Gradient regularization in discriminative and generative models

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Background

Regularization

Regularization: Any change to the model that makes it generalize better to unseen data.

- L2 weight decay (Plaut et al 1986)
- dropout (Srivastava et al 2014)
- label smoothing (Szegedy et al 2015)
- entropy regularization (Pereyra et al 2017)
- ...and hundreds of others

Data loss

Unregularized training: we are looking for optimal network parameters

$$\operatorname*{argmin}_{\Theta} L(f_\Theta(x), y)$$

where

- Θ are the network parameters,
- $f_\Theta(x)$ is the output of the network on input x,
- y is the expected output on input x.
- $L(\hat{y}, y)$ is the loss function that quantifies how much we like the network's output, the smaller the better.
- $(x, y) \sim (X, Y)$ is sampled from our training data.

Regularization term

Now we want to regularize, that is, improve generalization to unseen data. One standard class of methods works by adding a regularization term to the data loss that penalizes network settings that we want to avoid:

$$\underset{\Theta}{\operatorname{argmin}}[L(f_\Theta(x), y) + \lambda L_{reg}(\Theta)]$$

Weight decay

The archetypal regularization term, from 1986 but still widely used, is the *L2 weight decay*:

$$L_{reg}(\Theta) = \|\Theta\|_2^2$$

It punishes large network weights (strong neural connections), which helps to avoid memorizing superficial correlations.

Remark: For a single dense linear layer it is equal to the squared Frobenius norm of the weight matrix.

Method

Smoothness prior

- The core idea behind our project is to enforce a **smoothness** property of the neural network via a well-chosen regularization term.
- Tiny perturbations of the network input should not lead to large changes in network output.

Smoothness prior

- We formalize smoothness in several ways, leading to our *Spectral Regularizer*, that approximates the Frobenius norm of the Jacobian of the input-output mapping at the training examples:

$$L_{SpectReg}(x, \Theta) = \| \frac{\partial}{\partial x} f_\Theta(x) \|_F^2 = \mathbb{E}_{\epsilon \sim \mathcal{N}(0, I^m)} [\| \epsilon^T \frac{\partial}{\partial x} f_\Theta(x) \|_2^2]$$

- and the *DataGrad* regularizer that penalizes large changes of the loss function at the training examples:

$$L_{DataGrad}(x, y, \Theta) = \| \frac{\partial}{\partial x} L(f_\Theta(x), y) \|_2^2$$

DataGrad

For lack of time we will only talk about DataGrad in this talk. To the best of our knowledge, the Spectral Regularizer is our contribution, but DataGrad has a more complex background story.

DataGrad

$$L_{DataGrad}(x, y, \Theta) = \| \frac{\partial}{\partial x} L(f_\Theta(x), y) \|_2^2$$

- The *DataGrad* regularization term was introduced by (Ororbia et al 2016).
- Intuitively, DataGrad penalizes large changes in the performance of the classifier at the training examples.
- Interestingly, the authors do not analyze or even implement this method, arguably making this a case of *flag-planting*.
- Instead, they work with an finite-difference approximation, based on *adversarial sampling*, and demonstrate that it can make models more robust to adversarial sampling.

DataGrad

In relation to (Ororbia et al 2016), our contributions are twofold:

