Loss Surfaces & Mode Connectivity if DNN's

A short report on

Garipov et al.'18, arxiv 1802.10026,

Gotmare et al.'18, ICML (nothing new relatively to

Garipov)

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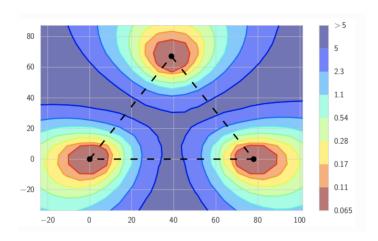
Skoltech

Moscow, 2018



Observation on Loss Surface

The cross-entropy loss $+ L_2$ reg surface of a deep residual network (ResNet-164) on CIFAR-100, as a function of network weights in a two-dimensional subspace.



Could we find path between nets with near constant low loss?

Problem formulation

Consider:

- ightharpoonup L(w) := DNN loss with fixed architecture and weigths w
- $lackbox{} \hat{\textit{w}}_1, \ \hat{\textit{w}}_2 \in \mathbb{R}^{|\mathsf{net}|}$
- $lacksquare \phi_{ heta}(t): [0;1]
 ightarrow \mathbb{R}^{|\mathsf{net}|}$
- $\phi_{\theta}(0) = \hat{w}_1; \ \phi_{\theta}(1) = \hat{w}_2$

What we really want to solve, as I suppose:

$$\min_{ heta} \max_{t} \mathit{L}(\phi_{ heta}(t))$$

Trivial Solution

Consider CNN with ReLU activations, $\hat{w}_1,~\hat{w}_2 \in \mathbb{R}^{|\mathsf{net}|}$, two nets.

- ► Connect both \hat{w}_i with 0 with constant loss, so have path with constant loss every where, expect 0
- $ightharpoonup o_i = W_i \text{ReLU}(o_{i-1}) + b_i, i = n \text{ correspond to logits}$
- ▶ Parametrization on *t*:
 - $ightharpoonup W_i(t) = W_i t$
 - $b_i(t) = b_i t^i$
- ▶ Then logist $o_n(t) = t^n o_n$ for $t \in (0, 1]$ prediction labels not change

Authors solve problem under another criteria, however, they are still find this trivial path. Now I formulate their optimization criteria and add some intuition about it.



Relaxed problem

Minimize average loss along curve:

$$egin{aligned} \min_{ heta} & rac{1}{\int d\phi} \int L(\phi) d\phi = \left[\int\limits_0^1 \|\phi_{ heta}'(t)\| dt
ight]^{-1} \int\limits_0^1 L(\phi_{ heta}(t)) \|\phi_{ heta}(t)'\| dt \Leftrightarrow \ & \Leftrightarrow \min_{ heta} \mathbb{E}_{t \sim U[\phi_{ heta}]} L(\phi_{ heta}(t)), \end{aligned}$$

where $U[\phi_{\theta}]:=$ uniform distribution on curve

However, we have some problems with normalization such distribution and hence taking gradients with respect to $\boldsymbol{\theta}$



More Relaxed problem

So, authors relax more:

$$\min_{ heta} \mathbb{E}_{t \sim U[0;1]} L(\phi_{ heta}(t))$$

Note, that they are quite different problems! But now we have very easy gradient estimation procedure:

$$\nabla_{\theta} \mathbb{E}_{t \sim U[0;1]} L(\phi_{\theta}(t)) = \nabla_{\theta} L(\phi_{\theta}(\hat{t})), \ \hat{t} \sim U[0;1]$$

Parametrization on $\phi, \ t \in [0; 1]$:

► Linear chain

$$\begin{cases} 2(t\theta + (0.5 - t)\hat{w}_1) & t \in [0; 0.5] \\ 2((t - 0.5)\hat{w}_2 + (1 - t)\theta) & t \in [0.5; 1] \end{cases}$$

