An empirical look at the loss landscape: shape, dynamics, and loose ends

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Loose Ends

Components of training an image classifier

For fixed architecture of ResNet 56 we have:

1. Preprocessing: normalize, shift and flip (show examples)
2. Momentum
3. Weight decay (aka L^2 regularization)
4. Learning rate scheduling

Components of training an image classifier

With all the ingredients (mom, wd, prep) we get 93.1% accuracy on C10!

- Remove momentum only: -1.5%
- Remove weight decay only: -3.2%
- Remove preprocessing only: -6.3%
- Remove all three: -12.5%

Expressivity and overfitting

- Regression vs. classification
- Memorizing the training set and 9 examples in CIFAR100
- Overfitting in loss vs. accuracy
- Cow on beach example (DLP)

Introduction to training

The Loss Function

1. Take a dataset and split it into two parts: $\mathcal{D}_{train}$ & $\mathcal{D}_{test}$
2. Form the loss using only $\mathcal{D}_{train}$:

$$\mathcal{L}_{train}(w) = \frac{1}{|\mathcal{D}_{train}|} \sum_{(x,y)\in\mathcal{D}_{train}} \ell(w;(x,y))$$

3. Find: $w^* = \arg\min \mathcal{L}_{train}(w)$
4. *...and hope that it will work on* $\mathcal{D}_{test}$.

The Loss Function

Some quantites:

- M : number of parameters $w \in \mathbb{R}^M$
- N : number of examples in the *training* set $|\mathcal{D}_{train}|$
- d : number of dimension in the input $x \in \mathbb{R}^d$
- k : number of classes in the dataset

Question: When do we call a model over-parametrized?

Question: How to minimize the high-dimensional, non-convex loss?

GD is bad use SGD

"Stochastic gradient learning in neural networks", Léon Bottou, 1991

- The total gradient (3) converges to a *local minimum* of the cost function. The algorithm then cannot escape this local minimum, which is sometimes a poor solution of the problem.

  In practical situations, the gradient algorithm may get stuck in an area where the cost is extremely ill conditionned, like a deep ravine of the cost function. This situation actually is a local minimum in a subspace defined by the largest eigenvalues of the Hessian matrix of the cost.

  The stochastic gradient algorithm (4) usually is able to escape from such bothersome situations, thanks to its random behavior (Bourrely, 1989).

GD is bad use SGD

Bourelly (1988)

5 CONCLUSION

It has been shown that the difficulty in parallel learning is due to the fact that the parallel algorithm does not really use the stochastic algorithm. Two solutions are presently proposed to prevent the system from falling into a local minimum.

1) Add momentum to the algorithm such that it can "roll past" a local minimum. Thus the algorithm then becomes:

$$W_{t+1} = (1-\alpha)\, W_t - \varepsilon\, \alpha\, f(W_t, X_t)$$

where f is the error gradient Q relative to W

2) One can add a random "noise" to the gradient calculations. One method of performing this task is to calculate the gradients in an approximate manner. This variation could be modelled as a type of 'Brownian motion', using a temperature function (similar to simulated annealing). This temperature could be lowered relative to the remaining system error. For example, the variation in gradients could follow a Gaussian distribution. Thus, for example:

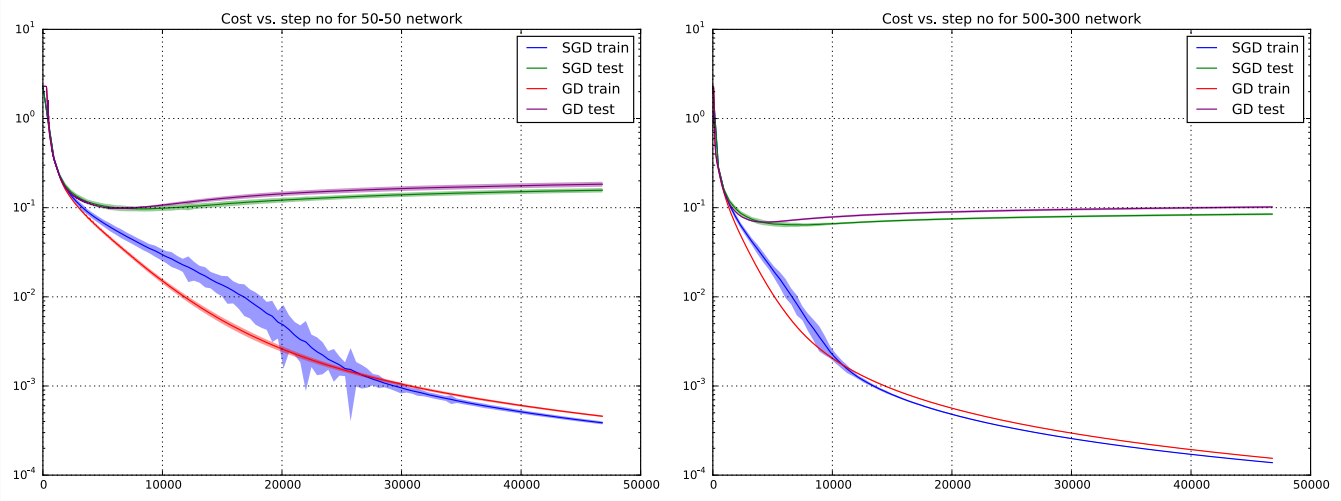
$$W_{t+1} = W_t - \varepsilon\, N\left(f(W_t, X_t),\ k\sqrt{Temp} \right)$$

where f is the error gradient Q relative to W
and N is a function giving a Gaussian random variable.

Both of these approaches are presently under research.

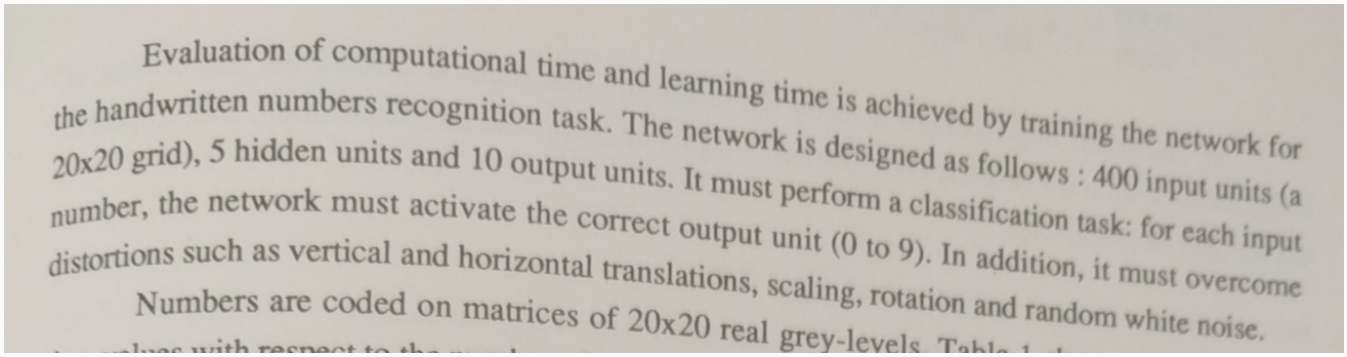
GD is bad use SGD

Simple fully-connected network on MNIST (S.-Guney-LeCun, 2014):
$M \sim 43$K (left) and $M \sim 450$K (right)



GD is bad use SGD

The network has only 5 neurons in the hidden layer!

