Controlling the Structure of Inference and Learning in Neural Networks

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Machine learning is transforming science



https://www.microsoft.com/en-us/research/project/crispr/





https://news.mit.edu/2020/artificial-intelligence-identifies-new-antibiotic-0220



Halicin: structurally new antibiotic

...and autonomous decision-making



MLNav: Learning to Safely Navigate on Martian Terrains https://arxiv.org/abs/2203.04563



Microsoft Azure Personalizer https://learn.microsoft.com/en-us/azure/cognitive-services/personalizer/how-personalizer-works



AlphaGo

...and creativity



https://www.vice.com/en/article/bvmvgm/an-ai-generated-artwork-won-first-place-at-a-state-fair-fine-arts-competition-and-artists-are-pissed

...and common-sense reasoning

Query: How many muffins can each kid have for it to be fair?



ViperGPT

https://viper.cs.columbia.edu/



Operationally: What is Machine Learning? (Optimization Perspective)



Tuning Neural Networks is Messy and Hard

Initialization, activation, loss, architecture type, depth & width, dropout rate, optimizer, learning rate, momentum, batch size, ...



(Brock et al, 2019)





Canonical View of ML Optimization



Canonical View of ML Optimization

• ^T In Theory:

Pai

- Set η via perturbation analysis
 - How much f can change w.r.t. θ
 - (e.g., global Lipschitz constant of f)

In Practice:

• Re-tune η if we change anything about learning setup!

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Looking Inside a Neural Network

Linear w/ ReLU activation

 $f(\mathbf{h}; \boldsymbol{\theta}) = [\boldsymbol{\theta}^T \mathbf{h}]_+$

Example:

(ignoring bias/offset)



Intuition (for binary classification)



Sequence of transformations

- Each dimension is a half-space mapping
- Goal: last layer is a separable space with perfect classification

Idea #1: Per-Layer Perturbation Analysis

• How does the layer's function change under parameter perturbation?



Potential Application: depth- & width-invariant learning rate η

Idea #2: Control Dynamics of Hidden Layers

Recall: we want each layer to push representation towards good answer





Goal: control sequence of hidden layers h_1, \dots, h_N

• quickly and robustly converge to low loss



How to exploit the structure of NNs to develop a more nuanced theory?

Control-Theoretic Shaping of Neural ODEs "Lyapunov Loss"



Warm-Up: Local Perturbation Analysis

- Linear approximation breaks down as $\Delta \theta$ increases!
- Understand rate of break-down via perturbation analysis.

Taylor Expansion:

$$L(\theta + \Delta \theta) = L(\theta) + \nabla_{\theta} L(\theta)^{T} \Delta \theta + \frac{1}{2} \Delta \theta^{T} \nabla_{\theta}^{2} \Delta \theta + \dots$$

Linear Approximation
$$I(\theta)$$



Majorize-Minimize in Action



Aside: Duality of Majorization & Trust Regions

$$\min_{\Delta \theta} \nabla_{\theta} L(\theta)^T \Delta \theta + \lambda |\Delta \theta|^2$$

Theoretical guidance via tivity, tant

• Closed-form solution:
$$\Delta \theta = -\begin{pmatrix} 2\\ \lambda \end{pmatrix} \nabla_{\theta} L(\theta)$$

• Implies GD update rule: $\theta \leftarrow \theta - \begin{pmatrix} 2\\ \lambda \end{pmatrix} \nabla_{\theta} L(\theta)$
• Analogous to: $\min_{\Delta \theta} \nabla_{\theta} L(\theta)^T \Delta \theta$ s.t. $|\Delta \theta|^2 \leq C$ "Trust Region"



Architecture-Naive Majorizations

- Deep networks have complicated optimization landscapes
- Using a single isotropic majorization can be very inefficient!



How to define a majorization that exploits NN structure?





