On the Expressive Power of Deep Neural Networks

Maithra Raj[1,2] Ben Poole[3] Jon Kleinberg[1] Surya Ganguli[3]
Jascha Sohl Dickstein[2]

[1]Cornell University

[2]Google Brain

[3]Stanford University

ICLR, 2017
Presenter: Ritambhara Singh

Outline

Outline

1. Introduction
   - Motivation
   - State-of-the-art
   - Contributions
2. Measures of Expressivity
   - Neuron Transitions and Activity Patterns
   - Trajectory length
3. Insights
   - Expressivity and Network Stability
   - Trajectory Regularization

Motivation

- Understanding of how and why neural networks achieve empirical success is lacking.

Motivation

- Understanding of how and why neural networks achieve empirical success is lacking.
- *Neural Network Expressivity*: To characterize how structural properties of neural network affect functions it is able to compute.

Motivation

- Understanding of how and why neural networks achieve empirical success is lacking.
- *Neural Network Expressivity*: To characterize how structural properties of neural network affect functions it is able to compute.
- Neural Network (NN) Architecture: A (certain depth, width, layer type)
- All parameters of the network: W
- Input: x
- Associated Function: $F_A(x; W)$

Motivation

- Understanding of how and why neural networks achieve empirical success is lacking.
- *Neural Network Expressivity*: To characterize how structural properties of neural network affect functions it is able to compute.
- Neural Network (NN) Architecture: A (certain depth, width, layer type)
- All parameters of the network: W
- Input: x
- Associated Function: $F_A(x; W)$
- **Goal:** To understand how behavior of $F_A(x; W)$ changes when A changes.

Outline

State-of-the-art

- Studying expressivity using highly theoretical approaches like, comparison to boolean circuits etc.
- **Drawback:** Results shown on shallow networks that are different from deep networks used today.
- Understanding benefits of depth for neural networks, showing separations between deep and shallow networks.
- **Drawback:** Results on very specific choice of weights (hand-coded) and focus on only lower bounds.

Outline

Contributions

- Propose easily computable measures of of NN expressivity.
- Study input transformation by the network by measuring *trajectory length*, find exponential depth dependence of these measures.
- Show that all weights are not equal and optimizing weights of lower layers matter more.
- Propose new method of *Trajectory Regularization*,which is as good as batch normalization but more computationally efficient.

Outline

Trajectory

Definition

Given two points, $x_0, x1 \in R^m$, $x(t)$ is a *trajectory* (between x_0 and x_1) if $x(t)$ is a curve parameterized by a scalar $t \in [0, 1]$, with $x(0) = x_0$ and $x(1) = x_1$.

Neuron Transitions

Definition

For fixed W, a neuron with piecewise linear region *transitions* between inputs $x, x+\delta$ if its activation function switches linear regions between x and $x+\delta$.

Activation Pattern

Definition

Activation pattern, $AP(F_A(x(t)); W))$, is a string of form $\{0,1\}^N$ (for ReLUs) and $\{-1,0,1\}^N$ (for hard tanh) of the network encoding the linear region of activation function of **every** neuron, for an input x and weights W .

(Tight) Upper Bound for Number of Activation Patterns

Theorem

Let $A_{(n,k)}$ denote a fully connected network with n hidden layers of width k, and inputs in R^m. Then the number of activation patterns $A(F_{A_{(n.k)}}(R^m; W))$ is upper bounded by $O(k^{mn})$ for ReLU activation, and $O((2k)^{mn})$ for hard tanh.

Regions in Input Space

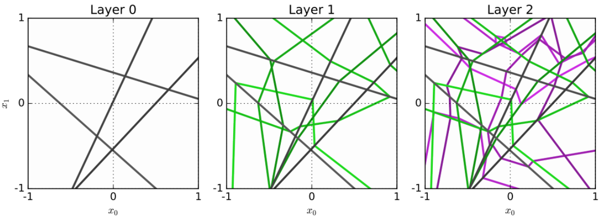
Theorem

Given the corresponding function of a neural network $F_A(R^m; W)$ with ReLU or hard tanh activations, the input space is partitioned into convex polytopes, with $F_A(R^m; W)$ corresponding to a different linear function on each region.

Regions in Input Space

Theorem

Given the corresponding function of a neural network $F_A(R^m; W)$ with ReLU or hard tanh activations, the input space is partitioned into convex polytopes, with $F_A(R^m; W)$ corresponding to a different linear function on each region.



Outline

Trajectory Length

Definition

Given a trajectory, $x(t)$, its length $l(x(t))$, is the standard arc length:

$$l(x(t)) = \int_t \left\| \frac{dx(t)}{dt} \right\| dt \tag{1}$$

Bound on Growth of Trajectory Length

- $A_{(n,k)}$ is fully connected network with n hidden layers of width k each.
- Initialize weights $\sim \mathcal{N}(0, \sigma_w^2/k)$ and biases $\sim \mathcal{N}(0, \sigma_b^2)$.

