KU LEUVEN

Avoiding local minima in Deep Learning: a nonlinear optimal control approach

Master's Thesis defence

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23 June 2021

0 Outline

1 Outline

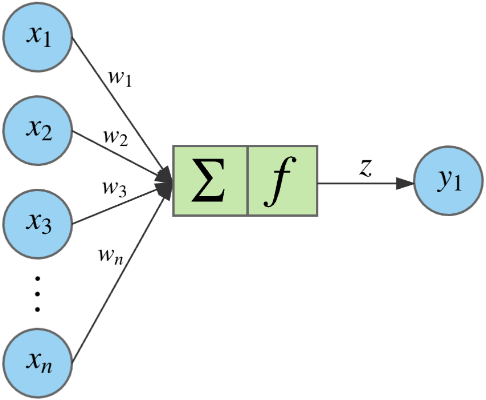
1 Machine Learning and Neural Networks

- Machine Learning
  - Subset of Artificial Intelligence
  - Learn relationships in data sets
  - Input features $\rightarrow$ Target output
  - Learn on Training Data, Apply to Test Data

- Artificial Neural Networks
  - Popular machine learning model
  - Very expressive
  - Suited for large data sets
  - Can model complex nonlinear relationships

- Focus on deep feedforward neural networks in this thesis

1 Neuron



Single Neuron - McCulloch–Pitts model [A. Dertat 2017].

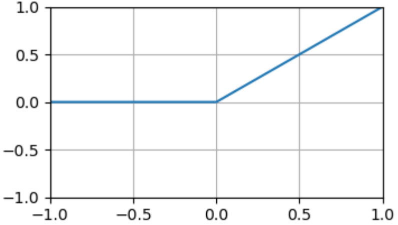
1 Activation Function

- McCulloch–Pitts neuron model

$$y = \sigma(w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$

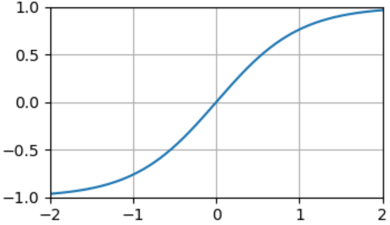
Rectified Linear Unit (ReLU)

$$\sigma(x) = x^+ = \max(0, x)$$

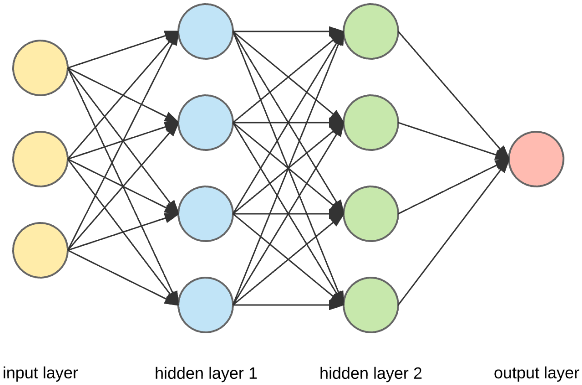


Hyperbolic Tangent (tanh)

$$\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \tanh(x)$$



1 Neural Network



Feedforward Deep Neural Network [A. Dertat 2017].

1 Neural Network Training

- Function definition of network with L layers

$$f_W(x) = W_L\sigma(W_{L-1}\sigma(...W_1\sigma(W_0x)...))$$

- Function application & matrix multiplication
- Training = unconstrained optimization problem over training set:

$$\underset{W}{\text{minimize}} \quad C(W) = \frac{1}{N}\sum_{j=0}^{N} l(f_W(x_j) - y_j)$$

- $f_W(x_j)$: prediction of network for x_j
- compare network prediction to target output y_j
- Minimize average loss for loss function $l(\cdot, \cdot)$
- Proxy for performance metric P defined over the test set

1 Gradient Descent

- Training problem is solved using Gradient Descent:

$$W_{k+1} = W_k - \eta_k \nabla C(W_k)$$

  - η_k: step size a.k.a. "learning rate"
  - Gradient is calculated using Backpropagation algorithm
- Cumbersome to calculate full gradient for large datasets
  - $\Rightarrow$ Approximate gradient over "mini-batch" of datapoints
  - Stochastic Gradient Descent
- Current best algorithms use adaptive learning rates
  - AdaGrad, Rmsprop, ADAM, ...
- Halting based on "early stopping" criterion
  - $\Leftrightarrow$ pure optimization halts on small gradient

1 Local Minima

- Gradient Descent is a locally converging algorithm
- Cost function will have highly non-convex surface
- Possibly uncountably many local minima
- Finding global minimum is intractible
  - "bad" local minima: have comparatively high cost value
  - Hard to define exactly
- " ... but experts now suspect that, for sufficiently large neural networks, most local minima have a low cost function value ... " [Goodfellow et. al. 2016]
- Other optimization challenges
  - Ill-conditioned Hessian matrix
  - Exploding/Vanishing gradients
  - "Dying" ReLU

1 Neural networks as Dynamical Systems

$$
\begin{aligned}
z_0 &= x \\
z_{k+1} &= \sigma_k(W_k z_k), \quad k = 0, ..., L \\
f_W(x) &= z_{L+1}
\end{aligned}
$$

- Neural networks are dynamical systems
  - Each layer is a state
- Optimal Control objective cost function:

$$E(\theta) = \sum_{s=1}^{L-1} g^s(a^s, \theta^s) + h(a^L)$$

- NN training only considers terminal cost

1 Training as Optimal Control Problem

$$
\begin{aligned}
\underset{W,z}{\text{minimize}} \quad & \sum_{j=0}^{n} ||\sigma_L(W_L z_L) - y_j||_2^2 \\
\text{subject to} \quad & z_{1,j} = \sigma_0(W_0, x_j), \qquad\qquad j = 1, \ldots, n \\
& z_{k+1,j} = \sigma_k(W_k z_{k,j}), \qquad k = 1, \ldots, L-1, j = 1, \ldots, n
\end{aligned}
$$

Optimal Control	Neural Network
decision variables	weight parameters
state variables	(neuron) activation
stage	layer

1 Goal of the thesis: Solving the OCP

- Optimal control theory: two direct approaches
- Sequential Approach
  - Direct Single Shooting
  - Eliminate states using dynamics
  - Reduces to unconstrained problem
  - Small, highly nonlinear NLP
  - Equivalent to backpropagation for NN [Dreyfus et al. 1990]
- Simultaneous Approach
  - Direct Multiple Shooting
  - Keep states as variables
  - Large, structured problem
  - Novel approach for NN
  - Topic of this thesis

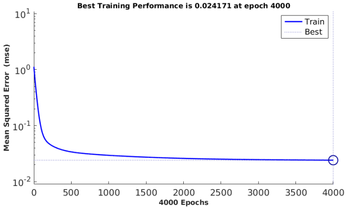
2 Outline

2 Multiple Shooting in MATLAB

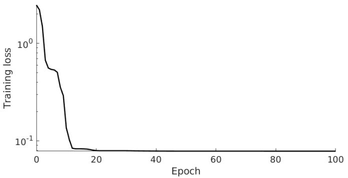
- Multiple shooting increases dimension of problem
  - For network of width W, depth L, N datapoints:
  - