A Numerical Analysis Perspective on Deep Neural Networks

Machine Learning for Physics and the Physics of Learning

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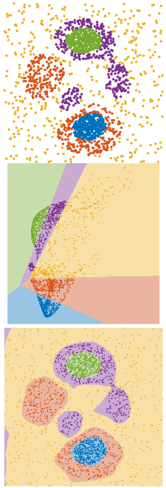
Agenda: Numerical Analysis of Deep Neural Networks

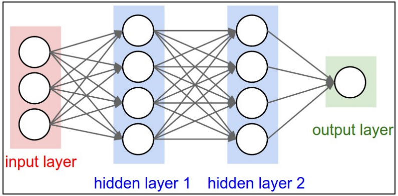
- **Notation: Deep Learning**
- **Case 1: Invertibility**
- **Case 2: Time Integrators**
  - Example: higher order or conservative?
- **Case 3: Discretize-then-Optimize**
  - Example: Neural ODEs
- **Case 4: Ill-conditioning**
  - Example: Single layer neural network
- **Conclusion and Summary**



Key question: What can numerical analysts do in the age of ML?

Deep Learning

Deep Learning Revolution (?)

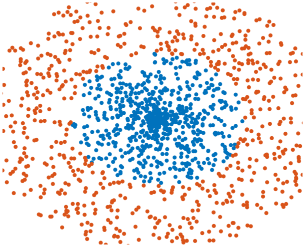


$$\begin{cases} \mathbf{Y}_{j+1} &= \sigma(\mathbf{K}_j\mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} &= \mathbf{Y}_j + \sigma(\mathbf{K}_j\mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} &= \mathbf{Y}_j + \sigma\left(\mathbf{K}_{j,2}\sigma(\mathbf{K}_{j,1}\mathbf{Y}_j + \mathbf{b}_{j,1}) + \mathbf{b}_{j,2}\right) \\ &\vdots \end{cases}$$

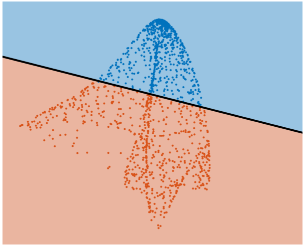
(Notation: $\mathbf{Y}_j$: features, $\mathbf{K}_j, \mathbf{b}_j$: weights, σ : activation)

- 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

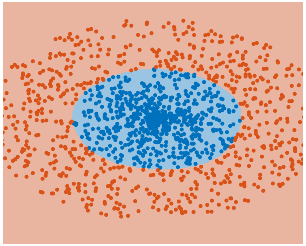
Optimal Control Framework for Deep Learning



training data, $\mathbf{Y}_0, \mathbf{C}$



prop. features, $\mathbf{Y}(T), \mathbf{C}$



classification result

Supervised Deep Learning Problem

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

$$\text{minimize}_{\boldsymbol{\theta},\mathbf{W},\boldsymbol{\mu}} \qquad \text{loss}[g(\mathbf{W}+\boldsymbol{\mu}), \mathbf{C}] + \text{regularizer}[\boldsymbol{\theta}, \mathbf{W}, \boldsymbol{\mu}]$$

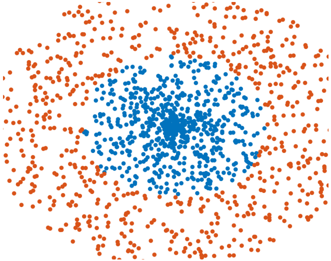
Deep Residual Neural Networks (simplified)

Award-winning forward propagation

$$\mathbf{Y}_{j+1} = \mathbf{Y}_j + h\mathbf{K}_{j,2}\sigma(\mathbf{K}_{j,1}\mathbf{Y}_j + \mathbf{b}_j), \quad \forall\, j = 0, 1, \ldots, N-1.$$

ResNet is forward Euler discretization of

$$\partial_t \mathbf{y}(t) = \mathbf{K}_2(t)\sigma\left(\mathbf{K}_1(t)\mathbf{y}(t) + \mathbf{b}(t)\right), \qquad \mathbf{y}(0) = \mathbf{y}_0.$$