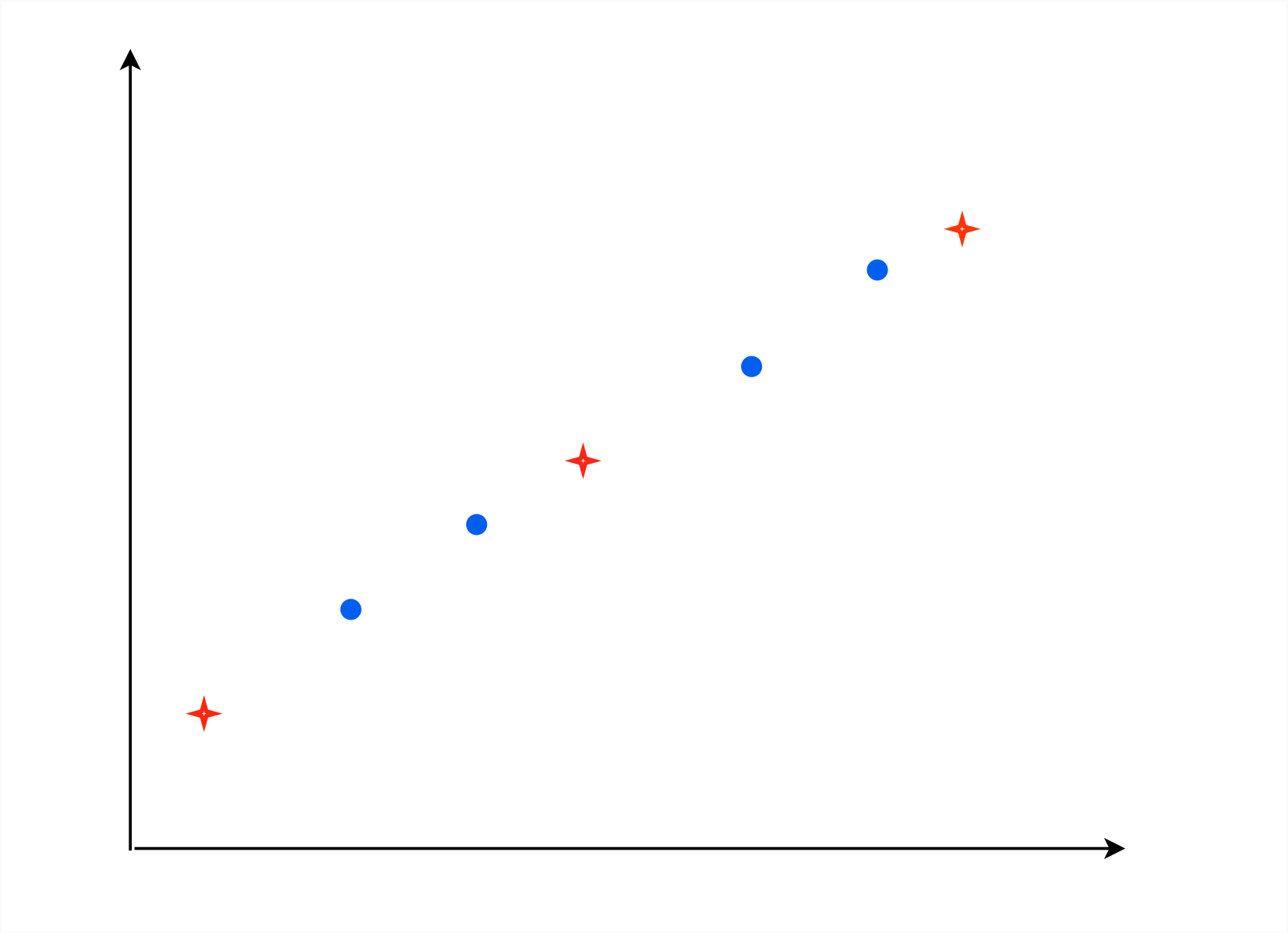
- We implement and investigate the symbolic, rather than adversarial sampling based version of DataGrad.
- We present detailed empirical evidence that the symbolic DataGrad method can improve classification accuracy, especially when the size of the training dataset is small.

Wait, this is not supposed to work!

$$L_{DataGrad}(x, y, \Theta) = \| \frac{\partial}{\partial x} L(f_\Theta(x), y) \|_2^2$$

- Did I say that the gradient norm is only controlled at the training examples?
- Yes. (And standard tricks like controlling it at noise-perturbed training examples did not help.)

Wait, this is not supposed to work!



