Mean-field theory and dynamical isometry of deep neural networks

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References list & slides can be find at

https://github.com/fwcore/mean-field-theory-deep-learning

Outlines

- > Introduction
- **➤** Mean-field theory framework and its predictions
 - ➤ Initialization strategies
 - > MLP
 - > CNN
 - ➤ Architectures
 - ResNet
 - > Dropout
 - batch normalization
- Details of the theory
 - ➤ Assumptions
 - ➤ Possible pitfalls

Introduction

Initialization

> He's & Xavier's

Activation functions

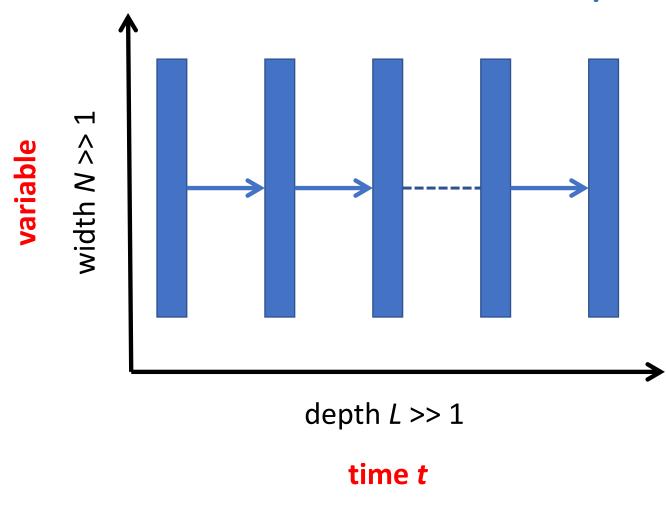
Dropout

BatchNorm

LSTM for RNN

To enhance the information propagation

Is there a theory for deep learning?



deep uniform neural networks

dynamical system

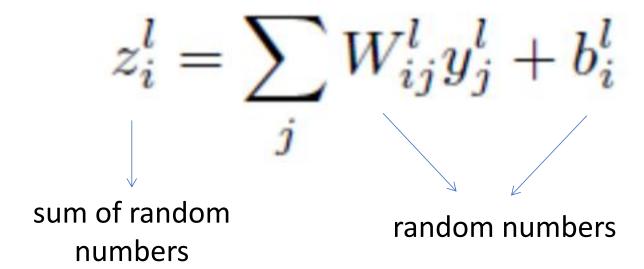
 $z_i^l = \sum_j W_{ij}^l y_j^l + b_i^l$

$$y_i^{l+1} = \phi(z_i^l)$$

But ...

z, y are random variables and hard to track

Mean-field theory for deep learning



Mean-field treatment

- > Replace z as Gaussian
- > Match z's mean and variance

- \rightarrow mean(z) = 0
- Hence we only need to track var(z)

Law of large numbers

Mean-field flow of var(z)

$\mathbb{E}[z_{i;a}^l z_{j;a}^l] = q_{aa}^l \delta_{ij}$

$$q_{aa}^{l} = \sigma_w^2 \int \mathcal{D}z \phi^2 \left(\sqrt{q_{aa}^{l-1}} z \right) + \sigma_b^2$$

i, j: neural index

I: layer index

a, b: sample index

covariance

$$\mathbb{E}[z_{i;a}^l z_{j;b}^l] = q_{ab}^l \delta_{ij}$$

$$q_{ab}^l = \sigma_w^2 \int \mathcal{D}z_1 \mathcal{D}z_2 \phi(u_1) \phi(u_2) + \sigma_b^2$$

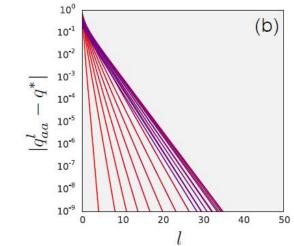
$$u_1 = \sqrt{q_{aa}^{l-1}} z_1$$

$$u_2 = \sqrt{q_{bb}^{l-1}} \left(c_{ab}^{l-1} z_1 + \sqrt{1 - (c_{ab}^{l-1})^2} z_2 \right)$$