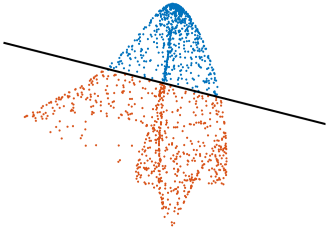


input features, $\mathbf{Y}_0$

Notation: $\boldsymbol{\theta}(t) = (\mathbf{K}_1(t), \mathbf{K}_2(t), \mathbf{b}(t))$ and

$$\partial_t \mathbf{y}(t) = f(\mathbf{y}, \boldsymbol{\theta}(t)), \quad \mathbf{y}(0) = \mathbf{y}_0$$

where $\quad f(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{K}_2(t)\sigma\left(\mathbf{K}_1(t)\mathbf{y}(t) + \mathbf{b}(t)\right).$



propagated features, $\mathbf{Y}_N$

K. He, X. Zhang, S. Ren, and J. Sun
Deep residual learning for image recognition.
IEEE Conf. on CVPR, 770–778, 2016.

(Some) Related Work

DNNs as (stochastic) Dynamical Systems

- **Weinan E**, *Proposal on ML via Dynamical Systems*, Commun. Math. Stat., 5(1), 2017.
- **E Haber, LR**, *Stable Architectures for DNNs*, Inverse Problems, 2017.
- **Q. Li, L. Chen, C. Tai, Weinan E**, *Maximum Principle Based Algorithms*, arXiv, 2017.
- **B. Wang, B. Yuan, Z. Shi, S. Osher**, *ResNets Ensemble via the Feynman-Kac Formalism*, arXiv, 2018.

Numerical Time Integrators

- **Y. Lu, A. Zhong, Q. Li, B. Dong**, *Beyond Finite Layer DNNs*, arXiv, 2017.
- **B. Chang, L. Meng, E. Haber, LR, D. Begert, E. Holtham**, *Reversible architectures for DNNs*, AAAI, 2018.
- **T. Chen, Y. Rubanova, J. Bettencourt, D. Duvenaud**, *Neural ODEs*, NeurIPS, 2018.
- **E. Haber, K. Lensink, E. Treister, LR**, *IMEXnet: Forward Stable DNN*. ICML, 2019.

Optimal Control

- **S. Günther, LR, J.B. Schroder, E.C. Cyr, N.R. Gauger**, *Layer-parallel training of ResNets*, arXiv, 2018.
- **A. Gholami, K. Keutzer, G. Biros**, *ANODE: Unconditionally Accurate Memory-Efficient Gradients for Neural ODEs*, arXiv, 2019.
- **T. Zhang, Z. Yao, A. Gholami, K. Keutzer, J. Gonzalez, G. Biros, M. Mahoney**, *ANODEV2: A Coupled Neural ODE Evolution Framework*, arXiv, 2019.

PDE-motivated Approaches

- **E. Haber, LR, E. Holtham**, *Learning across scales - Multiscale CNNs*, AAAI, 2018.
- **LR, E. Haber**, *DNNs motivated by PDEs*, arXiv, 2018.

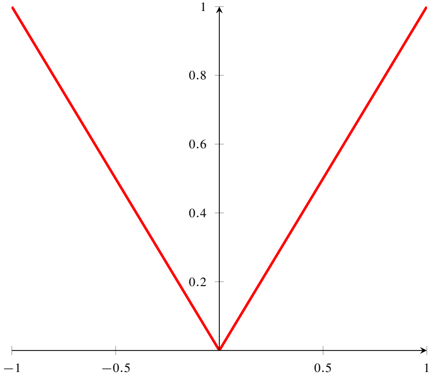
Numerical Methods for Deep Learning

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?

A Simple Example



Predict the output of:

```
x = param(0.0)
f = abs(x)
Tracker.back!(f)
Tracker.grad(x)
```

Case 1: Reversibility

Reversibility: Continuous vs. Discrete

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

Idea 1: ResNet

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

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

Idea 2: Hamiltonian NN

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

- discretize: Verlet, 32 time steps
- no padding, trivial inverse

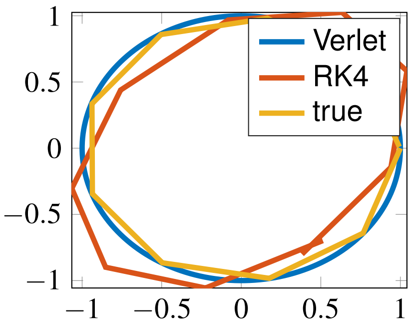
Case 2: Black-box

Example: High-order vs. Symplectic?