Jeremy Bernstein Kevin Huang



- (First) Key Idea: per-layer perturbation analysis
- Perturb entire layer's parameters => perturbation of final output

Thought Experiment



- Vary only n-th layer: $\theta_n + \Delta \theta_n$
- What is the Lipchitz constant of entire function f?
- Depends on parameters θ of other layers!
 - If other parameters are larger => perturbation is larger!

Architecture-Aware Perturbation Bounds

Lemmas 5.1 & 6.2 in https://arxiv.org/abs/2210.10101





Jeremy Bernstein Kevin Huang





Majorize-Minimize for Neural Networks



- Derive *majorization* of error
- Plug in *architecture perturbation bound*
- *Minimize* to obtain optimization algorithm

Related: "Automatically Bounding the Taylor Remainder Series: Tighter Bounds and New Applications" (https://arxiv.org/abs/2212.11429)



- "Clean" bound only for deep linear networks
 - Formula more complicated with non-linearities
 - First ever analysis even for deep linear networks
- Majorization has no (known) closed-form solution
 - Solving for the optimal $\Delta \theta$ is itself an optimization problem

First Result

Theorem 6.2 in https://arxiv.org/abs/2210.10101

- Key restriction: enforce relative update of each layer to be the same
 - Suboptimal but closed-form update rule



- Learning rate η transfers to wider & deeper networks!
 - (Related to mu-Parameterization by Greg Yang et al.)





Jeremy K Bernstein Hi

Kevin Huang Width:

64	— 1024
— 128	2048
256	4096
— 512	— 8192

Loss

Same learning rate is (near-)optimal across depth & width!

(ignoring stochastic aspect, i.e., full batch optimization)



Depth 6

Depth 8

Depth 10

Learning Rate

 10^{0}

 10^{-1}

Width:

64	— 1024
— 128	2048
256	4096
— 512	— 8192



Same learning rate is (near-)optimal across depth & width!

(ignoring stochastic aspect, i.e., full batch optimization)



Learning Rate

Width:

64	— 1024
—— 128	2048
256	4096
— 512	— 8192



Same learning rate is (near-)optimal across depth & width!

(ignoring stochastic aspect, i.e., full batch optimization)

Learning Rate

Case Study: Training Very Deep Networks

(Fully connected, no Skip Connections or Normalization Layers)



Training very deep networks is hard! Practitioners use techniques like skip connections & normalization layers.

https://arxiv.org/abs/2002.03432

Latest Result Automatic Gradient Descent

Initialize Weights:

- **for** layer *n* in {1, ..., *N*}:
 - $\theta_n \sim unif(orthogonal(dim_n, dim_{n-1}))$

$$\theta_n \sim \theta_n \cdot \sqrt{\frac{\dim_n}{\dim_{n-1}}}$$

Update Weights:

•
$$G \leftarrow \frac{1}{N} \sum_{n=1}^{N} |\nabla_{\theta_n} L|_F \cdot \sqrt{\frac{\dim_n}{\dim_{n-2}}}$$

- $\eta \leftarrow \log \frac{1 + \sqrt{1 + 4G}}{2}$
- **for** layer $n \text{ in } \{1, ..., N\}$:

•
$$\theta_n \leftarrow \theta_n - \frac{\eta}{N} \cdot \frac{\nabla_{\theta_n} L}{|\nabla_{\theta_n} L|_F} \cdot \sqrt{\frac{\dim_n}{\dim_{n-1}}}$$

$$\Rightarrow \qquad |\theta_n| = \sqrt{\frac{\dim_n}{\dim_{n-1}}}$$



Jeremy Chris Bernstein Mingard

$$\Rightarrow \qquad |\Delta \theta_n| = \frac{\eta}{N} \cdot \sqrt{\frac{\dim_n}{\dim_{n-1}}}$$

https://arxiv.org/abs/2304.05187

AGD trains without hyperparameters





Different Ways to Design Optimizers





Different Ways to Design Optimizers

- Fromage: Per-layer was our first foray
 - <u>https://arxiv.org/abs/2002.03432</u>
- Nero: Per-neuron
 - Also constrain per-neuron weight norm
 - Connections to batch-norm
 - Connections to generalization
 - <u>https://arxiv.org/abs/2102.07227</u>