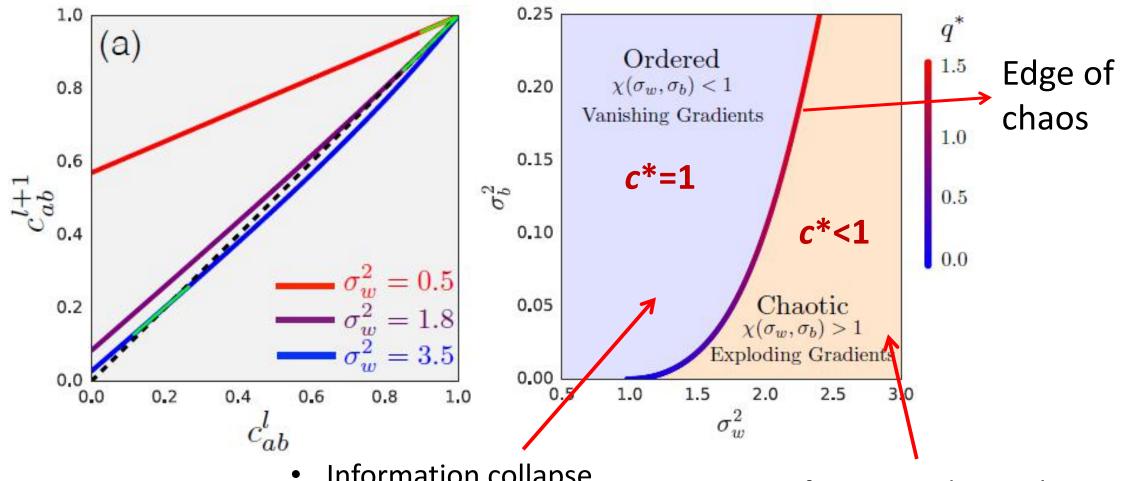
$$c_{ab}^l = q_{ab}^l / \sqrt{q_{aa}^l q_{bb}^l}$$

 $q^* = \lim_{l \to \infty} q_{aa}^l$ is a smooth function.

However, *limit c is differen*t



Mean-field flow of c: a phase transition

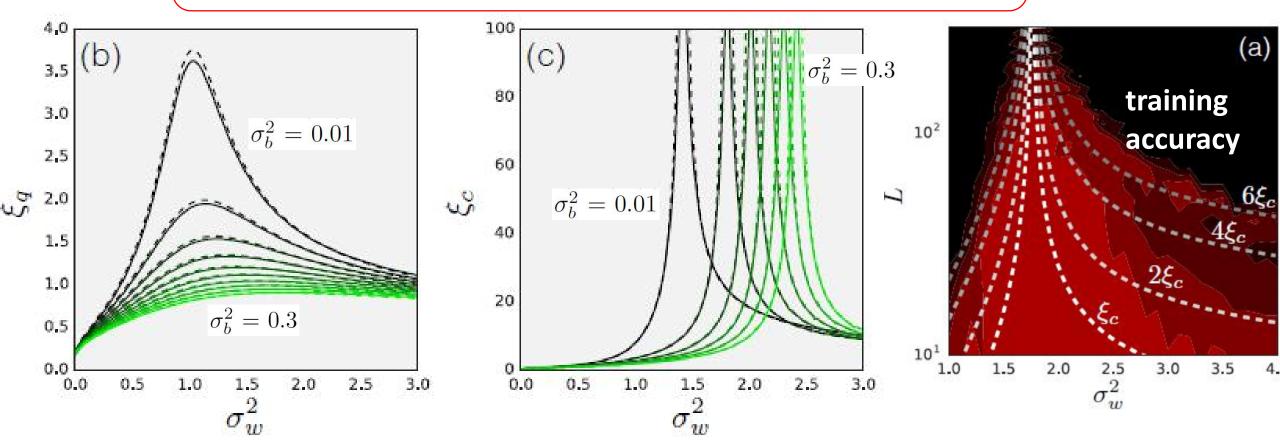


- Information collapse.
- Gradients vanish.