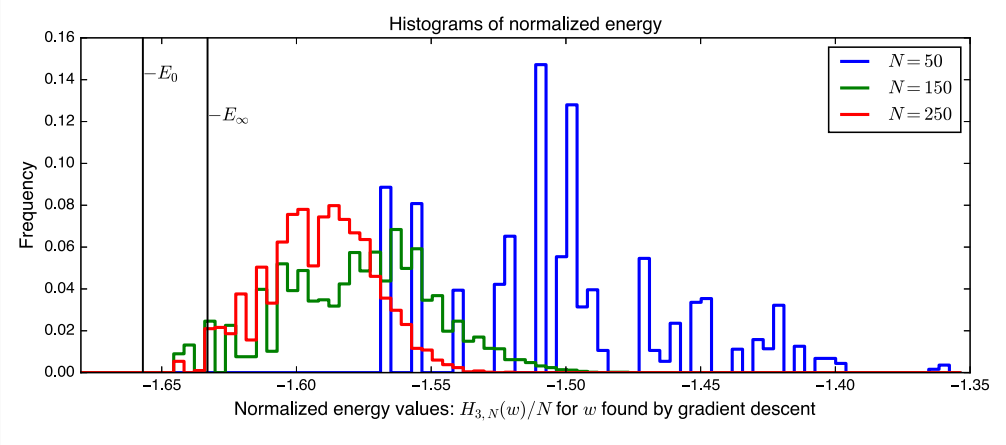


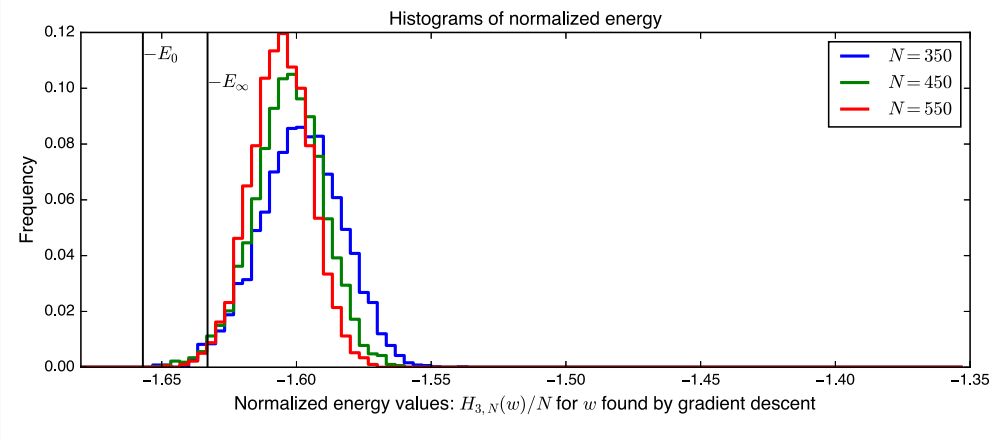
Evaluation of computational time and learning time is achieved by training the network for the handwritten numbers recognition task. The network is designed as follows : 400 input units (a 20x20 grid), 5 hidden units and 10 output units. It must perform a classification task: for each input number, the network must activate the correct output unit (0 to 9). In addition, it must overcome distortions such as vertical and horizontal translations, scaling, rotation and random white noise.

Numbers are coded on matrices of 20x20 real grey-levels. Table 1

Why dimensionality matters?

GD on the 3-spin model (S., Guney, Ben Arous, LeCun - 2014)





More counter-examples

Training is easy when M is large (S.-Bottou 2016, Zhang et. al. 2016)

- Corrupt data
- Scramble labels
- More complex data
- Random polynomials

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How about generalization?

SGD is really special

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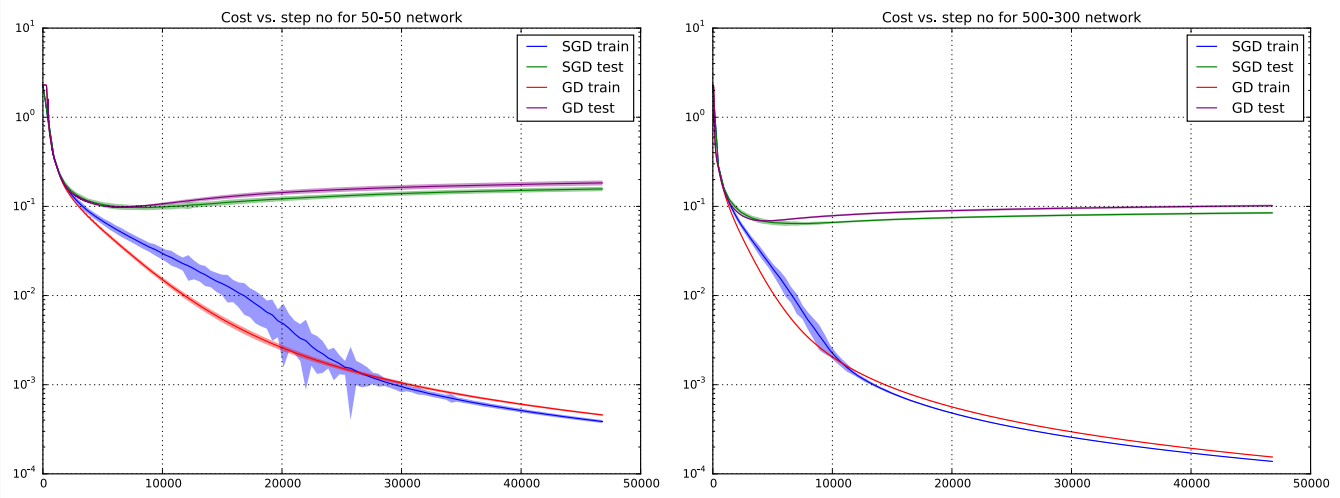
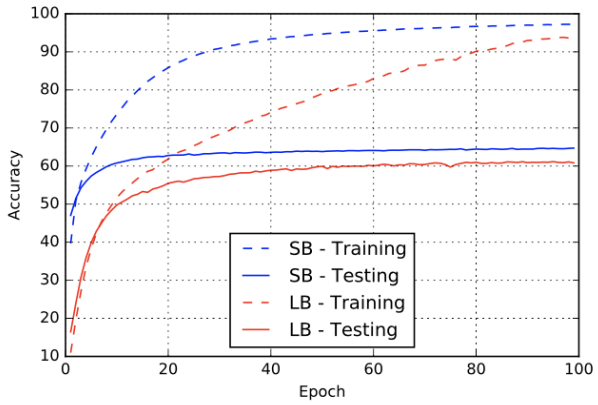


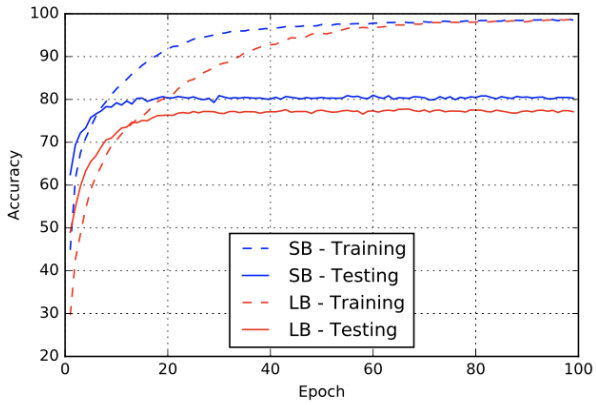
Average number of misclassifications:
small-SGD: 256, small-GD: 299, large-SGD: 174, large-GD: 194

SGD is really special

Where common wisdom may be true (Keskar et. al. 2016.):



(a) F_2



(b) C_1

Figure 2: Convergence trajectories of training and testing accuracy for SB and LB methods

F2: fully connected, TIMIT ($M = 1.2$M)

C1: conv-net, CIFAR10 ($M = 1.7$M)

- Similar training error, but gap in the test error.