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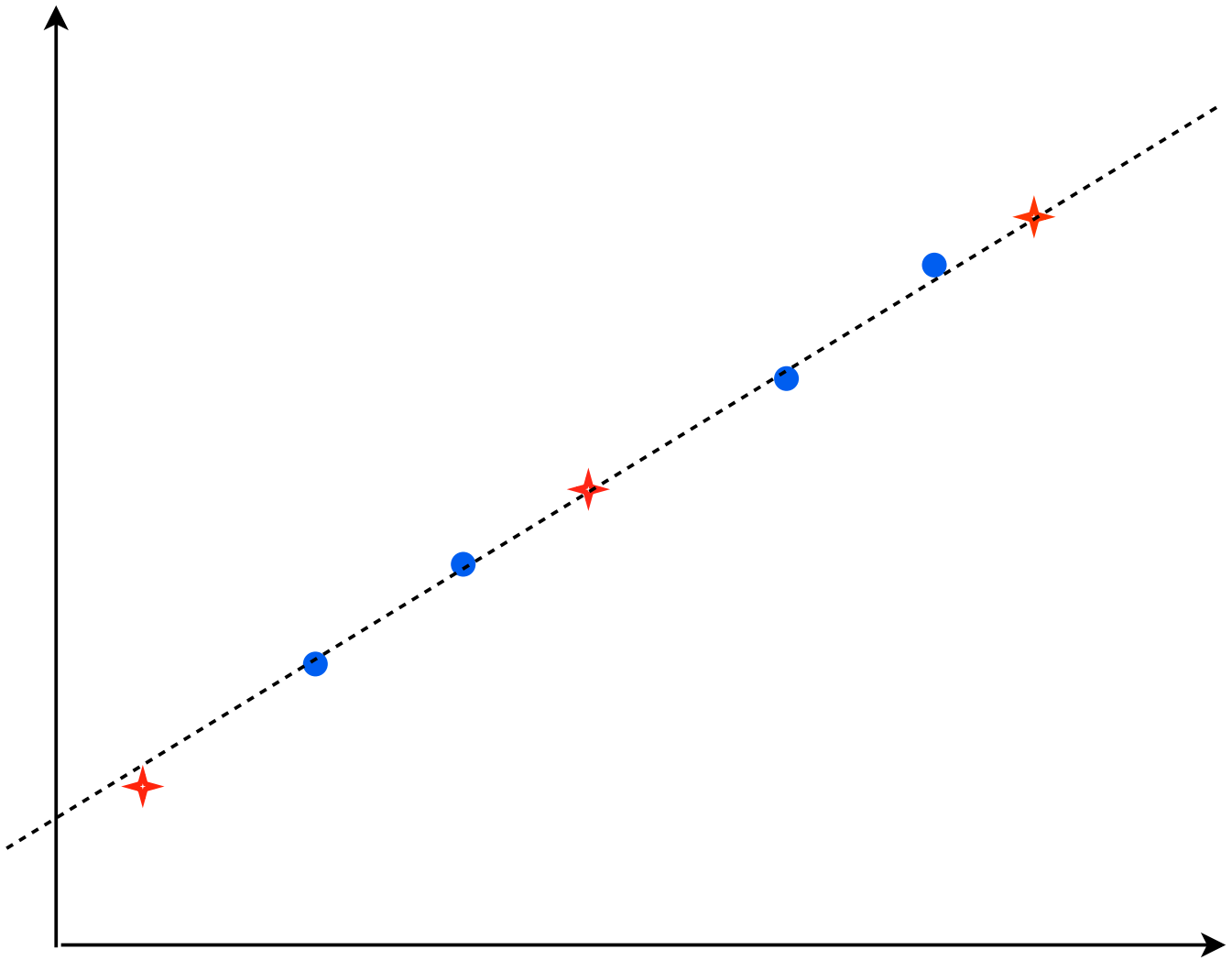