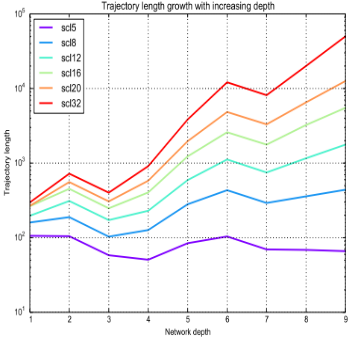
Theorem

Let $F_A(x', W)$ be a ReLU or hard tanh random neural network and $x(t)$ a one dimensional trajectory with $x(t+\delta)$ having a non-trivial perpendicular component to $x(t)$ for all t and δ (i.e, not a line). Then defining $z^{(d)}(x(t)) = z^{(d)}(t)$ to be the image of the trajectory in layer d of the network:

$$E[l(z^{(d)}(t)] \geq O\left(\frac{\sigma_w\sqrt{k}}{\sqrt{k+1}}\right)^d l(x(t))[ReLUs] \tag{2}$$

$$E[l(z^{(d)}(t)] \geq O\left(\frac{\sigma_w\sqrt{k}}{\sigma_w^2+\sigma_b^2+k\sqrt{\sigma_w^2+\sigma_b^2}}\right)^d l(x(t))[hardtanh] \tag{3}$$

Bound on Growth of Trajectory Length



Transitions proportional to trajectory length

Theorem

Let $F_{A_{(n,k)}}$ be a hard tanh network with n hidden layers each of width k. And let

$$g(k, \sigma_w, \sigma_b, n) = O\left(\frac{\sqrt{k}}{\sqrt{1 + \frac{\sigma_w^2}{\sigma_b^2}}}\right)^n \tag{4}$$

Then $T(F_{A_{(n,k)}}(x(t); W)) = O(g(k, \sigma_w, \sigma_b, n))$ for W initialized with weight and bias scales σ_w, σ_b.

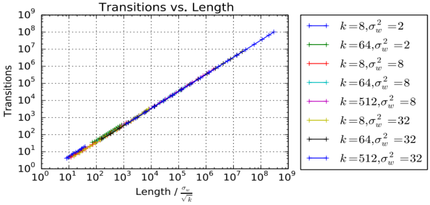
Transitions proportional to trajectory length

Theorem

Let $F_{A_{(n,k)}}$ be a hard tanh network with n hidden layers each of width k. And let

$$g(k, \sigma_w, \sigma_b, n) = O\left(\frac{\sqrt{k}}{\sqrt{1 + \frac{\sigma_w^2}{\sigma_b^2}}}\right)^n \tag{4}$$

Then $T(F_{A_{(n,k)}}(x(t); W)) = O(g(k, \sigma_w, \sigma_b, n))$ for W initialized with weight and bias scales σ_w, σ_b.



Outline

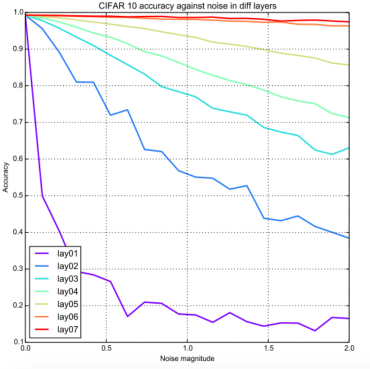
1. Introduction
   - Motivation
   - State-of-the-art
   - Contributions
2. Measures of Expressivity
   - Neuron Transitions and Activity Patterns
   - Trajectory length
3. Insights
   - Expressivity and Network Stability
   - Trajectory Regularization

Expressivity and Network Stability

- A perturbation at a layer grows exponentially in the remaining depth after that layer

Expressivity and Network Stability

- A perturbation at a layer grows exponentially in the remaining depth after that layer



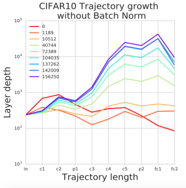
Outline

Trajectory Regularization

- Initial growth of trajectory length enables greater functional expressivity, however, large trajectory growth in the learnt representation results in unstable representation.

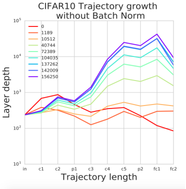
Trajectory Regularization

- Initial growth of trajectory length enables greater functional expressivity, however, large trajectory growth in the learnt representation results in unstable representation.



Trajectory Regularization

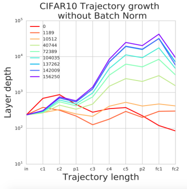
- Initial growth of trajectory length enables greater functional expressivity, however, large trajectory growth in the learnt representation results in unstable representation.



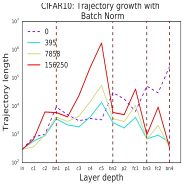
- Batch normalization layers reduce trajectory length, helping stability

Trajectory Regularization

- Initial growth of trajectory length enables greater functional expressivity, however, large trajectory growth in the learnt representation results in unstable representation.



- Batch normalization layers reduce trajectory length, helping stability



Summary

- Presented interrelated measures of expressivity of NN.
- Analysis of trajectories gives insight for performance of trained NNs.
- Developed new regularization method, trajectory regularization.
- Future work
  - Linking measures of expressivity to other properties of NN performance.
  - Natural connection between adverserial samples and trajectory length.