SGD is really special

Moreover, Keskar et. al. (2016) observe that:

- LB $\rightarrow$ sharp minima
- SB $\rightarrow$ wide minima

Considerations around the idea of sharp/wide minima:

$$\tilde{H}_{\Lambda,f}(R) \equiv f^{-1}\Big\{\int S_\Lambda(R-R')f[H(R')]dR'\Big\} \tag{2}$$

where R is a multidimensional vector representing all the coordinates in the molecule.

One of the simplest and most useful forms for S_Λ is a Gaussian

$$\begin{aligned} S_\Lambda(R) &\equiv C(\Lambda)e^{-R\Lambda^{-2}R} \\ C(\Lambda) &\equiv \pi^{-d/2}Det^{-1}(\Lambda) \end{aligned} \tag{3}$$

where d is the total dimensionality of R. The function f included in (2) allows for non-linear averaging. Two choices motivated by physical considerations are $f(x) = x$ and $f(x) = e^{-x/k_BT}$. These choices correspond respectively to the "diffusion equation" and "effective energy" methods which are described below. Wu [77] has presented a general discussion of transformations of the form of (2).

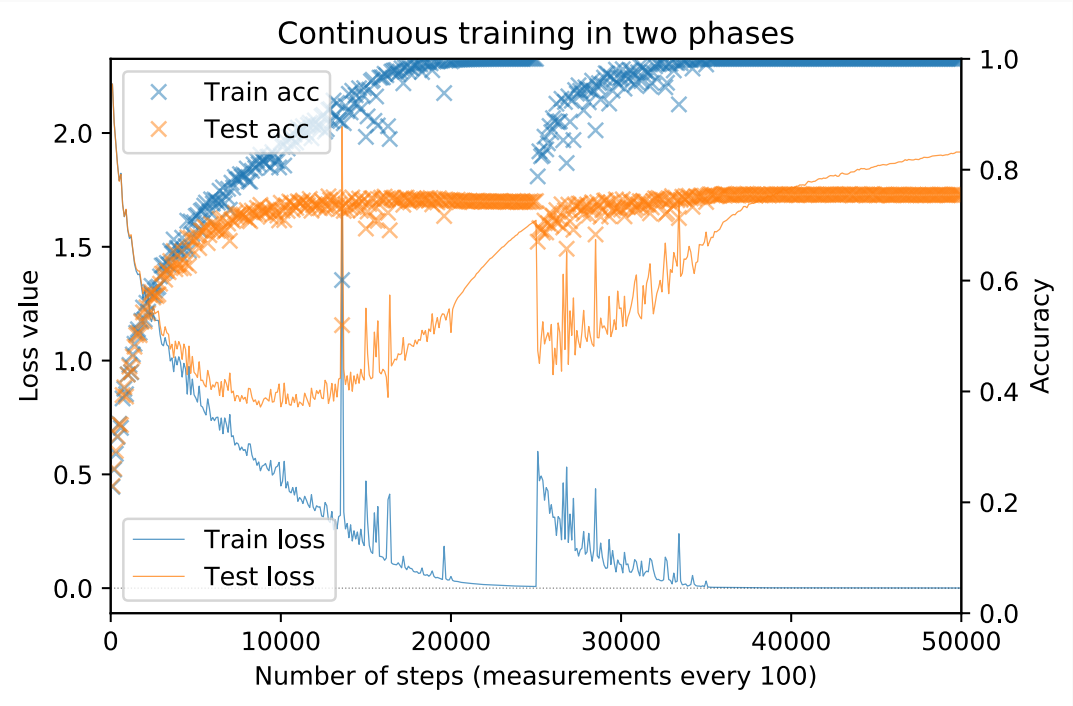
A highly smoothed $\tilde{H}_{\Lambda,f}$ (from which all high spatial-frequency components have been removed) will in most cases have fewer local minima than the unsmoothed ("bare") function, so it will be much easier to identify its global minimum. If the strong spatial-scaling hypothesis is correct, the position of this minimum can then be iteratively tracked by local-minimization as Λ decreases. As $\Lambda \rightarrow 0$, the position will approach the global minimizer of the bare objective function.

Pardalos et. al. 1993 (*More recently:* Zecchina et. al., Bengio et. al., ...)

Searching for sharp basins

Repeating the LB/SB with a twist (S. et. al. 2017).

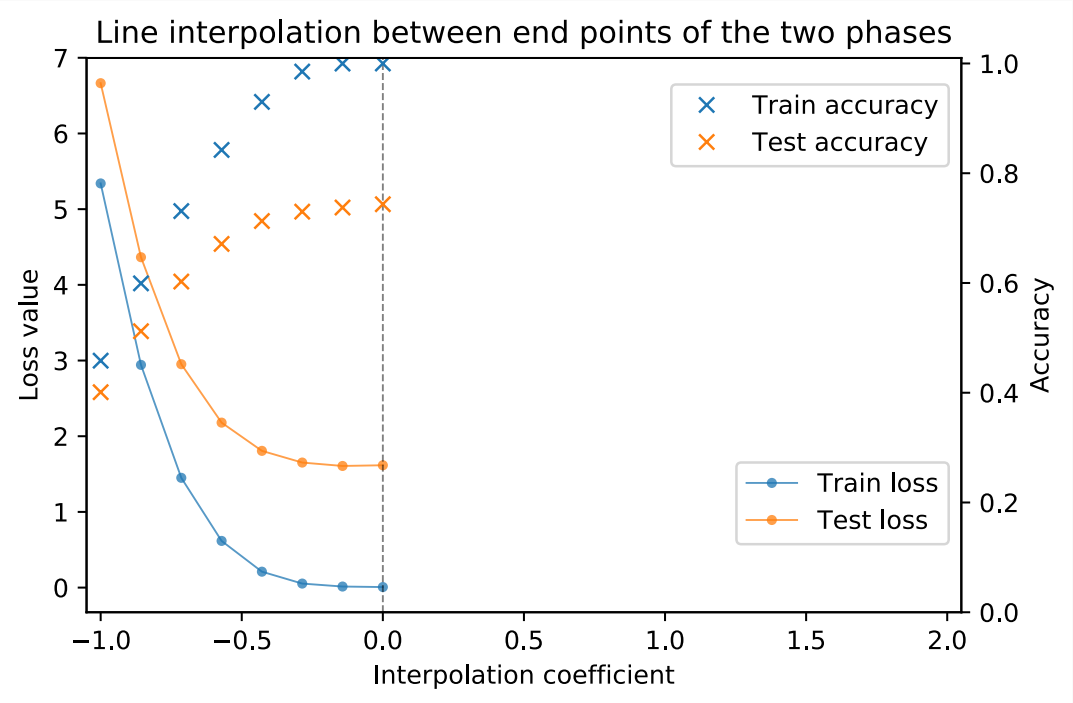
1. Train a large batch CIFAR10 on a *bare* AlexNet
2. At the end point switch to small batch



Searching for sharp basins

Keep the two points: end of LB training and end of SB continuation.