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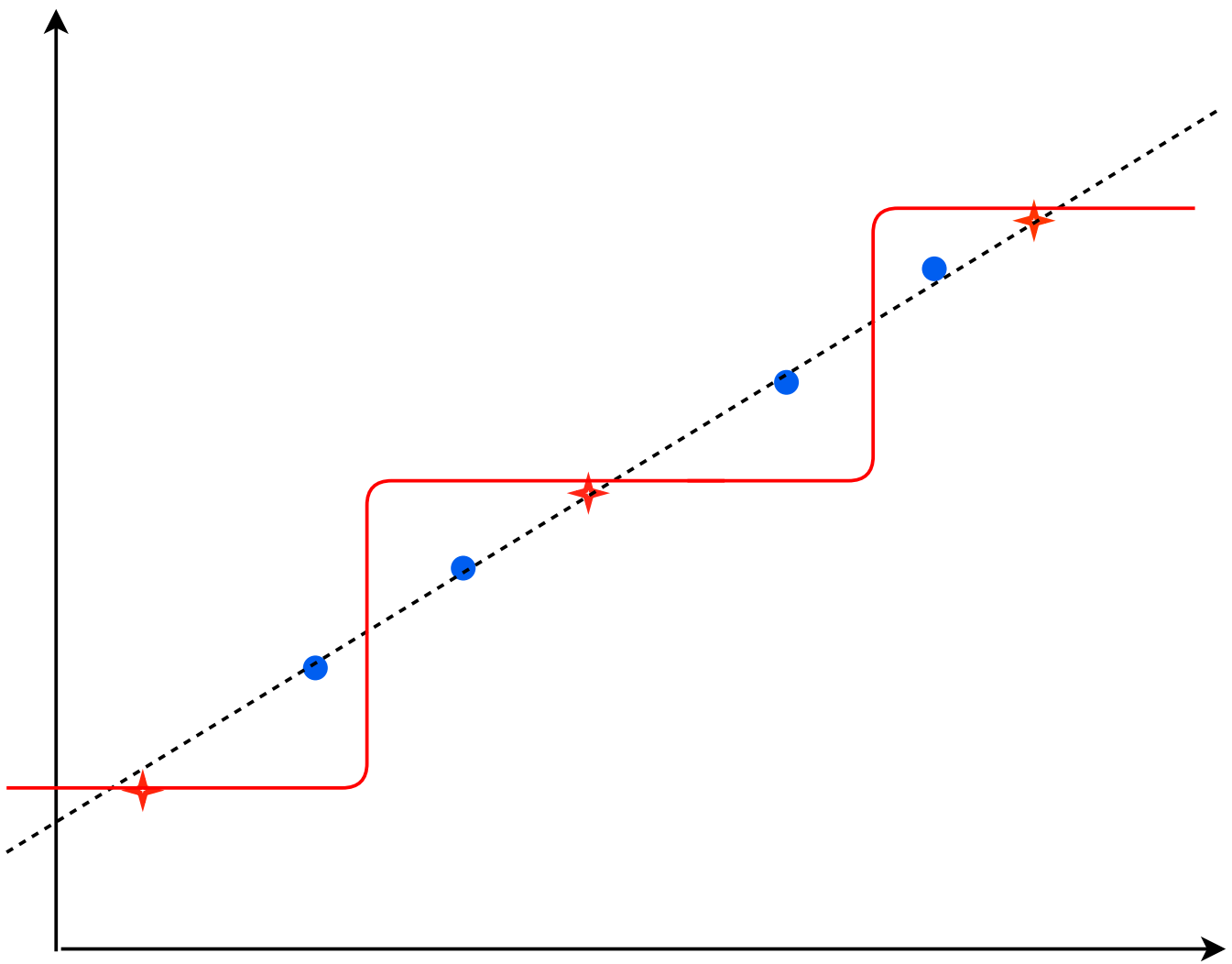


...But it does work.

- We are still in the process of understanding the phenomenon better,
- ...but apparently the low-dimensional intuition of the previous slides does not generalize to complex high-dimensional loss surfaces,
- ...especially not when our method of discovery of these surfaces is the gradient descent.
- Gradient descent does not converge to step function-like solutions such as seen on the previous slide.
- It is probably better to think of gradient regularization as "smarter weight decay". It influences the gradient norm at points far away from the training dataset.