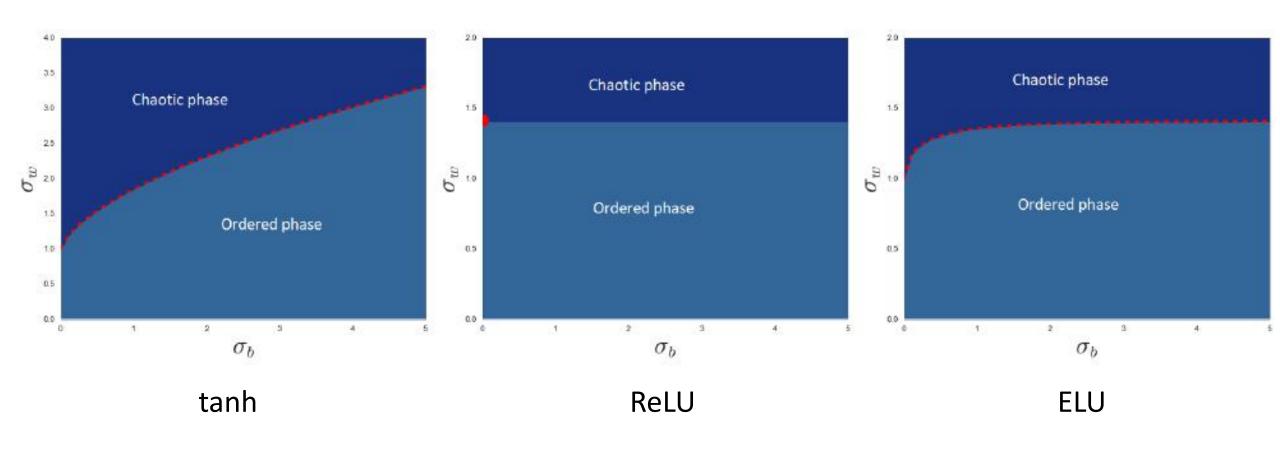
- Information decorrelates.
- Gradients explode.

Perturbation around c* = asymptotic behavior near the edge of chaos

$$\epsilon^{l+1} = \epsilon^l \left[\sigma_w^2 \int \mathcal{D} z_1 \mathcal{D} z_2 \phi'(u_1^*) \phi'(u_2^*) \right] + \mathcal{O}((\epsilon^l)^2) \sim e^{-l/\xi_c}$$



Activation functions



Gaussian initialization is enough?

 $\xi_{\rm c}$ controls information propagation depth, and determines training accuracy,

How about *training speed* & *generalization*?

Edge of chaos

guarantees slow changes of correlation

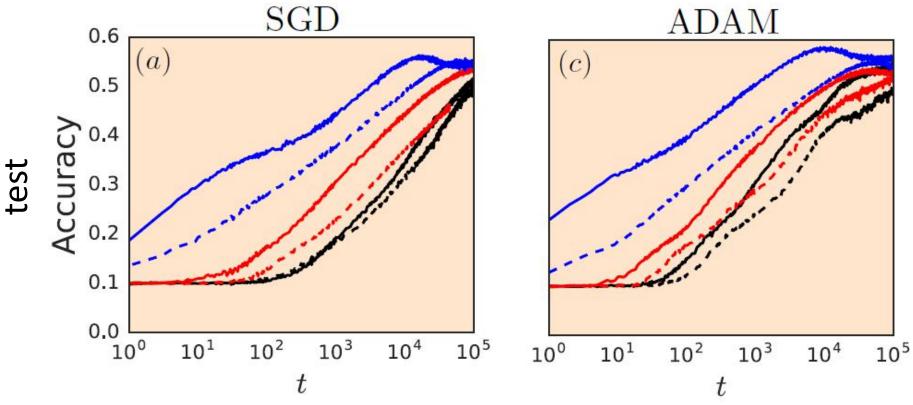
Dynamical isometry

guarantees correlation preservation

$$\mathbf{J} = \frac{\partial \mathbf{x}^L}{\partial \mathbf{h}^0} = \prod_{l=1}^L \mathbf{D}^l \mathbf{W}^l \qquad D_{ij}^l = \phi'(h_i^l) \, \delta_{ij}$$

All singular values have norm 1

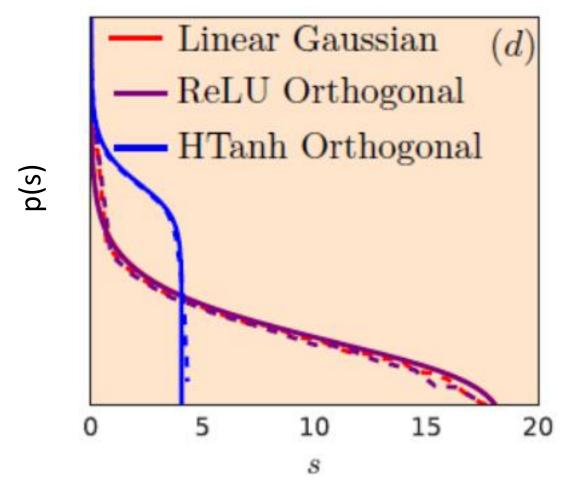
Dynamical isometry initialization speeds up training



dashed line: Gaussian solid line: orthogonal

tanh with $\sigma_w^2 = 1.05$ (close to EOC) tanh with $\sigma_w^2 = 2$ (far away from EOC) ReLU with $\sigma_w^2 = 2$ (at critical point)

