Introduction to Deep Neural Networks

Numerical Methods for Deep Learning

Why Deep Networks?

- Universal approximation theorem of NN suggests that we can approximate **any** function by two layers.
- But - The width of the layer can be very large $\mathcal{O}(n \cdot n_f)$
- Deeper architectures can lead to more efficient descriptions of the problem.
  (No real proof but lots of practical experience)

Deep Neural Networks

How deep is deep?
We will answer this question later ...

Until recently, the standard architecture was

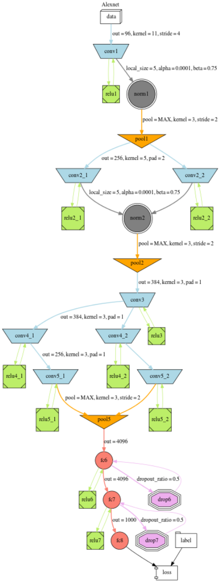
$$
\begin{aligned}
\mathbf{Y}_1 &= \sigma(\mathbf{K}_0\mathbf{Y}_0 + \mathbf{b}_0) \\
\vdots &= \vdots \\
\mathbf{Y}_N &= \sigma(\mathbf{K}_{N-1}\mathbf{Y}_{N-1} + \mathbf{b}_{N-1})
\end{aligned}
$$

And use $\mathbf{Y}_N$ to classify. This leads to the optimization problem

$$
\min_{\mathbf{K}_{0,\ldots,N-1},\mathbf{b}_{0,\ldots,N-1},\mathbf{W}} \; E\left(\mathbf{W}\mathbf{Y}_N(\mathbf{K}_1,\ldots,\mathbf{K}_{N-1},\mathbf{b}_1,\ldots,\mathbf{b}_{N-1}),\mathbf{C}^{\rm obs}\right)
$$

Example: The Alexnet [8] for Image Classification

- Complex architectures
- trained on multiple GPUs
- $\approx$ 60 million weights

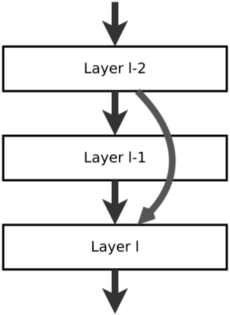


Deep Neural Networks in Practice

(Some) challenges:

- Computational costs (architecture have millions or billions of parameters)
- difficult to design
- difficult to train (exploding/vanishing gradients)
- unpredictable performance

In 2015, He et al. [6, 7] came with a new architecture that solves many of the problems



Simplified Residual Neural Network

Residual Network

$$
\begin{aligned}
\mathbf{Y}_1 &= \mathbf{Y}_0 + \sigma(\mathbf{K}_0 \mathbf{Y}_0 + \mathbf{b}_0) \\
\vdots &= \vdots \\
\mathbf{Y}_N &= \mathbf{Y}_{N-1} + \sigma(\mathbf{K}_{N-1} \mathbf{Y}_{N-1} + \mathbf{b}_{N-1})
\end{aligned}
$$

And use $\mathbf{Y}_N$ to classify. This leads to the optimization problem

$$
\min_{\mathbf{K}_{0,\dots,N-1}, \mathbf{b}_{0,\dots,N-1}, \mathbf{W}} \; E\left(\mathbf{W}\mathbf{Y}_N(\mathbf{K}_1, \dots, \mathbf{K}_{N-1}, \mathbf{b}_1, \dots, \mathbf{b}_{N-1}), \mathbf{C}^{\mathrm{obs}}\right)
$$

Leads to smoother objective function [9].

Stability of Deep Residual Networks

Why are ResNets more stable?
A small change

$$\begin{aligned} \mathbf{Y}_1 &= \mathbf{Y}_0 + h\sigma(\mathbf{K}_0\mathbf{Y}_0 + \mathbf{b}_0) \\ \vdots &= \vdots \\ \mathbf{Y}_N &= \mathbf{Y}_{N-1} + h\sigma(\mathbf{K}_{N-1}\mathbf{Y}_{N-1} + \mathbf{b}_{N-1}) \end{aligned}$$

This is nothing but a forward Euler discretization of the Ordinary Differential Equation (ODE)

$$\partial_t \mathbf{Y}(t) = \sigma(\mathbf{K}(t)\mathbf{Y}(t) + \mathbf{b}(t)), \qquad \mathbf{Y}(0) = \mathbf{Y}_0$$

Get intuition about ResNet behavior by using tools from nonlinear ODEs [5, 4]. A word of warning is [**?**].