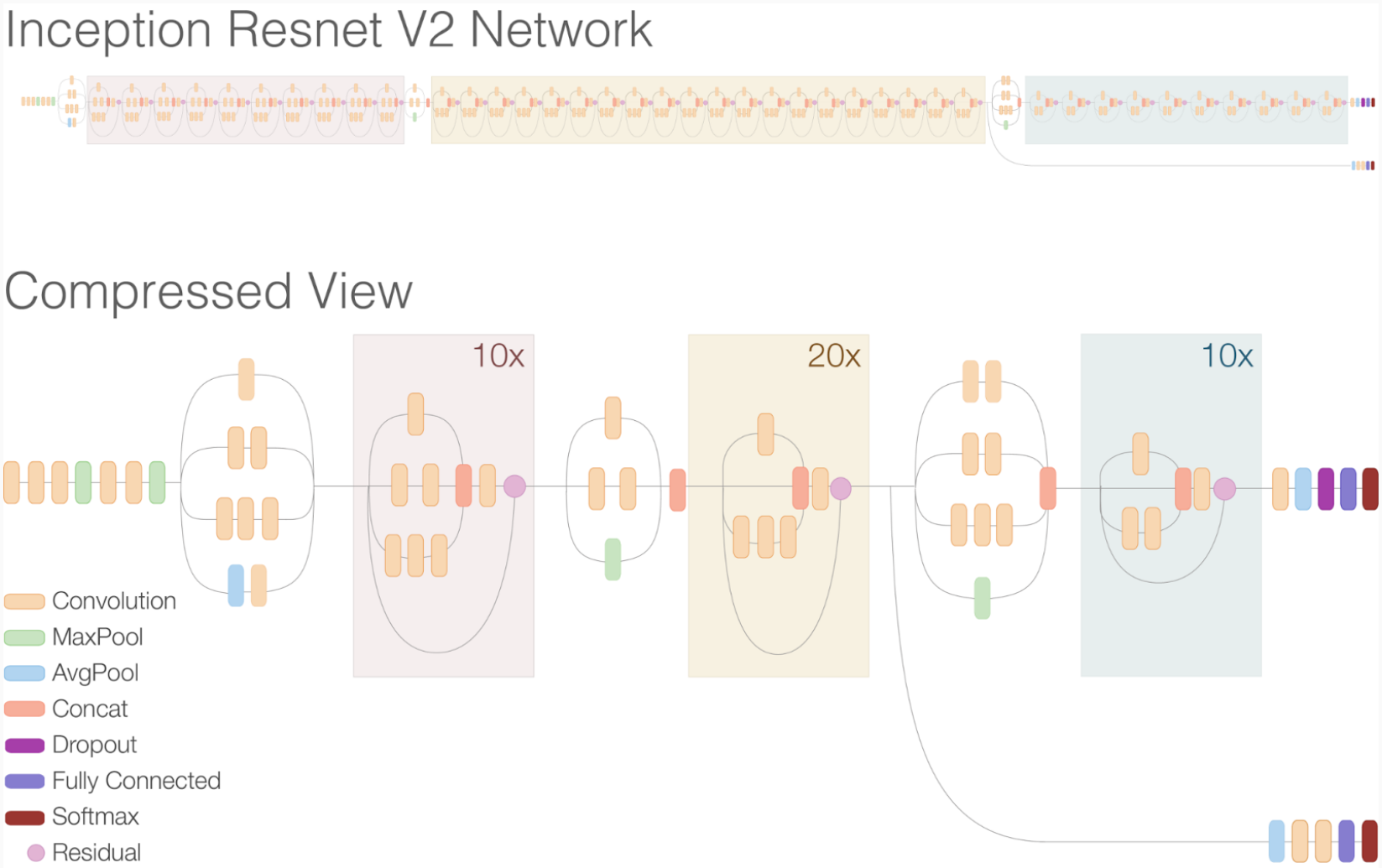
Symbolic differentiation

An implementation issue

- How do we calculate the gradient norms required for our Symbolic DataGrad and SpectReg regularizations?

Symbolic differentiation

Modern neural networks are big and complex beasts:



(Szegedy et al 2016)

Symbolic differentiation

- ...but at the end of the day they are still just formulae (or more precisely, straight line programs).
- They are built up from a small class of operations such as matrix-vector multiplication, vector addition, and elementwise maximum of vectors.
- Modern tensor software libraries such as Tensorflow and PyTorch are designed to manipulate such formulae symbolically. We can build the formula for $\frac{\partial}{\partial x} f(x)$ with a single operation:

```
tf.gradients(f, [x])
```

Symbolic differentiation

```
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)
```

Experimental Results

MNIST – training on 2000 randomly chosen samples, interaction with weight decay

Weight decay	NoGR	SpectReg	DataGrad
LeNet			
no WD	97.15	97.55 ($\lambda = 0.03$)	**97.93** ($\lambda = 20$)
WD=0.0005	97.32	97.67 ($\lambda = 0.05$)	**97.93** ($\lambda = 50$)