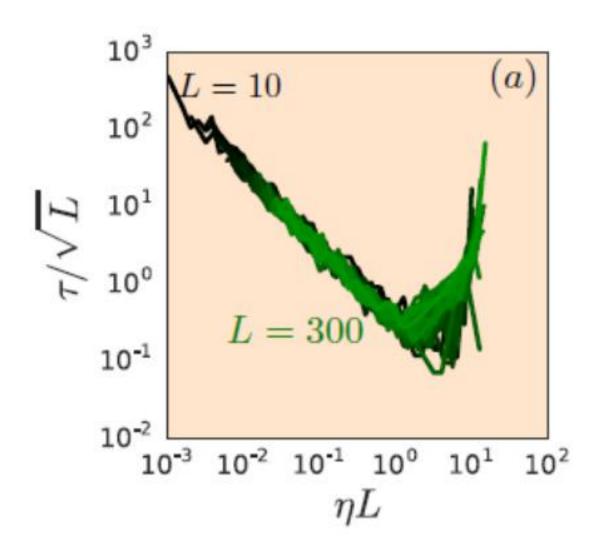
Activation functions



singular values of J

- > ReLU has no dynamical isometry
- > tanh is better to be initialized by Orthogonal scheme with a slightly small σ_b^2

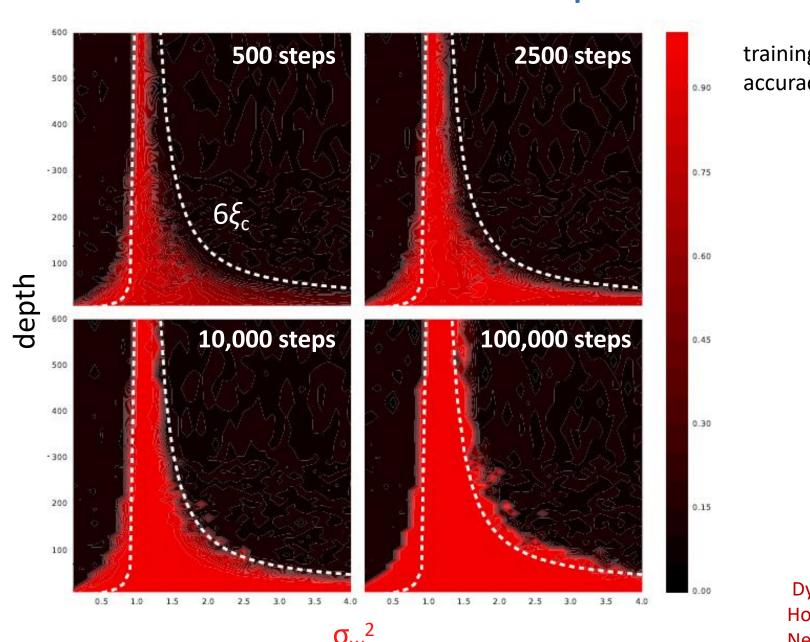
Scaling of training time



Under dynamical isometry

- > training time grows slower than L
- \triangleright optimal training rate $\eta \sim 1/L$