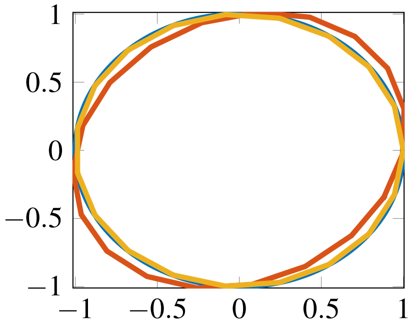
Consider linear harmonic oscillator

$$\partial_t \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \quad \text{associated with} \quad H(p,q) = p^2 + q^2$$

h large



h small



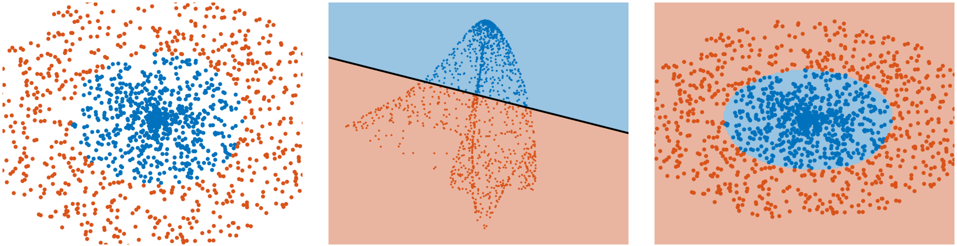
Use the right (in this case lower-order) integrators $\rightsquigarrow$ more bang for the buck!

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



training data, $\mathbf{Y}_0, \mathbf{C}$ prop. features, $\mathbf{Y}(T), \mathbf{C}$ classification result

Supervised Deep Learning Problem

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

$$\text{minimize}_{\boldsymbol{\theta},\mathbf{W},\boldsymbol{\mu}} \quad \text{loss}[g(\mathbf{W}+\boldsymbol{\mu}), \mathbf{C}] + \text{regularizer}[\boldsymbol{\theta}, \mathbf{W}, \boldsymbol{\mu}]$$

Optimal Control Background: Diff→Disc vs. Disc→Diff

$$\begin{aligned} \text{minimize}_{\boldsymbol{\theta},\mathbf{W},\boldsymbol{\mu}} \quad & \text{loss}[g(\mathbf{W}\mathbf{Y}(T)+\boldsymbol{\mu}),\mathbf{C}] + \text{regularizer}[\boldsymbol{\theta},\mathbf{W},\boldsymbol{\mu}] \\ \text{subject to} \quad & \partial_t \mathbf{Y}(t) = f\left(\mathbf{Y}(t),\boldsymbol{\theta}(t)\right), \ \mathbf{Y}(0)=\mathbf{Y}_0. \end{aligned}$$

- **First-Differentiate-then-Discretize (Diff→Disc)**
  - Keep $\boldsymbol{\theta}, \mathbf{b}, \mathbf{Y}$ continuous in time
  - Euler-Lagrange-Equations $\rightsquigarrow$ 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 $\boldsymbol{\theta}, \mathbf{b}, \mathbf{Y}$ 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.
NeurIPS, 2018.

A Gholami, K Keutzer, G Biros
ANODE: Unconditionally Accurate Memory-Efficient Gradients for Neural ODEs.
arXiv:1902.10298

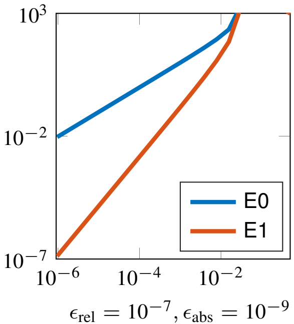
Example: Gradient Test Disc→Diff

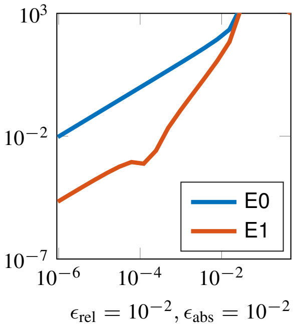
Goal: Find weights of neural network $F(\mathbf{u}, \theta)$ such that