1. Extend a line away from the LB solution



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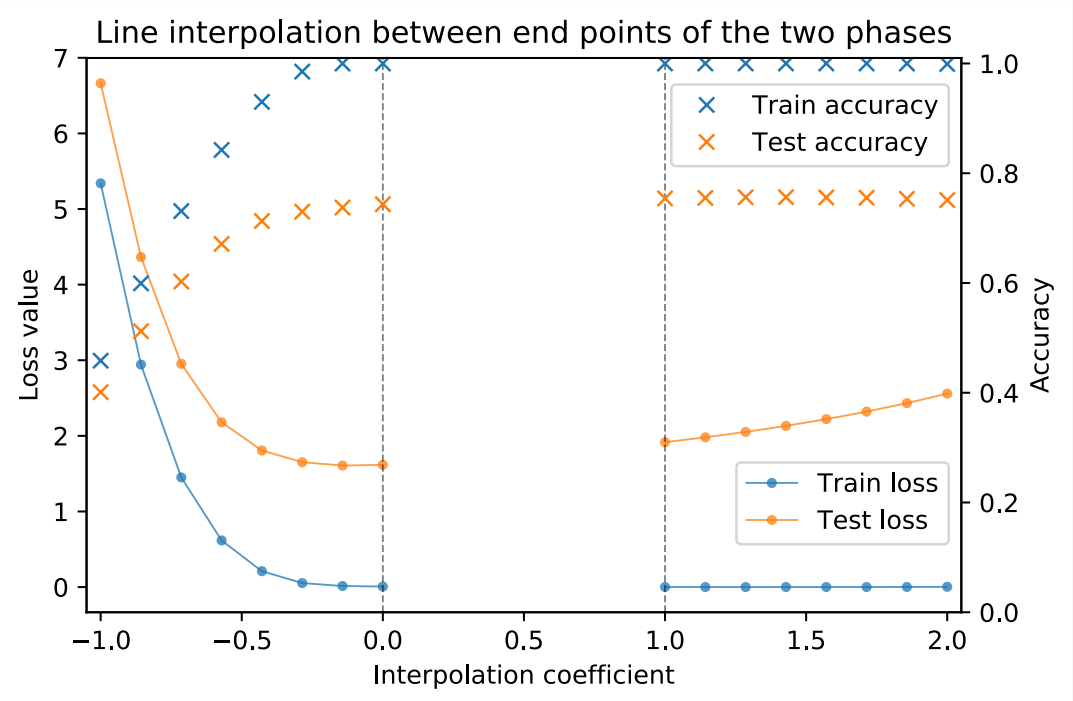

Searching for sharp basins

Keep the two points: end of LB training and end of SB continuation.

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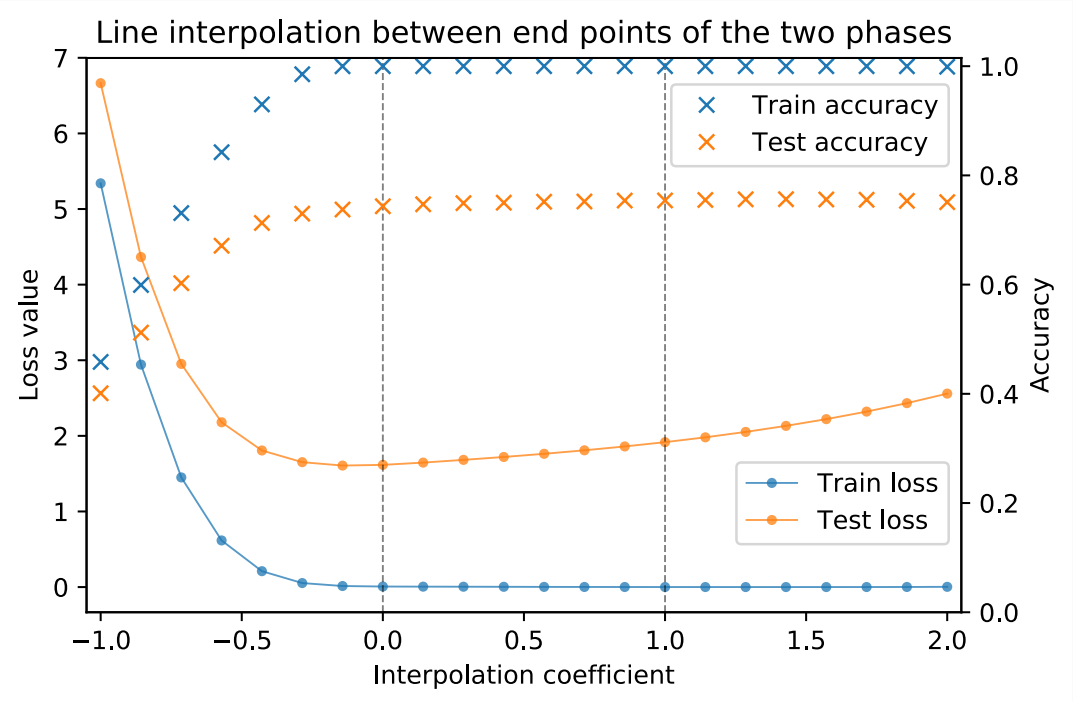
2. Extend a line away from the SB solution
3. Extend a line away between the two solutions



Geometry of redundant over-parametrization

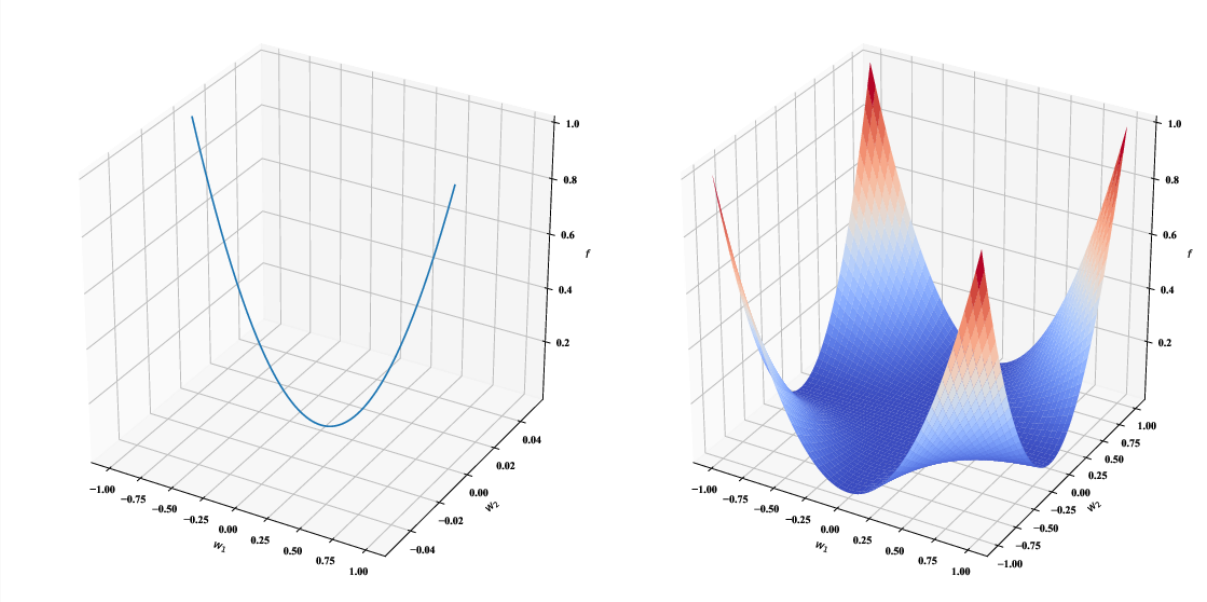
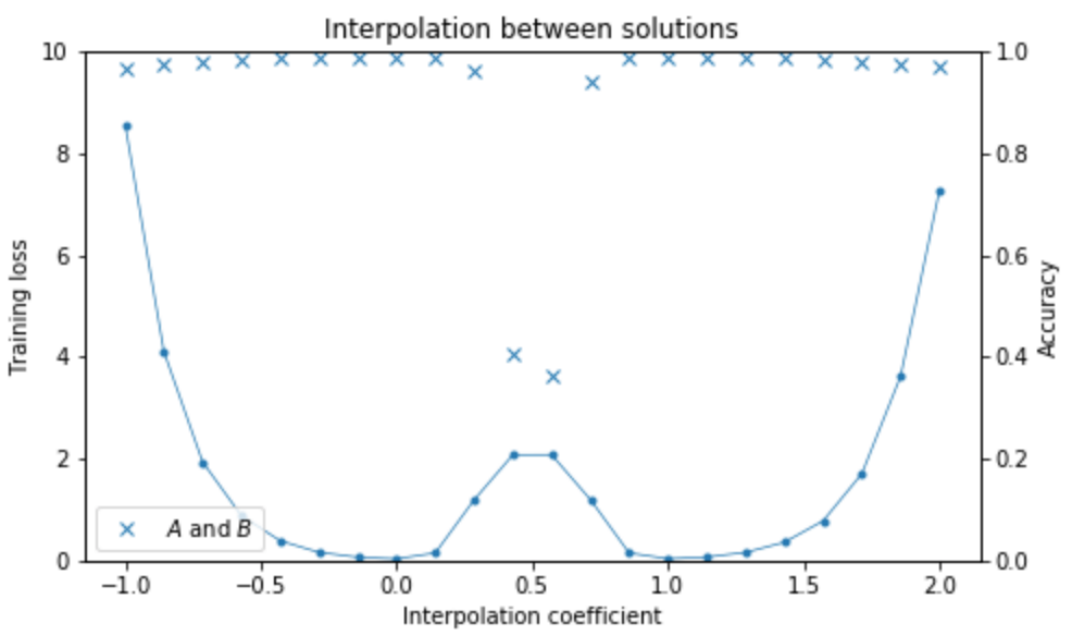