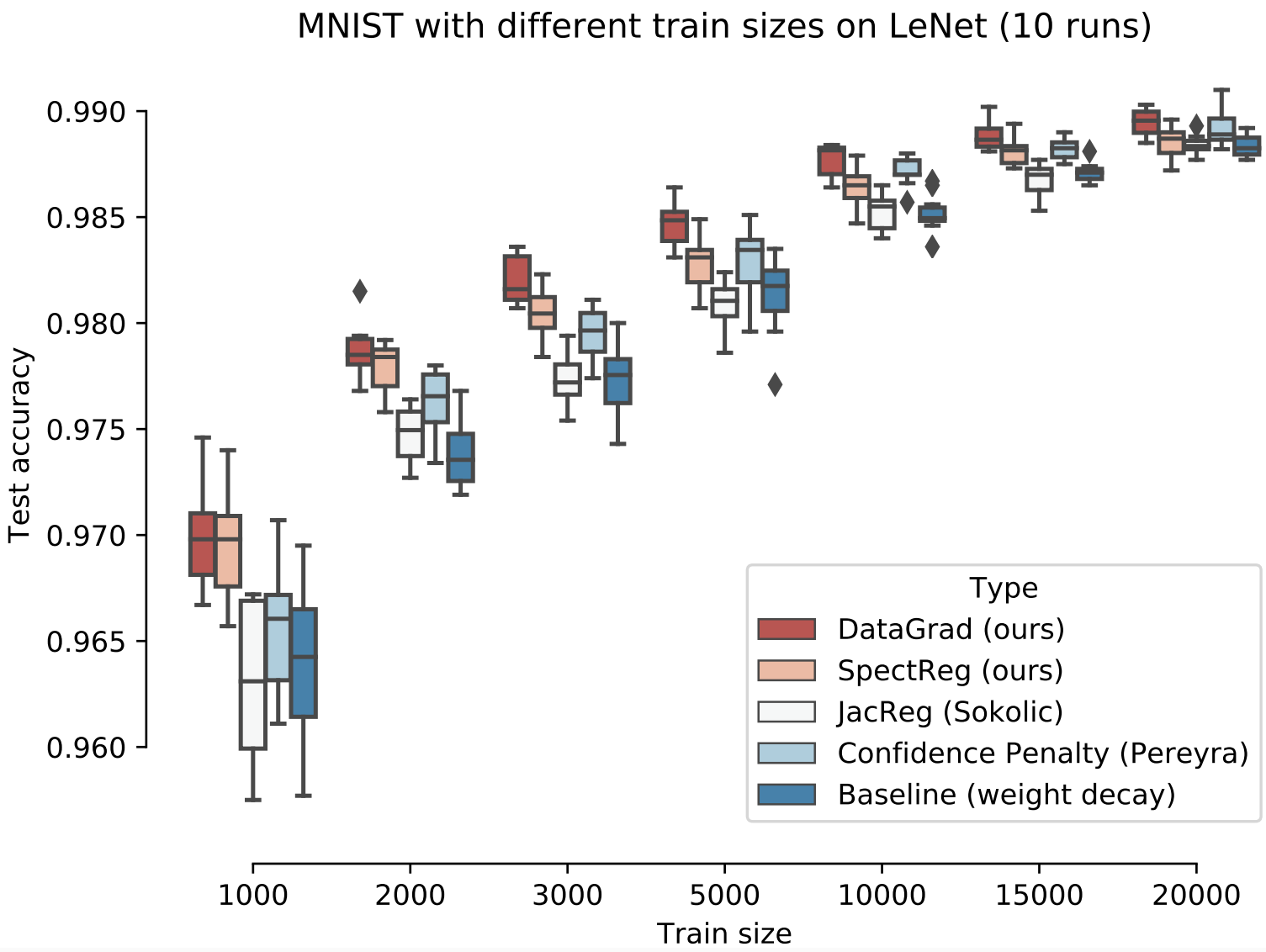
Dropout is on in all of these runs, dropout rate 0.5.