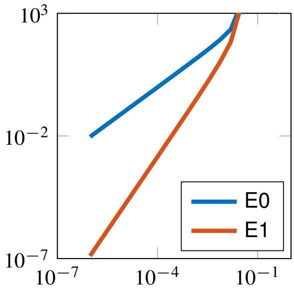
$$\partial_t \mathbf{u} = F(\mathbf{u}, \theta), \quad \mathbf{u}(0) = \mathbf{u}_0$$

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

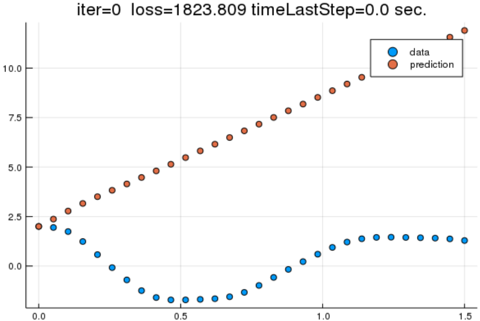
Question: How does accuracy of ODE solvers impact the quality of gradient?

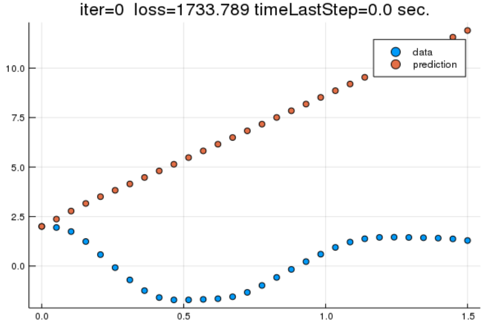






C Rackauckas, M Innes, Y Ma, J Bettencourt, L White, V Dixit
DiffEqFlux.jl - A Julia Library for Neural Differential Equations.
arXiv:1902.02376

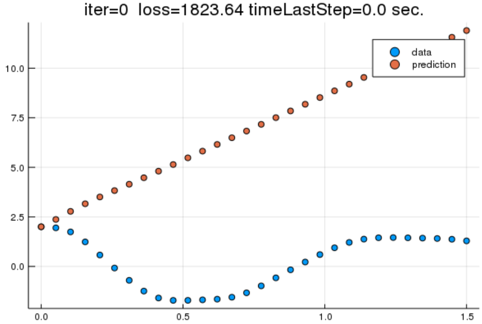


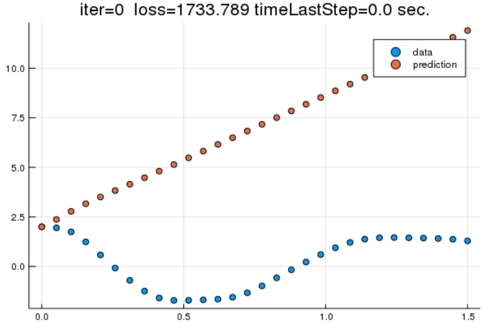


Neural ODE, $\epsilon_{\text{rel}} = 10^{-7}, \epsilon_{\text{abs}} = 10^{-9}$

Disc$\rightarrow$Diff, RK4, 30 steps

Training: ADAM with default setting, same initialization





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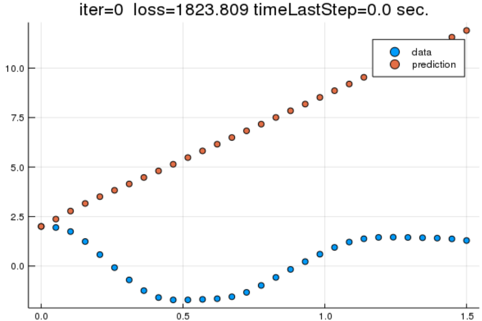
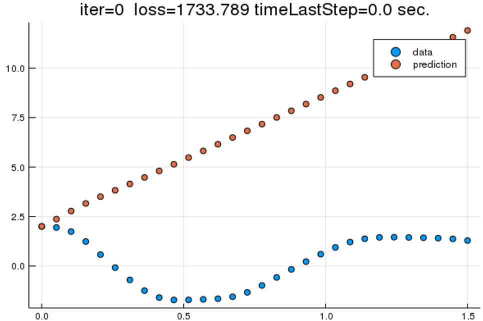




