A Numerical Analysis Perspective on Deep Neural Networks

Machine Learning for Physics and the Physics of Learning

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Agenda: Numerical Analysis of Deep Neural Networks

- Notation: Deep Learning
- Case 1: Invertibility
- Case 2: Time Integrators
  - Example: higher order or conservative?
- Case 3: Discretize-then-Optimize
  - Example: Neural ODEs
- Case 4: Ill-conditioning
  - Example: Single layer neural network
- Conclusion and Summary

Key question: What can numerical analysts do in the age of ML?
Deep Learning
Deep Learning Revolution (?)

\[
\begin{align*}
Y_{j+1} &= \sigma(K_j Y_j + b_j) \\
Y_{j+1} &= Y_j + \sigma(K_j Y_j + b_j) \\
Y_{j+1} &= Y_j + \sigma(K_{j,2} \sigma(K_{j,1} Y_j + b_{j,1}) + b_{j,2}) \\
&\vdots
\end{align*}
\]

(Notation: \( Y_j \): features, \( K_j, b_j \): weights, \( \sigma \): activation)

- deep learning: use neural networks (from \( \approx 1950\)'s) with many hidden layers
- able to "learn" complicated patterns from data
- applications: image classification, face recognition, segmentation, driverless cars, ...
- recent success fueled by: massive data sets, computing power
- A few recent references:
  - A radical new neural network design could overcome big challenges in AI, MIT Tech Review '18
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17
Optimal Control Framework for Deep Learning

Supervised Deep Learning Problem

Given training data, $\mathbf{Y}_0$, and labels, $\mathbf{C}$, find network parameters $\theta$ and classification weights $\mathbf{W}$, $\mu$ such that the DNN predicts the data-label relationship (and generalizes to new data), i.e., solve

$$\text{minimize}_{\theta, \mathbf{W}, \mu} \quad \text{loss}[g(\mathbf{W} + \mu), \mathbf{C}] + \text{regularizer}[\theta, \mathbf{W}, \mu]$$
Deep Residual Neural Networks (simplified)

Award-winning forward propagation

\[ Y_{j+1} = Y_j + hK_{j,2}\sigma(K_{j,1}Y_j + b_j), \quad \forall j = 0, 1, \ldots, N - 1. \]

ResNet is forward Euler discretization of

\[ \frac{\partial t}{t}y(t) = K_2(t)\sigma(K_1(t)y(t) + b(t)), \quad y(0) = y_0. \]

Notation: \( \theta(t) = (K_1(t), K_2(t), b(t)) \) and

\[ \frac{\partial t}{t}y(t) = f(y, \theta(t)), \quad y(0) = y_0 \]

where

\[ f(y, \theta) = K_2(t)\sigma(K_1(t)y(t) + b(t)). \]

K. He, X. Zhang, S. Ren, and J. Sun

*Deep residual learning for image recognition.*

(Some) Related Work

**DNNs as (stochastic) Dynamical Systems**

**Numerical Time Integrators**

**Optimal Control**

**PDE-motivated Approaches**
Numerical Methods for Deep Learning

An (almost perfectly) true statement

\[
\text{backpropagation} + \text{GPU} + \left\{ \begin{array}{c}
\text{TensorFlow} \\
\text{Caffe} \\
\text{Torch}
\end{array} \right\} \implies \text{success}
\]

So, why study numeric methods for deep learning?
A Simple Example

![Graph showing a V-shape function]

Predict the output of:

```python
x = param(0.0)
f = abs(x)
Tracker.back!(f)
Tracker.grad(x)
```
Case 1: Reversibility
Reversibility: Continuous vs. Discrete

Goal: If $Y = \text{NN}(X, \theta)$, want $X = \text{NN}^{-1}(Y, \theta)$!

**Idea 1: ResNet**

$$\partial_t Y = \tanh(K(t)Y + b(t))$$

- discretize: RK4, 16 time steps
- 4 channels, pad inputs with 0
- inverse: integrate backward in time

**Idea 2: Hamiltonian NN**

$$\partial_t \begin{pmatrix} Y \\ Z \end{pmatrix} = \begin{pmatrix} \tanh(K(t)Z + b(t)) \\ -\tanh(K(t)^\top Y + b(t)) \end{pmatrix}$$

- discretize: Verlet, 32 time steps
- no padding, trivial inverse
Case 2: Black-box
Example: High-order vs. Symplectic?