Figure: w^2 (left) vs. $(w_1 w_2)^2$ (right)

Connecting arbitrary solutions

1. Take two networks at arbitrary initial points
2. Train them to get two different solutions A and B
3. Flip the nodes of B to make it similar to A (network is unchanged)
4. Evaluate a straight between the solutions and look at angles



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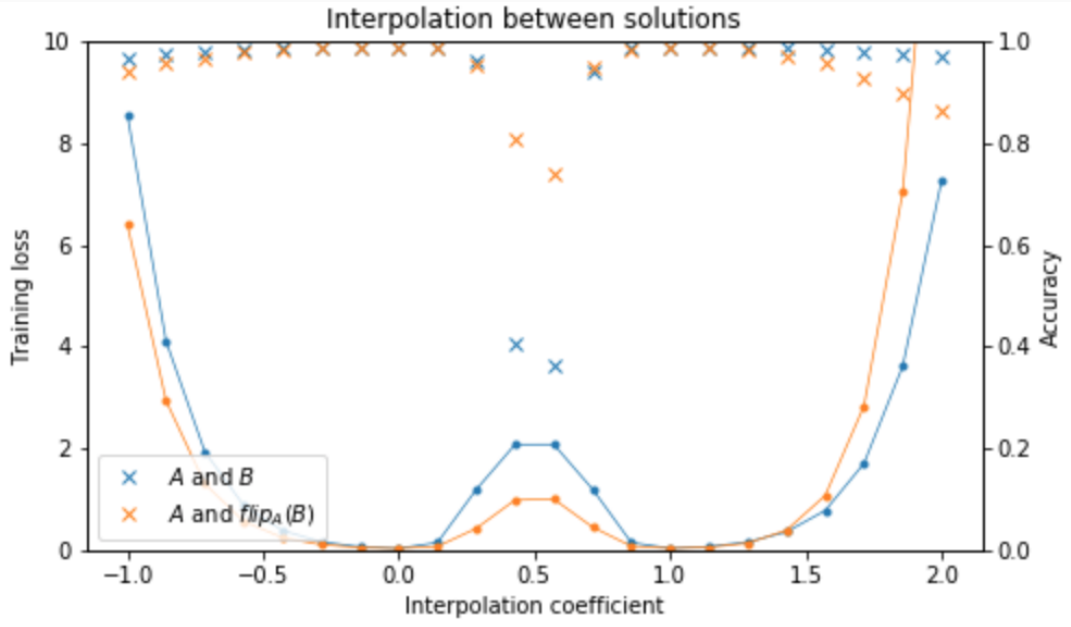
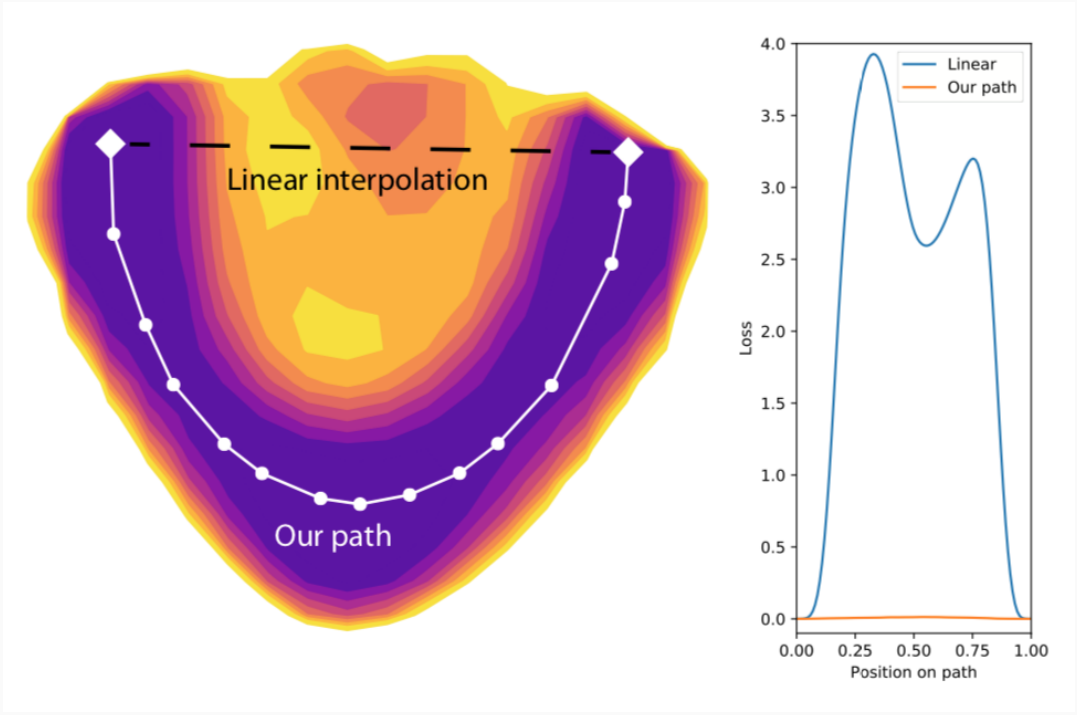


Connecting arbitrary solutions

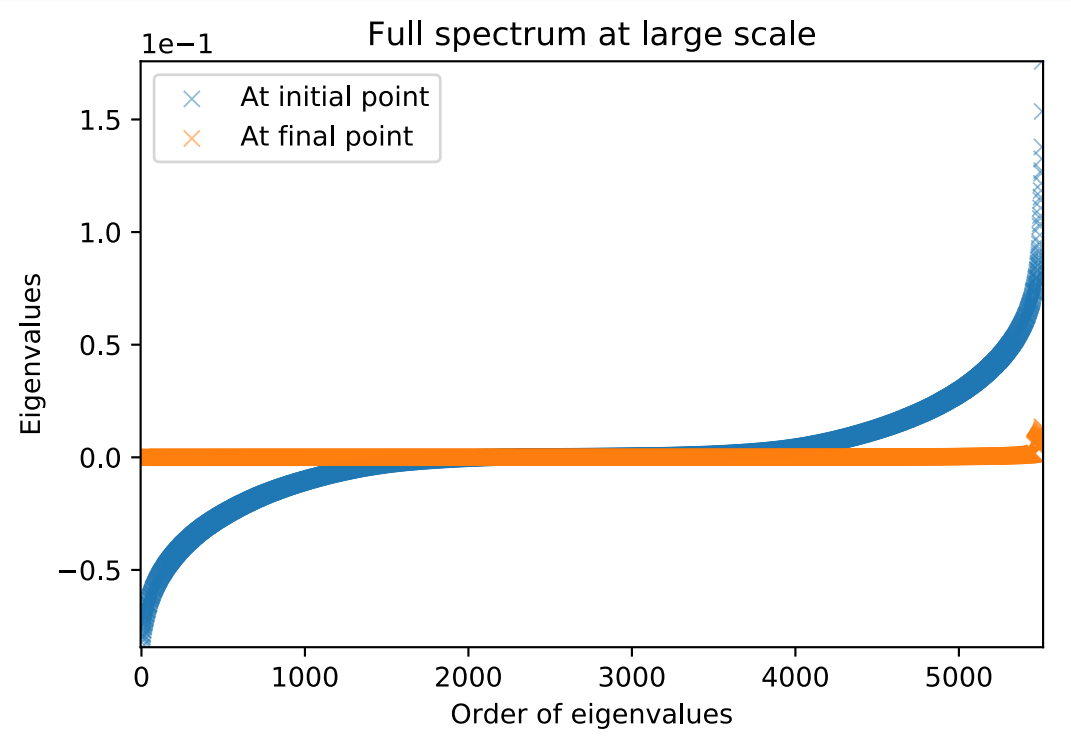
1. Freeman and Bruna 2017: barriers of order $1/M$
2. Draxler et. al. 2018: no barriers between solutions