Neural ODE, $\epsilon_{\text{rel}} = 10^{-2}, \epsilon_{\text{abs}} = 10^{-2}$

Disc→Diff, RK4, 30 steps

Training: ADAM with default setting, same initialization

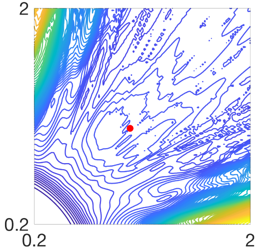
Impact of Network Architecture on Optimization - 1

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

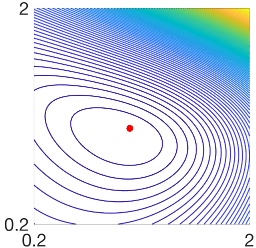
where $\mathbf{C} = \mathbf{Y}_{200}(1,1)$, $\mathbf{Y}_0 \sim \mathcal{N}(0,1)$, and

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

loss, $N = 5$

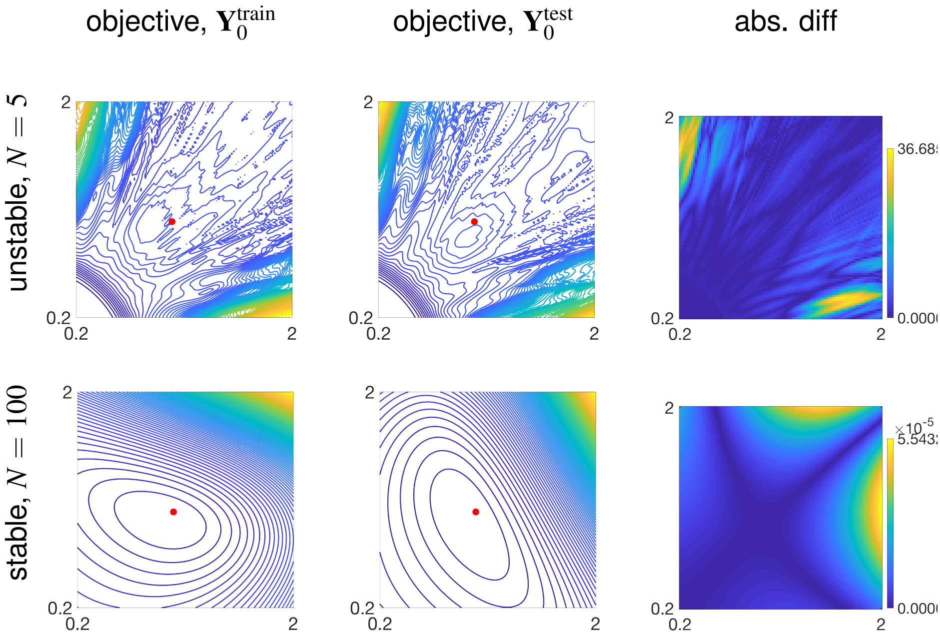


loss, $N = 100$



Next: Compare examples for different inputs $\sim$ generalization

Impact of Network Architecture on Optimization - 2



Case 4: Conditioning

Conditioning of the Learning Problem

Consider the regression problem with a single neural network layer

$$\min_{\mathbf{W},\mathbf{K}} \frac{1}{2s}\|\mathbf{R}(\mathbf{W},\mathbf{K})\|^2, \quad \text{where} \quad \mathbf{R}(\mathbf{W},\mathbf{K}) = \mathbf{W}\sigma(\mathbf{K}\mathbf{Y}) - \mathbf{C}$$