Bezier Curve

$$\phi_{\theta}(t) = (1-t)^2 \hat{w}_1 + 2t(1-t)\theta + t^2 \hat{w}_1$$

Experiments only for two nets, but can be generalized



Some intuition on problem formulation

We have trivial upper bound:

$$\min_{w} L(w) \leq \mathbb{E}_{w \sim p(w|\theta)} L(w), \ \forall w, \theta$$

Now we can make it thinner:

$$\min_{w} L(w) \leq \min_{\theta} \mathbb{E}_{w \sim p(w|\theta)} L(w)$$

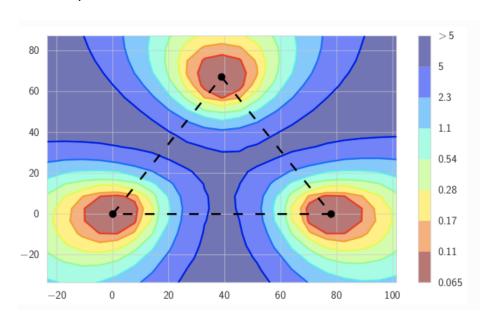
It's common trick in bayesian/variational optimization. Now we just reparametrize our distribution $p(w|\theta)$ with $t \sim U[0;1]$; $\phi(t)$

Note, that even as we don't averaging uniformly along curve it's upper ubond, that we minimizing.

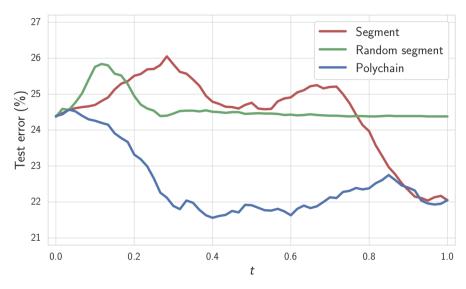


Experiments: Path

ResNet-164, CIFAR 10, plane of curve



 $\mathsf{Green} := \mathsf{step} \ \mathsf{on} \ \mathsf{random} \ \mathsf{angle}, \ \mathsf{blue} := \mathsf{our} \ \mathsf{ensambling}, \ \mathsf{red} := \mathsf{straight} \ \mathsf{line}$



VGG16 model architecture, CIFAR 10

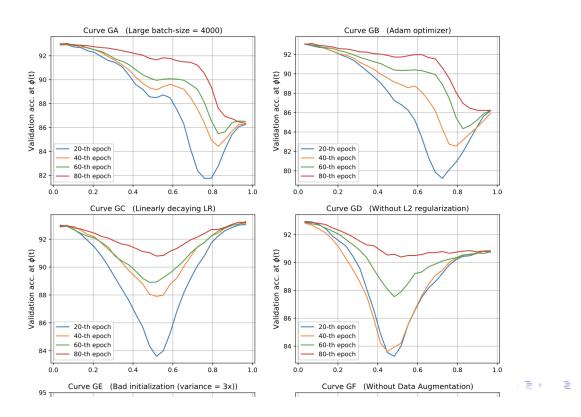
Strategies to make different nets:

Base net, G 200 epochs with SGD. The learning rate is ini- tialized to 0.05 and scaled down by a factor of 5 at epochs 60, 120, 160 (step decay). We use a training batch size of 100, momentum of 0.9, and a weight decay of 0.0005.

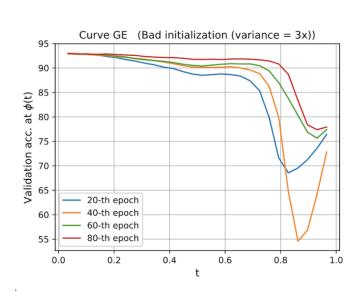
- ► A using a training batch size of 4000
- ▶ B by using the Adam optimizer instead of SGD
- ► C with a linearly decaying LR scheme
- ▶ D using a smaller weight decay, no l2 reg.
- ▶ E by increasing the variance of initialization distribution
- ▶ F using no data augmentation

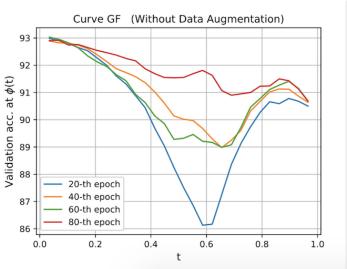
And ensamble with different t, G and any other one





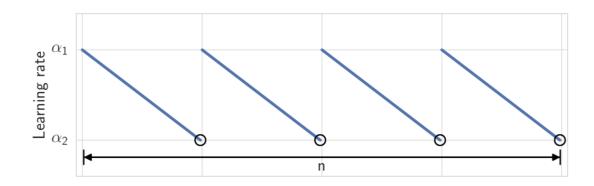
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Experiments: Online Ensemble learning

It's fine, but we should learn 2 nets instead of one. We can use cycling learning rate and ensemble online.



But it is not work much:)

Next time

Prediction of flat/sharp minimum convergence by largest eigenvalue of Hessian dynamic