ODE Crash Course

Consider the ODE

$$\partial_t \mathbf{y}(t) = f(\mathbf{y}(t))$$

with f differentiable and Jacobian

$$\mathbf{J}(\mathbf{y}) = \left(\frac{\partial f}{\partial \mathbf{y}}\right)^\top$$

Then (see also [2, 3, 1])

- If $Re(\mathrm{eig}(\mathbf{J})) > 0$ $\quad \rightarrow$ Unstable
- If $Re(\mathrm{eig}(\mathbf{J})) < 0$ $\quad \rightarrow$ Stable (converge to a stationary point)
- If $Re(\mathrm{eig}(\mathbf{J})) = 0$ $\quad \rightarrow$ Stable, energy bounded

Reality: f time-dependent ($\rightsquigarrow$ penalize time derivatives of weights or use heavier tools, e.g., kinematic eigenvalues)

Stability of Residual Network

Assume forward propagation of single example $\mathbf{y}_0$

$$\partial_t \mathbf{y}(t) = \sigma(\mathbf{K}(t)\mathbf{y}(t) + \mathbf{b}(t)), \qquad \mathbf{y}(0) = \mathbf{y}_0$$

The Jacobian is

$$\mathbf{J}(t) = \mathrm{diag}\left(\sigma'(\mathbf{K}(t)\mathbf{y}(t) + \mathbf{b}(t))\right)\mathbf{K}(t)$$

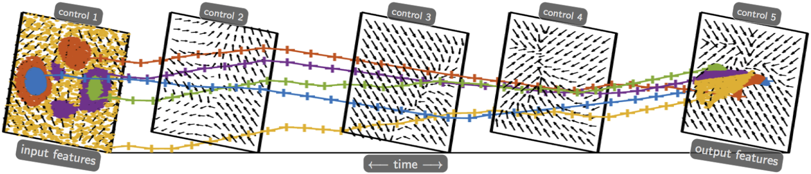
Here, $\sigma'(x) \geq 0$ for tanh, ReLU, ...

Hence, we need to enforce stability. One option:

1. $\mathbf{J}$ constant in time (or changes slowly)
2. $Re(\mathrm{eig}\mathbf{K}(t)) = 0$ for every t

Remember that we learn $\mathbf{K}$ $\leadsto$ ensure stability by regularization/constraints!

Residual Network as a Path Planning Problem



Forward propagation in residual network (continuous)

$$\partial_t \mathbf{Y}(t) = \sigma(\mathbf{K}(t)\mathbf{Y}(t) + \mathbf{b}(t)), \qquad \mathbf{Y}(0) = \mathbf{Y}_0$$

The goal is to plan a path (via $\mathbf{K}$ and b) such that the initial data can be linearly separated

Question: What is a layer, what is depth?

Stability: Continuous vs. Discrete

Assume $\mathbf{K}$ is chosen so that the (continuous) forward propagation is stable

$$\partial_t \mathbf{Y}(t) = \sigma(\mathbf{K}(t)\mathbf{Y}(t) + \mathbf{b}(t)), \qquad \mathbf{Y}(0) = \mathbf{Y}_0$$

And assume we use the forward Euler method to discretize

$$\mathbf{Y}_{l+1} = \mathbf{Y}_l + h\sigma(\mathbf{K}_l\mathbf{Y}_l + \mathbf{b}_l)$$

Is the network stable?

Not always ...

Stability: A Simple Example

Look at the simplest possible forward propagation

$$\partial_t \mathbf{Y}(t) = \lambda \mathbf{Y}(t), \qquad \lambda \in \mathbb{C}$$

And assume we use the forward Euler to discretize

$$\mathbf{Y}_{l+1} = \mathbf{Y}_l + h\lambda \mathbf{Y}_l = (1 + h\lambda)\mathbf{Y}_l$$

Then the method is stable only if

$$|1 + h\lambda| \leq 1$$

Not every network is stable! Time step size depends on λ (which depends on $\mathbf{K}$ that is trained).