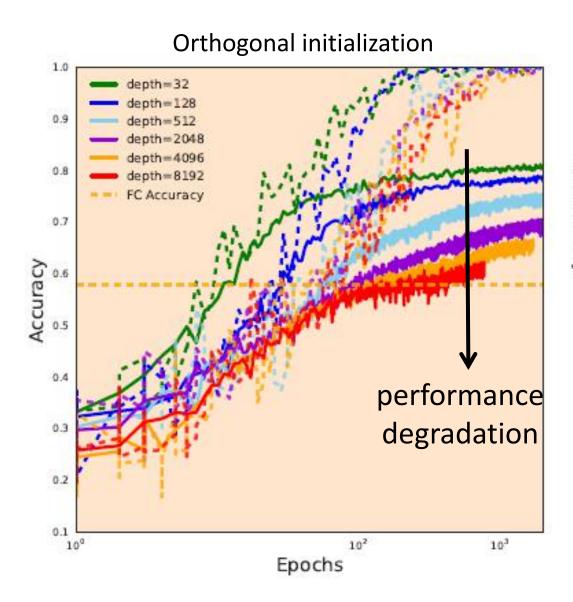
Deep ConvNet

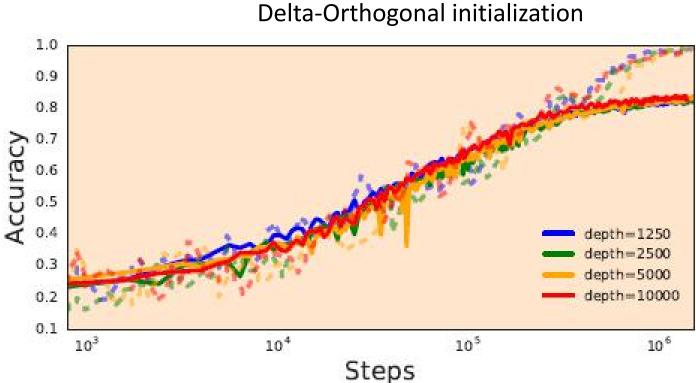


training accuracy

> Dynamical Isometry and a Mean Field Theory of CNNs: How to Train 10,000-Layer Vanilla Convolutional Neural Networks | arXiv:1806.05393

Dynamical isometry for deep ConvNet

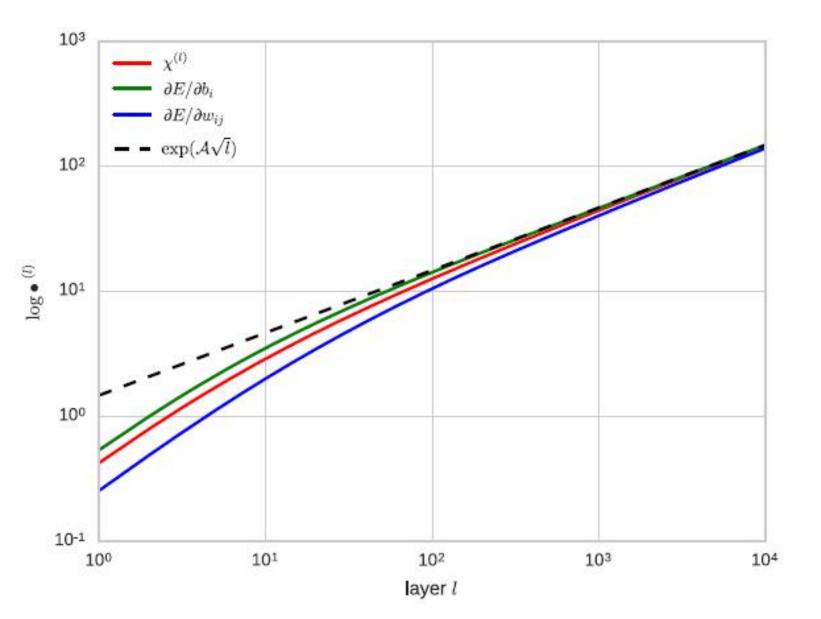




Dynamical isometry prevents performance degradation caused by increasing depth.

Reminder: ResNet is an alternative

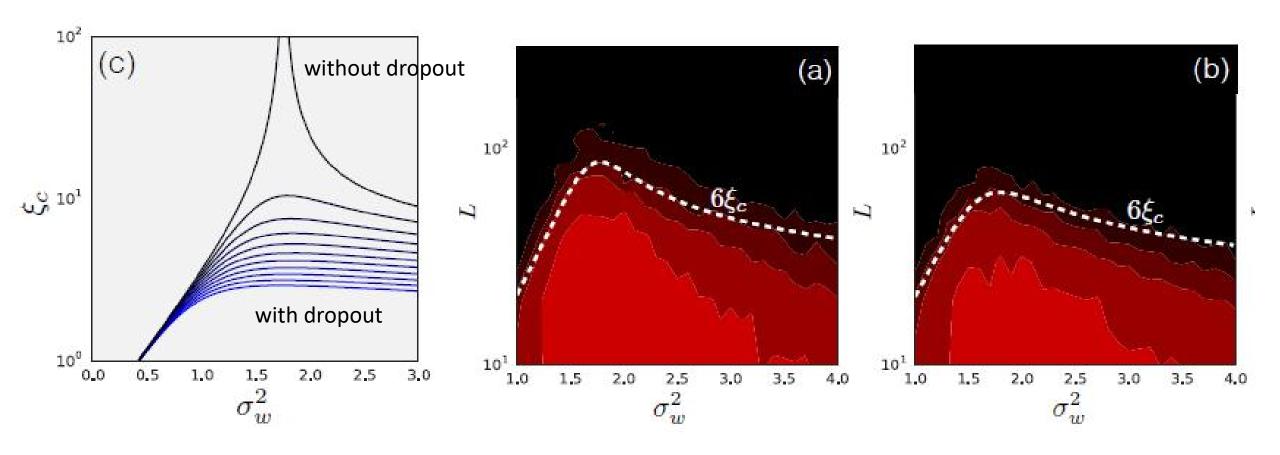
Why ResNet?