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

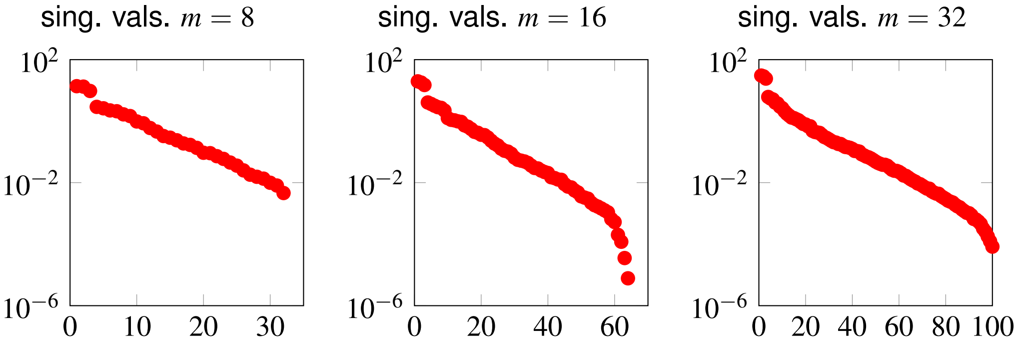
The problem above is a non-linear least squares problem (NNLS). Common to look at the Jacobian of $\mathbf{r}$, i.e., $\mathbf{J} = [\mathbf{J}_\mathbf{W}\ \mathbf{J}_\mathbf{K}]$ where

$$\mathbf{J}_\mathbf{W} = \sigma(\mathbf{K}\mathbf{Y})^\top \otimes \mathbf{I}, \quad \text{and} \quad \mathbf{J}_\mathbf{K} = (\mathbf{I}\otimes\mathbf{W})\,\mathrm{diag}(\sigma'(\mathbf{K}\mathbf{Y}))\,(\mathbf{Y}^\top \otimes \mathbf{I})$$

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

Q: What are the properties of $\mathbf{J}$?

Example: Condition Numbers



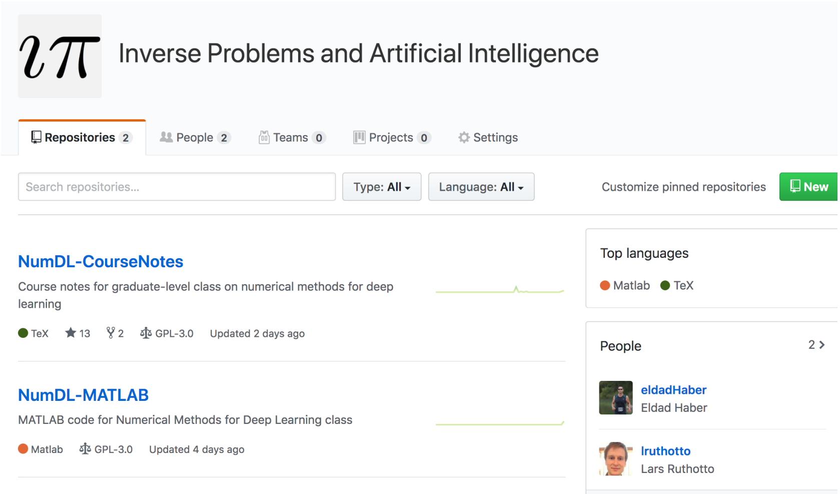
$$\mathbf{R}(\mathbf{K}, \mathbf{W}) = \mathbf{W}\sigma(\mathbf{KY}) - \mathbf{C}$$

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

Discussion:

- problem is ill-posed $\rightsquigarrow$ regularize!
- $\mathrm{cond}(\mathbf{J})$ large $\rightsquigarrow$ 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

$$\text{backpropagation} + \text{GPU} + \left\{ \begin{array}{c} \text{TensorFlow} \\ \text{Caffe} \\ \text{Torch} \\ \vdots \end{array} \right. \Rightarrow \text{success}$$

So, why study numeric methods for deep learning?

Transfer Learning

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

Do More With Less

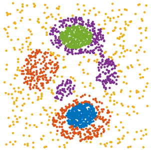
- Better modeling and algorithms $\rightsquigarrow$ process more data, use less resources
- How about 3D images and videos?

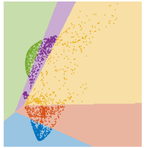
Power Of Abstraction

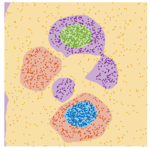
- Use continuous interpretation to design/relate architectures

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