Consider linear harmonic oscillator

\[
\partial_t \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}
\]

associated with

\[ H(p, q) = p^2 + q^2 \]

\( h \) large

\( h \) small

Use the right (in this case lower-order) integrators \( \Rightarrow \) more bang for the buck!

U Ascher

*Numerical methods for evolutionary differential equations.*

SIAM, 2008

S Greydanus, M Dzamba, J Yosinski

*Hamiltonian Neural Networks.*

arXiv:1906.01563
Case 3: Discrete vs. Continuous
Optimal Control Framework for Deep Learning

Supervised Deep Learning Problem

Given training data, \( Y_0 \), and labels, \( C \), find network parameters \( \theta \) and classification weights \( W, \mu \) such that the DNN predicts the data-label relationship (and generalizes to new data), i.e., solve

\[
\text{minimize}_{\theta, W, \mu} \quad \text{loss}[g(W + \mu), C] + \text{regularizer}[\theta, W, \mu]
\]
Optimal Control Background: Diff→Disc vs. Disc→Diff

minimize$_{\theta,W,\mu}$ \[ \text{loss}[g(WY(T) + \mu), C] + \text{regularizer}[\theta, W, \mu] \]
subject to \[ \partial_t Y(t) = f(Y(t), \theta(t)), \ Y(0) = Y_0. \]

**First-Differentiate-then-Discretize (Diff→Disc)**
- Keep $\theta, b, Y$ continuous in time
- Euler-Lagrange-Equations $\Rightarrow$ adjoint equation ($\approx$ backprop)
- Flexible choice of ODE solver in forward and adjoint
- Gradients only useful if fwd and adjoint solved well
- Use optimization to obtain discrete solution of ELE

**First-Discretize-then-Differentiate (Disc→Diff)**
- Discretize $\theta, b, Y$ in time (could use different grids)
- Differentiate objective (e.g., use automatic differentiation)
- Gradients related to adjoints but no choice of solver
- Gradients useful even if discretization is inaccurate
- Use nonlinear optimization tools to approximate minimizer

MD Gunzburger
*Perspectives in flow control and optimization.*
SIAM, 2013.

TQ Chen et al.,
*Neural Ordinary Differential Equations.*

A Gholami, K Keutzer, G Biros
*ANODE: Unconditionally Accurate Memory-Efficient Gradients for Neural ODEs.*
arXiv:1902.10298
Example: Gradient Test Disc $\rightarrow$ Diff

Goal: Find weights of neural network $F(u, \theta)$ such that

$$\partial_t u = F(u, \theta), \quad u(0) = u_0$$

fits true ODE at $0 < t_1 < t_2 < \cdots < t_n \leq 1.5$; details Sec. 8 from paper below.

Question: How does accuracy of ODE solvers impact the quality of gradient?

C Rackauckas, M Innes, Y Ma, J Bettencourt, L White, V Dixit

*DiffEqFlux.jl - A Julia Library for Neural Differential Equations.*

arXiv:1902.02376
Neural ODE, $\varepsilon_{\text{rel}} = 10^{-7}, \varepsilon_{\text{abs}} = 10^{-9}$

Training: ADAM with default setting, same initialization
Neural ODE, $\epsilon_{\text{rel}} = 10^{-7}$, $\epsilon_{\text{abs}} = 10^{-9}$

Training: ADAM with default setting, same initialization
Neural ODE, $\epsilon_{\text{rel}} = 10^{-2}$, $\epsilon_{\text{abs}} = 10^{-2}$