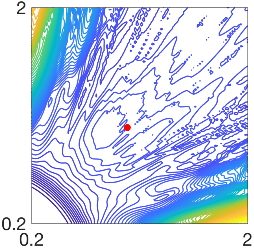
Why you should care about stability - 1

$$\min_{\theta} \frac{1}{2}\|\mathbf{Y}_N(\theta) - \mathbf{C}\|_F^2 \qquad \mathbf{Y}_{j+1}(\theta) = \mathbf{Y}_j(\theta) + \frac{10}{N}\tanh\left(\mathbf{K}\mathbf{Y}_j(\theta)\right)$$

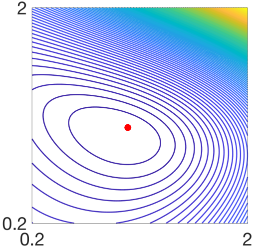
where $\mathbf{C} = \mathbf{Y}_{200}(1,1)$, $\mathbf{Y}_0 \sim \mathcal{N}(0,1)$, and

$$\mathbf{K}(\theta) = \begin{pmatrix} -\theta_1 - \theta_2 & \theta_1 & \theta_2 \\ \theta_2 & -\theta_1 - \theta_2 & \theta_1 \\ \theta_1 & \theta_2 & -\theta_1 - \theta_2 \end{pmatrix}$$

objective, $N = 5$

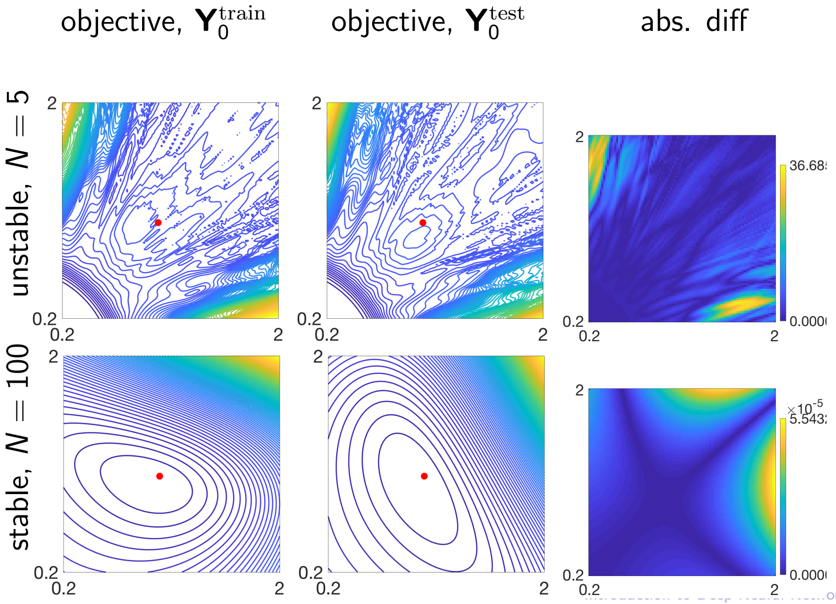


objective, $N = 100$



Next: Compare different inputs $\sim$ generalization

Why you should care about stability - 2



Stability: A Non-Trivial Example

Consider the antisymmetric kernel model

$$\mathbf{K}(t) = \mathbf{K}(t) - \mathbf{K}(t)^\top.$$

Here, $Re(\mathrm{eig}(\mathbf{J}(t))) = 0$ for all $\boldsymbol{\theta}$.

Assume we use the forward Euler to discretize

$$\mathbf{Y}_{l+1} = \mathbf{Y}_l + h\sigma((\mathbf{K}_l - \mathbf{K}_l^\top)\mathbf{Y}_l + \mathbf{b}_l).$$

Tricky question: How to pick h to ensure stability?
Answer: Impossible since eigenvalues of Jacobian are imaginary. Need other method than forward Euler.

References

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[6] K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 770–778, 2016.

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[9] H. Li, Z. Xu, G. Taylor, and T. Goldstein. Visualizing the Loss Landscape of Neural Nets. 2017.