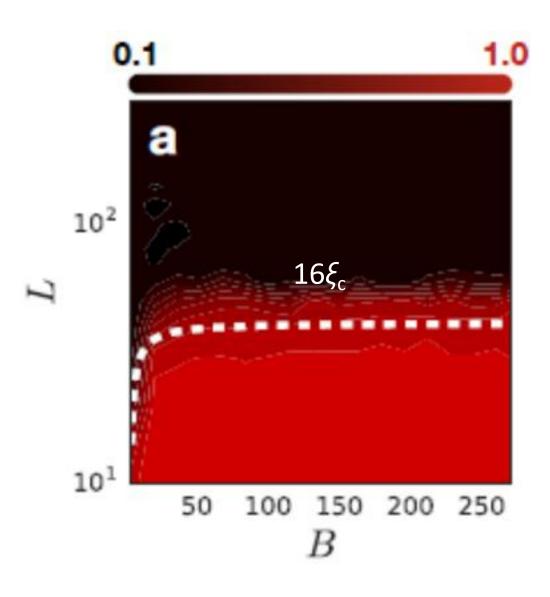
- Xavier or the He initializations are not optimal for residual networks
- the optimal initialization variances depend on the depth

Mean Field Residual Networks: On the Edge of Chaos | arXiv:1712.08969

Dropout limits the depth



Batch normalization limits the depth



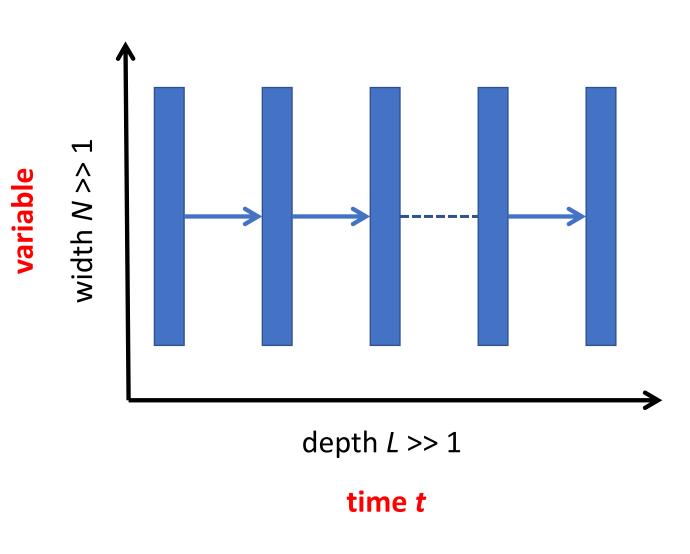
Method to overcome

Gradient explosion can be **reduced** by tuning the network close to the **linear** regime

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Mean-field theory Assumptions



deep uniform neural networks

dynamical system

Assumptions

- Uniform layers (constant N)
- independent weights for forward & back propogation
- > N >> 1
- > L >> 1
- theory works only for untrained model (time t = layer number ≠ epoch)

Mean-field theory limitations/pitfalls

- Theory works only for untrained model (time t = layer number ≠ epoch)
- ➤ Orthogonal initialization ≠ dynamical isometry necessary but not sufficient
- ➤ May not work if width is small
- ➤ May not work for shallow networks
- ➤ Not theory on generalization/test performance, training speed only on information propagation

Summary

- ➤ Mean-field theory (MFT) describes information propogation.
- ➤ MFT determine the maximal training depth.
- ➤ Initialization at the edge of chaos unlimits the training depth.
- ➤ Dynamical isometry speeds up training, and prevents test accuracy degradation with depth.
- ➤ Orthogonal initialization is a powerful scheme to reach dynamical isometry.
- > BatchNorm and dropout limit the training depth.
- > ReLU has no dynamical isometry.