are small: after Bonferroni correction, the only statistically significant difference is between SpectReg and JacReg. We conclude that 1) we do not lose accuracy by minimizing a random projection of the Jacobian of the logits and that 2) it is better to minimize the Jacobian on the logits, rather than on the probabilities.

We compare SpectReg, which applies a random projection on the Jacobian of the logits, to JacReg which minimizes the full Frobenius norm of the Jacobian of the probabilities, and FrobReg which minimizes the full Frobenius norm of the Jacobian of the logits. We can see from Table 6 that it is somewhat more beneficial to control the Jacobian on the logits, rather than on the probabilities. We also conclude that minimizing a random projection of the Jacobian does not lead to a loss in accuracy, compared to the expensive full calculation of the Jacobian.

### 6.2.7 DataGrad’s Effect on the Magnitude of Network Parameters

Figure 4 shows the effect of DataGrad loss term weight $\lambda$ on two values: accuracy shown in blue, and the sum of squares of network parameters, shown in black. Each chart was created using a different L2 regularization weight. We can see that the correlation between DataGrad weight and model accuracy is positive until a phase transition point is reached where accuracy collapses. For the task at hand, this phase transition point was around DataGrad weight 20, unaffected by the amount of weight decay.

Let us now investigate how the amount of DataGrad regularization affects the magnitude of network weights for the trained network. For the model with no weight decay, DataGrad acts as a kind of weight decay itself, inasmuch as increasing the DataGrad weight $\lambda$ decreases the weight loss of the trained network. For models with weight decay, the relationship is more complex: below the phase transition DataGrad counteracts weight decay, above the phase transition it reinforces its effect.

The fact that DataGrad regularization affects a global attribute of the network such as total weight loss is evidence of the hypothesis that its effect is global, not limited to the immediate neighborhood.
Figure 4: Black: weight loss, primary y-axis. Blue: accuracy, secondary y-axis. Increasing the DataGrad weight increases accuracy, until a phase transition where accuracy collapses. Below this transition point, the weight loss of the trained network increases with the DataGrad weight, except for the case of zero weight decay, where DataGrad takes the role of weight decay.

| SpectReg $\lambda$ | 0   | 0.001 | 0.003 | 0.01 | 0.03 | 0.1  | 1   | 3   | 10  |
|---------------------|-----|-------|-------|------|------|------|-----|-----|-----|
| MSE (1e-5)          | 16.6| 24.5  | 2.5   | 2.3  | **1.6** | 3.4  | 74.9| 497.7| 1264.4| 2002.2|

Table 7: Mean squared error (MSE) on SIN for various SpectReg weights. The optimal weight is 0.03 which yields a reduction in MSE by a factor of 10.

of the training points where the gradient norm is regularized. In the next subsection we give a clear demonstration of this phenomenon on our synthetic task.

6.2.8 **Local gradient control does not lead to globally pathological gradient landscape**

A reasonable objection to gradient regularization methods is that they control the gradients only in the training points. A highly overparametrized network is capable of representing a "step function" that is extremely flat around the training points and contains unwanted sudden jumps elsewhere. Such a solution results in low gradient loss with high actual gradients in some points. However, all our experiments indicate that the learning process of neural networks is unable to find such pathological solutions and instead converges to truly smooth functions.

We demonstrate this on the SIN dataset. Note that our training set is small and noisy, so a good fit is likely to be curvy and steep. Figure 5 shows our training set and the functions learned by the network regularized with SpectReg using different weights. (Using DataGrad produces very similar graphs.) We observe that increasing the SpectReg weight makes the output smoother, not only around the training points, but globally as well.

Note that the bandwidth of the network does not limit its ability to learn the aforementioned pathological step-function like solutions. We verified this by training a modified version of the dataset: in this SIN2 dataset, we have two datapoints $(x, y)$ and $(x + 0.001, y)$ for each $(x, y)$ element of the original SIN. The network managed to reconstruct this function. We conclude that it is the optimization process rather than the network’s bandwidth that prevents the model from reaching a solution that has zero gradients near the training points.

While extremely large SpectReg weights clearly degrade the learned function, a well tuned SpectReg regularizer can provide much better fit to our target function. This is demonstrated in Figure 6, where we zoom into a small portion of the domain. Table 7 shows the mean squared error on the test set for the various SpectReg weights. SpecReg can reduce the mean squared error of the baseline model by a factor of 10.

### 7 Conclusion, Future Work

The paper presents evidence that gradient regularization can increase classification accuracy in vision tasks. We compare several gradient regularization schemes empirically on small-scale vision tasks, and observe that two of these outperform strong baselines: *Double Backpropagation (DataGrad)* and *Spectral Regularization*. The improvement is most pronounced for smaller training set sizes.
The effect of SpectReg on function approximation

Figure 5: This figure shows how increasing the weight of the SpectReg regularizer forces the network to learn an increasingly flat function. Note that the effect is global: although the gradient is controlled only on 100 training points, the whole manifold becomes smoother.

The smoothening effect of SpectReg

Figure 6: Zooming into a small portion of the domain, we observe that SpectReg allows for achieving a better fit to the target function.
Despite the fact that gradient control is applied only at the training points, our paper demonstrates that stochastic gradient descent converges to a solution where gradients are globally controlled. Even for very small training set sizes, the regularized models become smoother on the whole data manifold.

Below we list some of what we see as promising further research on gradient regularization:

- DataGrad is very sensitive to the choice of its coefficient. Understanding the relationship between the magnitude of the main loss term and the DataGrad loss term could help scaling the magnitude, leading to more robust behavior.
- In our applications, gradients were calculated with respect to inputs. We plan to investigate regularization terms where gradients are calculated with respect to hidden activations.
- Our understanding of the counterintuitive interaction between gradient regularization and stochastic gradient descent is still limited. A full-blown theory may yet be out of sight, but it is reasonable to expect that well-chosen experiments on synthetic benchmarks will lead to important new insights.

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