Local shape of the loss

Hessian of the loss: An example

2-hidden layer ReLU net, 50 categories of Gaussian blobs in 100 dimensions, SGD with constant step size



All zero, with some outliers...

Gauss-Newton decomposition of the Hessian

Loss functions between the output, s, and label, y

- MSE $\ell(s, y) = (s - y)^2$
- Hinge $\ell(s, y) = \max\{0, sy\}$
- NLL $\ell(s_y, y) = -s_y + \log \sum_{y'} \exp s_{y'}$

are all convex in their output: $s = f(w; x)$

Gauss-Newton decomposition of the Hessian

With $\ell \circ f$ in mind, the gradient and the Hessian per loss:

$$\nabla \ell(f(w)) = \ell'(f(w)) \nabla f(w)$$
$$\nabla^2 \ell(f(w)) = \ell''(f(w)) \nabla f(w) \nabla f(w)^T + \ell'(f(w)) \nabla^2 f(w)$$

then average over the training data:

$$\nabla^2 \mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^{N} \ell''(f(w)) \nabla f(w) \nabla f(w)^T + \frac{1}{N} \sum_{i=1}^{N} \ell'(f(w)) \nabla^2 f(w)$$

First term of the decomposition

Take the first term:

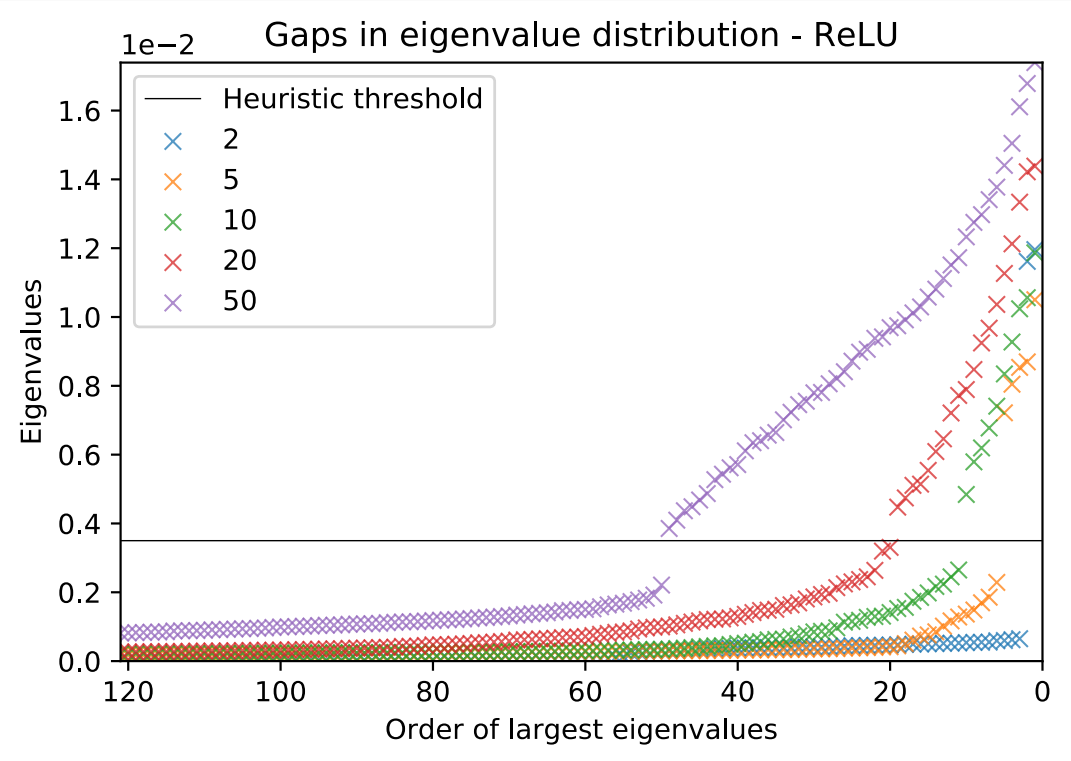
$$\nabla^2 \mathcal{L}(w) \approx \underbrace{\frac{1}{N} \sum_{i=1}^{N} \ell''(f(w)) \nabla f(w) \nabla f(w)^T}_{X(w)X(w)^T}$$

where $X(w)$ is an $M \times N$ matrix with $min\{M, N\}$ non-trivial eigenvalues.

- Suppose the data has k clusters each with small variance
- Redundancy in N examples (even when N is too large)
- Would $X(w)X(w)^T$ have order k non-trivial eigenvalues?

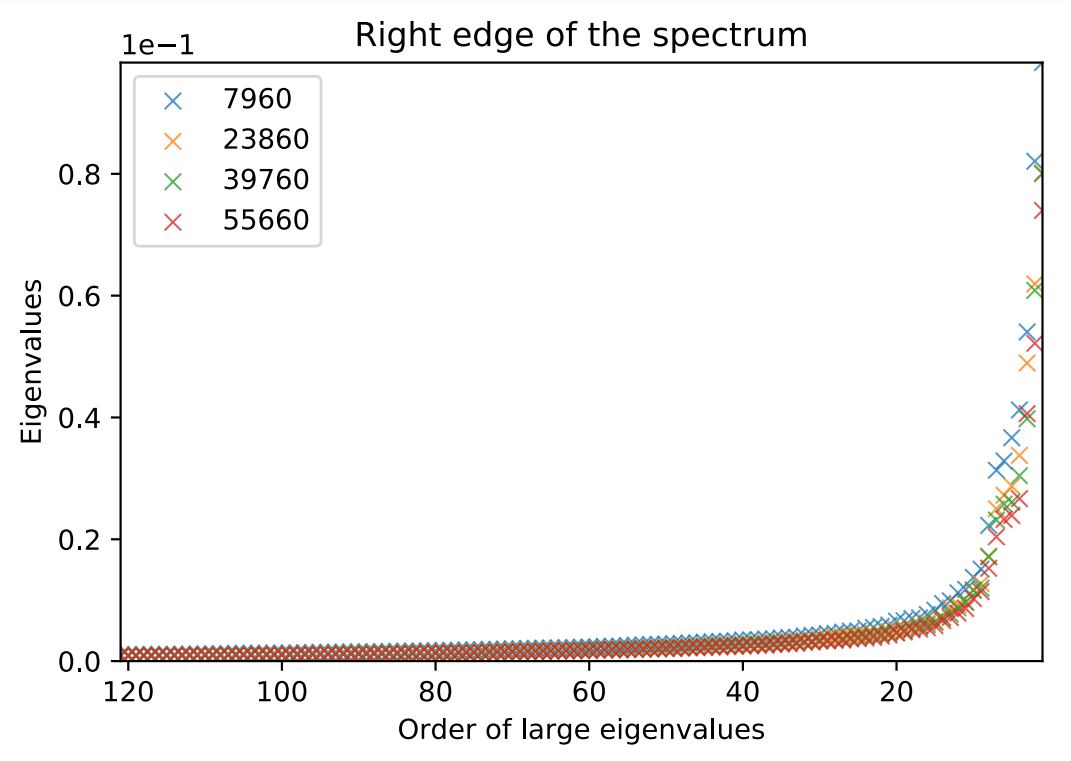
Closer look: (1) data and outliers

Random data of k-blobs for fixed ReLU architecture, fixed learning rate, and batch-size. Changing k gives rise to roughly k large eigenvalues:



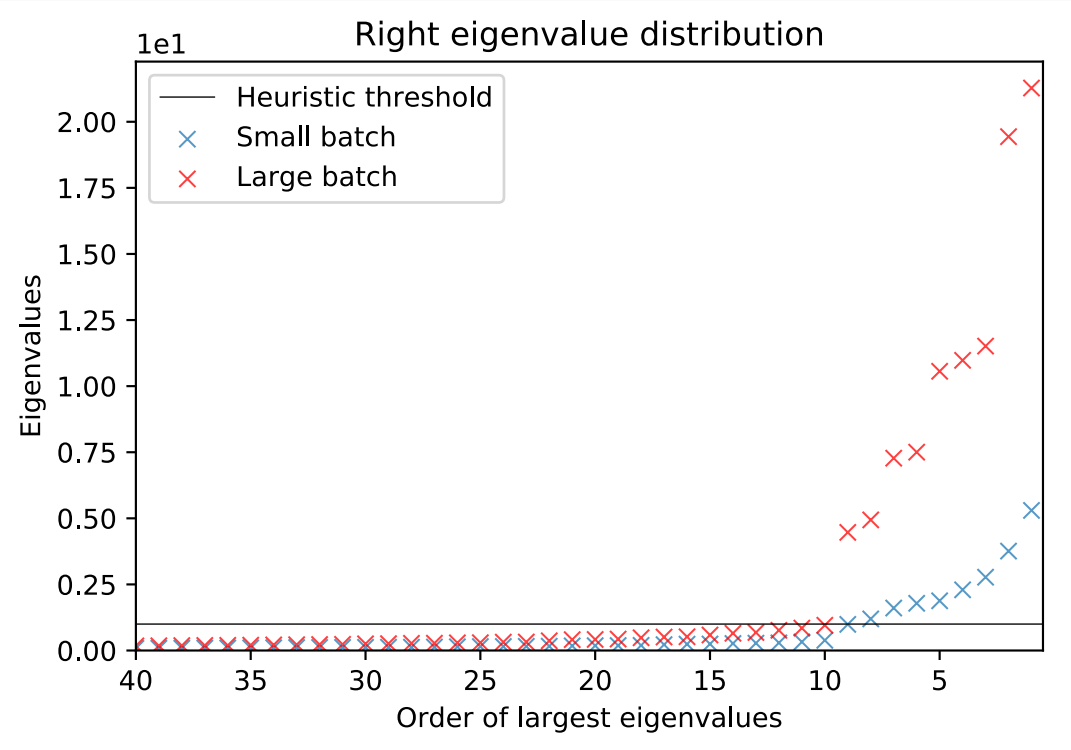
Closer look: (2) number of parameters and outliers

MNIST on a simple fully-connected network. Increasing the size of the network doesn't change the outliers.



Closer look: (3) algorithm and outliers

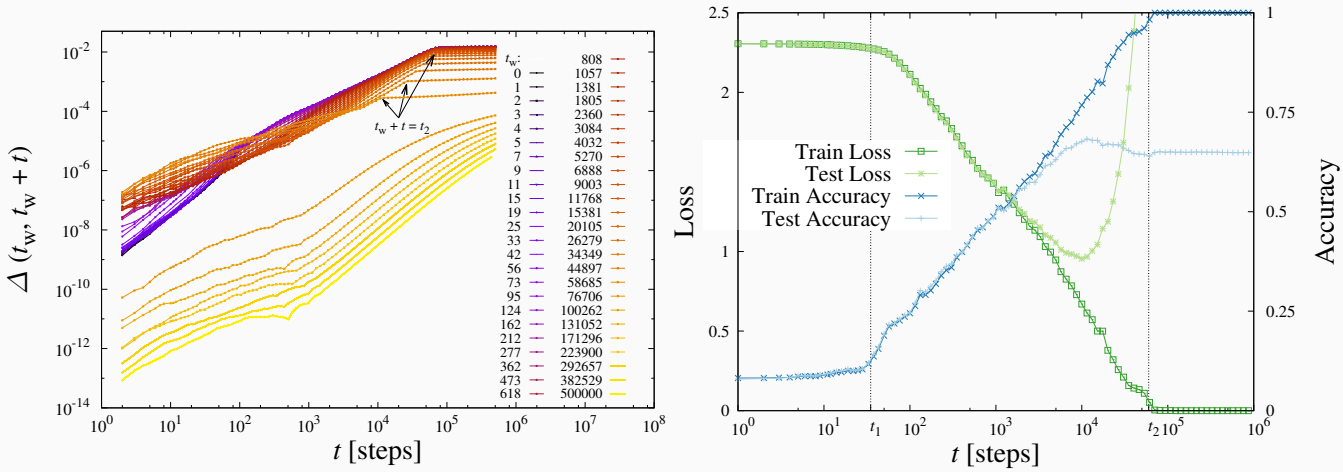
MNIST on a simple fully-connected network. Increasing the batch-size leads to larger outlier eigenvalues.



SGD dynamics

Loss and weights during the dynamic process

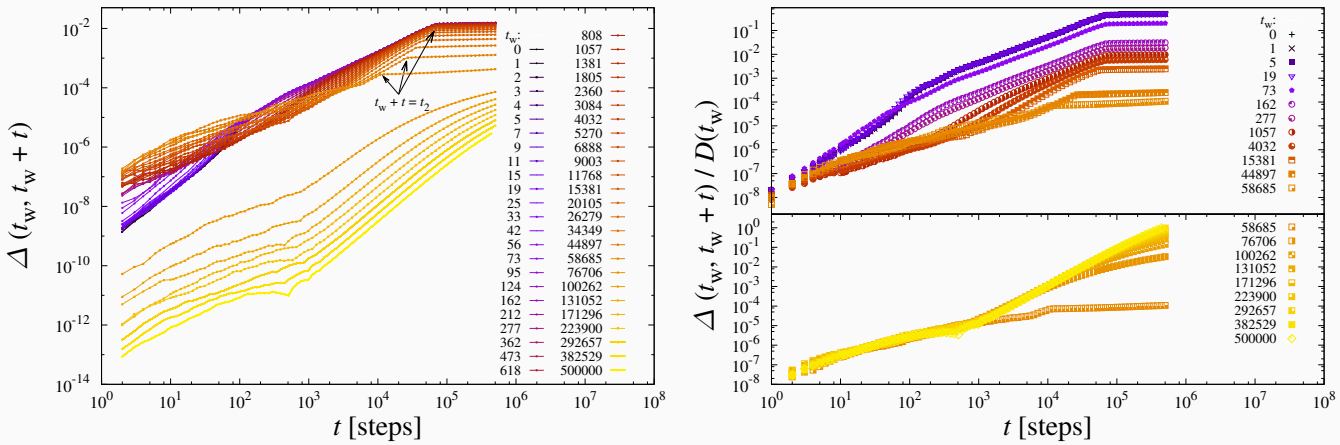
A small convolutional network trained on CIFAR-10



where $\Delta(t_w, t_w + t) = \frac{1}{M} \sum_i (w_i(t_w) - w_i(t_w + t))^2$

Collapse in the diffusive phase

Same MSD profile as above (left), scaled with the diffusion coeff (right)