Training: ADAM with default setting, same initialization
Impact of Network Architecture on Optimization - 1

\[
\min_{\theta} \frac{1}{2} \| Y_N(\theta) - C \|^2_F \quad \quad Y_{j+1}(\theta) = Y_j(\theta) + \frac{10}{N} \tanh (K Y_j(\theta))
\]

where \( C = Y_{200}(1, 1) \), \( Y_0 \sim \mathcal{N}(0, 1) \), and

\[
K(\theta) = \begin{pmatrix}
-\theta_1 - \theta_2 & \theta_1 & \theta_2 \\
\theta_2 & -\theta_1 - \theta_2 & \theta_1 \\
\theta_1 & \theta_2 & -\theta_1 - \theta_2
\end{pmatrix}
\]

Next: Compare examples for different inputs \( \sim \) generalization
Impact of Network Architecture on Optimization - 2

objective, \( Y_{0}^{\text{train}} \)  

unstable, \( N = 5 \)  

stable, \( N = 100 \)  

objective, \( Y_{0}^{\text{test}} \)  

abs. diff

\[
\begin{array}{c c c}
\text{unstable, } N = 5 & \text{stable, } N = 100 & \text{abs. diff} \\
\end{array}
\]
Case 4: Conditioning
Conditioning of the Learning Problem

Consider the regression problem with a single neural network layer

$$\min_{W,K} \frac{1}{2s} \|R(W,K)\|^2,$$

where \( R(W,K) = W\sigma(KY) - C \)

- \( Y \in \mathbb{R}^{d\times s} \) - input features
- \( C \in \mathbb{R}^{n\times s} \) - output features
- \( K \in \mathbb{R}^{m\times d}, W \in \mathbb{R}^{n\times m} \) - weights for fully-connected transformation
- \( \sigma : \mathbb{R} \rightarrow \mathbb{R} \) - activation function (applied to each element)

The problem above is a non-linear least squares problem (NNLS). Common to look at the Jacobian of \( r \), i.e., \( J = [J_W J_K] \) where

$$J_W = \sigma(KY)^\top \otimes I, \quad \text{and} \quad J_K = (I \otimes W) \text{diag}(\sigma'(KY)) (Y^\top \otimes I)$$

(here, we vectorized \( R, I \) is identity, and \( \otimes \) is the Kronecker product)

Q: What are the properties of \( J \)?
Example: Condition Numbers

\[ R(K, W) = W \sigma(KY) - C \]

- \( d = \frac{3}{n} = 1 \) input/output features
- \( s = 100 \) examples \( \sim \mathcal{U}([-1, 1]^d) \)
- \( m = \{8, 16, 32\} \) width of network
- \( \sigma = \tanh \)
- \( K, W \sim \mathcal{N}(0, 1) \)

Discussion:
- problem is ill-posed \( \leadsto \) regularize!
- \( \text{cond}(J) \) large \( \leadsto \) smart LinAlg
- how about single/half precision?
- NNLS solvers will not be effective
- need better initialization / method
Conclusion
course launched Spring 18 at Emory and UBC
slides + simple MATLAB codes available (pyTorch to come)
next offerings: Fall ’19 at UBC and Spring ’20 at Emory

check it out: https://github.com/IPAIOpen
Numerical Methods for Deep Learning

An (almost perfectly) true statement

\[
\text{backpropagation} + \text{GPU} + \begin{cases} \text{TensorFlow} \\ \text{Caffe} \\ \text{Torch} \\ \vdots \end{cases} \Rightarrow \text{success}
\]

So, why study numeric methods for deep learning?

**Transfer Learning**
- DL is similar to path planning, optimal control, differential equations . . .

**Do More With Less**
- Better modeling and algorithms \(\rightsquigarrow\) process more data, use less resources
- How about 3D images and videos?

**Power Of Abstraction**
- Use continuous interpretation to design/relate architectures
Σ: Numerical Analysis of Deep Neural Networks

- **Case 1: Invertibility**
  - often but not always important
  - it does not come for free

- **Case 2: Time integrators**
  - conserving physical quantities can simplify numerics

- **Case 3: Discretize-then-Optimize**
  - Neural ODE: need high accuracy to obtain good gradients
  - Disc→Diff: can be more efficient/predictable

- **Case 4: Ill-conditioning**
  - even simple learning problems can be ill-posed
  - need more analysis, especially in low-precisions

There are a lot of challenges in ML for computational and applied mathematicians