Gradient regularization's interaction with DO and BN

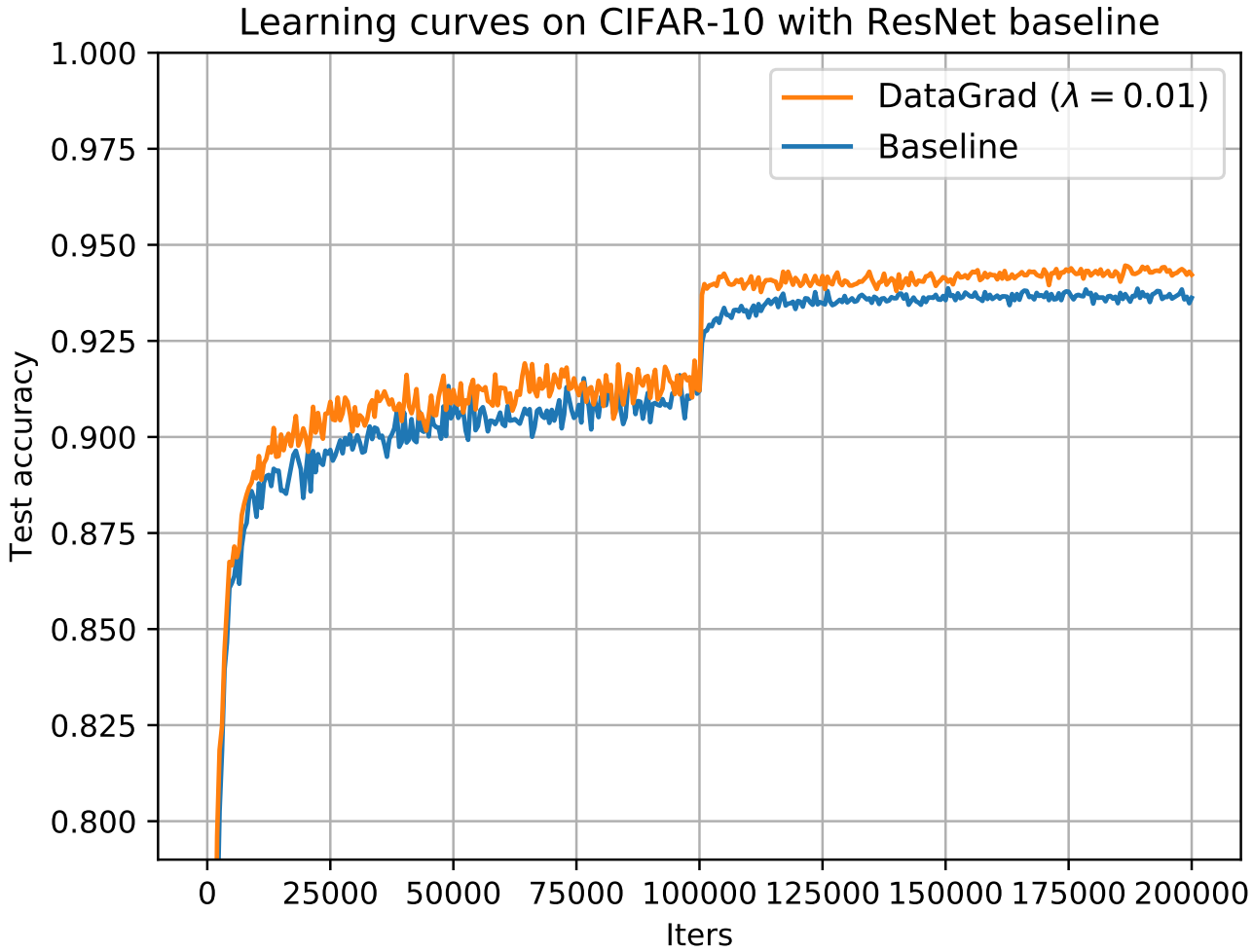
	NoGR	SpectReg	DataGrad
LeNet unreg	96.99	*97.59*	97.56
Lenet BatchNorm	96.89	*96.94*	96.89
Lenet Dropout	97.29	97.67	**97.93**

Comparison of dropout, batch normalization and two variants of gradient regularization: symbolic DataGrad and SpectReg. Train size was set to 2000. Each hyperparameter was tuned individually on a development set.

Comparison of various regularization methods on MNIST



DataGrad learning curve on full CIFAR-10



Improvements even on full CIFAR-10 with data augmentation.

Generative models

Gradient regularization in generative models

Unfortunately I do not have the time to talk about gradient regularization in generative models, but aren't these artificial bedrooms nice?

Summary

Summary

- We propose the symbolic *DataGrad* and *SpectReg* regularization methods,
- present them in a more general framework of Jacobian-based regularizers,
- and experimentally demonstrate that they very consistently improve test accuracy on variations of standard low-resolution image recognition benchmarks,
- especially when the size of the training set is small.