• Madam: Per-synapse

- Also sign-constrain weights
- Leads to multiplicative update rule
- Connections to biological synapses
- <u>https://arxiv.org/abs/2006.14560</u>













Summary: Architecture-Aware Perturbation Bounds



Architectural perturbation bound $\|\Delta f(x)\| \leq C \cdot \left[\prod_{I} \left(1 + \frac{\|\Delta W_{I}\|}{\|W_{I}\|} \right) - 1 \right]$



Towards A Practical Theory of Deep Learning Optimization

$$-M_{1} = R_{1} + R_{2} + R_{3}$$



 $1/R = 1/R_1 + 1/R_2 + 1/R_3$



Theory of Composite Functions?

- Learning Rate
- Learning Rate Decay
- Momentum

...

- Gradient Averaging
- Warm-up Iterations

Optimisation & Generalisation in Networks of Neurons

Thesis by Jeremy Bernstein

In Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy





Jeremy Bernstein

Error $L(\theta)$ $H_{1} = \theta_{0}$ H_{2} H_{2}

How to exploit the structure of NNs to develop a more nuanced theory?



Recall Idea #2: Control Dynamics of Hidden Layers

We want each layer to push representation towards good answer





Goal: control sequence of hidden layers h_1, \dots, h_N

• quickly and robustly converge to low loss

Warm Up: Deep Networks



Warm Up: ResNets



Functional Form:

 $h_0 = f_{in}(x)$ $h_n = h_{n-1} + f_n(h_{n-1})$ $y = f_{out}(h_N)$

ResNets => Continuous-in-Depth => Neural ODEs



"Euler Integration Step Size"

$$\begin{array}{c} & \downarrow \\ h_n = h_{n-1} + \delta f(h_{n-1}) \end{array} \xrightarrow{\lim_{\delta \to 0}} & \frac{\partial h}{\partial t} = f(h)
\end{array}$$

Neural Ordinary Differential Equations (NODEs)

https://arxiv.org/abs/1806.07366

$$h_0 = f_{in}(x)$$

Input Layer

Comments:

• Forward pass requires ODE solve

 $\frac{\partial h}{\partial t} = f(h, x)$ Continuum of hidden layers
"Dynamics"

$$y(t) = f_{out}(h(t))$$

WLOG: $t \in [0,1]$

- Can evaluate output at any time
 - E.g., y(0.5)
- Includes continuous normalizing flows & other generative models

("augmented" NODE since f depends on x -- https://arxiv.org/abs/1904.01681)

Output Layer

Using Control Theory to Shape Learning

Control can shape dynamical systems (most commonly ODEs)



Why Shape Dynamics of NODEs?

2D state space, Red Class is correct Showing inference trajectories under perturbations



Ivan Jimenez Rodriguez





Our Approach Lyapunov Loss

What dynamics can we shape?

$$h_0 = f_{in}(x)$$



• (too unwieldy)



 $y(t) = f_{out}(h(t))$

• **Projection**: $V(h(t)) \equiv L(y(t))$

1

- Dynamics of the training loss
- 1-D projection of state space

WLOG: $t \in [0,1]$





Ivan

Jimenez Rodriguez

Exponential Convergence in Action

CIFAR-10



LyaNet is trained to optimize for exponential convergence

https://arxiv.org/abs/2202.02526

Measuring Progress via Contraction Condition



Contraction Satisfied Everywhere => Exponential Stability!

Lyapunov Loss

• Point-wise Lyapunov Loss

$$L_{V}(x, y, h) \equiv \max\left\{0, \frac{\partial V_{y}^{T}}{\partial h}f(h) + \kappa V_{y}(h)\right\}$$

Contraction condition violation

• Lyapunov Loss:

$$L_V(\theta) \equiv \boldsymbol{E}_{x,y} \left[\int_0^1 L_V(x, y, h(t)) dt \right]$$

Achieving zero Lyapunov Loss (almost) everywhere implies exponential stability!

Satisfaction:

 $\frac{\partial V^T}{\partial h} f(h) \le -\kappa V(h)$

Violation:

 $\frac{\partial V^T}{\partial h} f(h) > -\kappa V(h)$



3. Optimize Lyapunov Loss everywhere

N I

$$L_V(x, y, h) \equiv \max\left\{0, \frac{\partial V_y^T}{\partial h}f(h) - \kappa V_y(h)\right\}$$

$$Interpret training loss as potential function. V(n(t)) = L()$$

1. Interpret training loss as potential function:
$$V(h(t)) \equiv L(y(t))$$



lvan Jimenez Rodriguez

Optimization Considerations

$$L_V(\theta) \equiv \boldsymbol{E}_{x,y} \left[\int_0^1 L_V(x, y, h(t)) dt \right]$$

Lyapunov Loss



- Evaluating integral exactly is hard
- Approximate by sampling (simplest is Monte Carlo)
 - Sample (x,y,h) uniformly at random
 - Backprop on point-wise Lyapunov Loss

$$L_V(x, y, h) \equiv \max\left\{0, \frac{\partial V_y}{\partial h}^T f(h) - \kappa V_y(h)\right\}$$

Point-wise Lyapunov Loss

https://arxiv.org/abs/2202.02526

Benefits of Sampling

• Avoids expensive ODE solve

• Goal is to minimize Lyapunov Loss everywhere

$$L_V(\theta) \equiv \boldsymbol{E}_{x,y} \left[\int_0^1 L_V(x, y, h(t)) dt \right]$$

Achieving $L_V(\theta) = 0$ under uniform measure implies $L_V(\theta) = 0$ in original measure

• Similar idea used in Score-Based Generative Models & Moser Flows

https://arxiv.org/abs/2202.02526

Connection to Control Theory

https://ieeexplore.ieee.org/document/6709752

• V is an *Exponentially-Stabilizing Control Lyapunov Function (ES-CLF)* for a controllable ODE if for all states *h* ∈ *H*:

$$\min_{\theta} \left[\frac{\partial V^T}{\partial h} f(h; \theta) + \kappa V(h) \right] \le 0$$

Equivalent to Lyapunov Loss

- Can we find a controller θ that makes V an ES-CLF?
 - In control, f has uncontrolled dynamics and θ is low-dim
- Connection between controllability & learnability
 - Can we find a θ that achieves zero Lyapunov Loss?
 - For NODEs, f is fully controlled and over-parameterized



Comments & Extensions

- Stabilize to sets rather than points
 - E.g., under adversarial perturbations, can still stabilize to a region of low loss
 - Sets need not be convex
- Combinations of conditions (multiple invariances)



Motivating Application: Continuous Control

Note: Dynamics of Control System included in Neural ODE



Neural Gaits

Learn policy to satisfy composition of continuous-time conditions Implies indefinite walking (forward-invariance)





Ivan Jimenez Rodriguez Noel Csomay-Shanklin





https://arxiv.org/abs/2204.08120



Certified Forward-Invariance in NODEs









Certified Robust Forward Invariance (First Ever Result)

https://arxiv.org/abs/2210.16940

Summary: Control-Theoretic Shaping of Neural ODEs









Aside: Symbolic Music Generation via Stochastic Control

Yujia Huang





Symbolic Music Generation with Non-Differentiable Rule-Guided DiffusionYujia Huang, et al., arXivhttps://scg-rule-guided-music.github.io/



Towards Structure-Aware Theory of Deep Learning

- Neural Nets are not arbitrary black-box functions
 - Analyzing structure can lead to more nuanced theory
 - Can unlock new connections



Contraction Analysis & Control Theory





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Thanks!



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