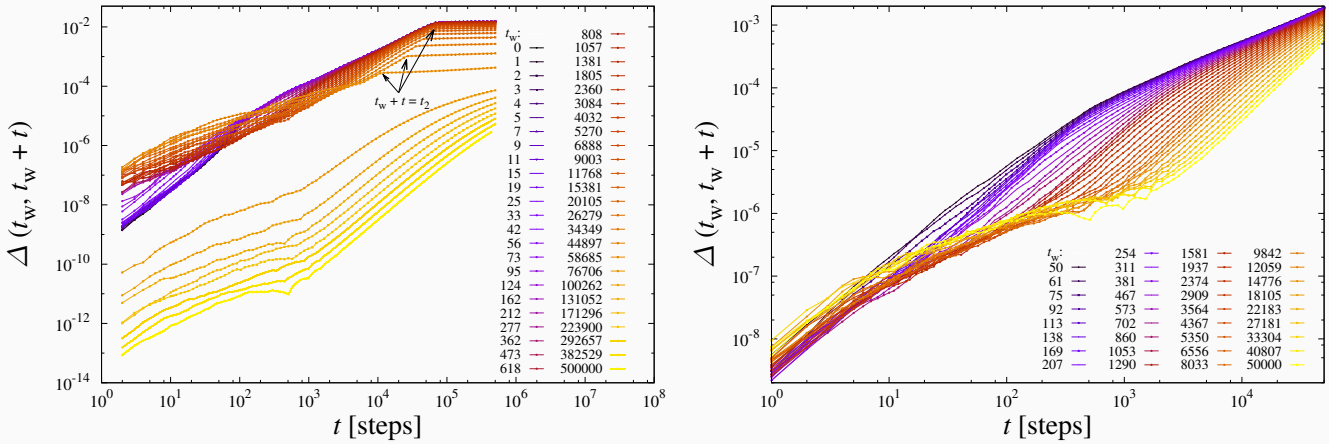


where the diffusion constant is given by $\frac{1}{N} \sum_i ||grad_i - \langle grad \rangle||^2$

Phase transition from under- to over-parametrized

Similar loss and MSD profiles can be found for: a toy model inspired by Freeman & Bruna, Fully Connected model, Larger ConvNet, ResNet.

However, this breaks down in smaller networks! (Wyart's talk)



Same model (left), small model (right)

Concluding remarks

- Loss landscape appears to be quite flat
- Connected topology of the solution space
- SGD may not be special for the reasons we thought it was
- No apparent reason for glassy landscape

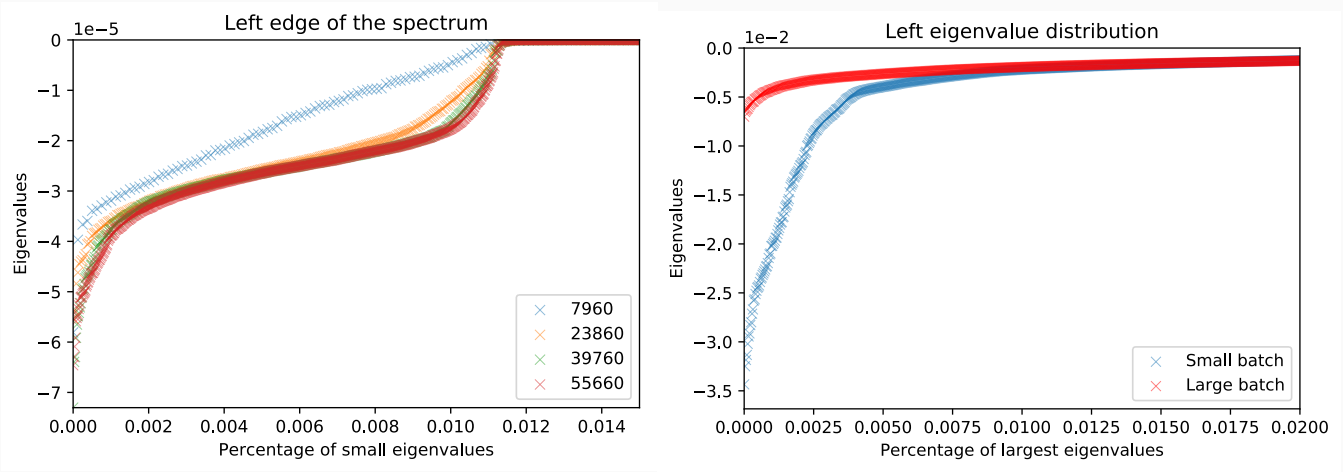
Future directions

- Understand the nature of the phase transition
- The link between loss, architecture and the algorithm
- Data dependent measure of architecture complexity
- And architecture dependent data complexity

Thank you!

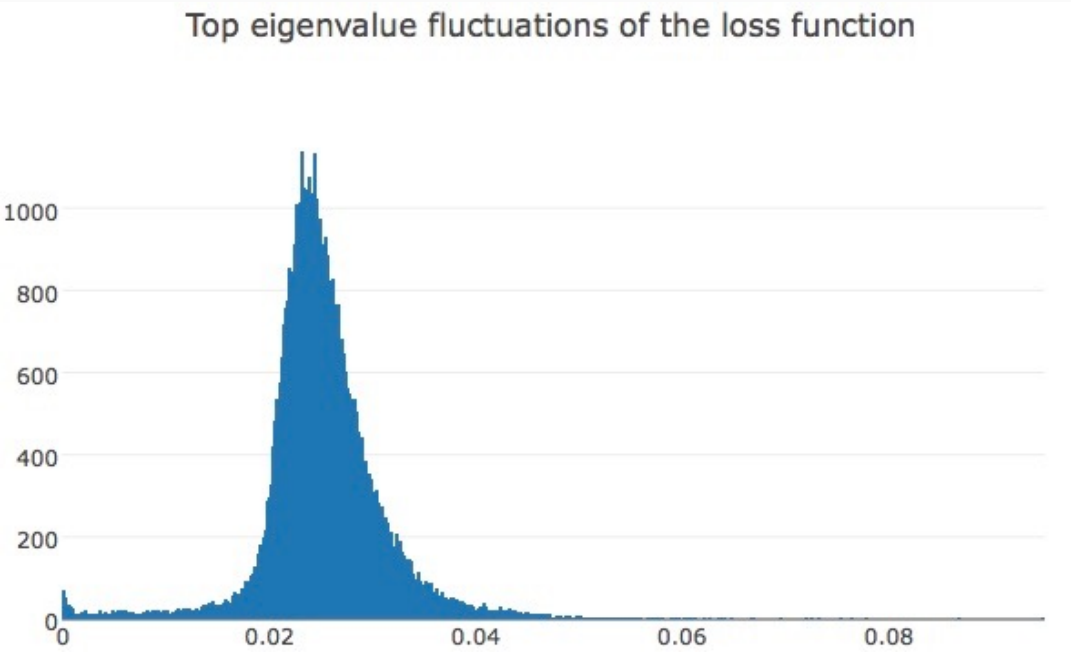
Further look at the negative eigenvalues

Negative eigenvalues in increasing the size of the hidden layer (left) and changing the algorithm (right): x-axis is the *ratio* among all



Further observations

For fixed M, train a system for a given number of iterations, and calculate the top eigenvalue at the end (50K times).



Remark: Kurt Johansson "From Gumbel to Tracy-Widom" (2005)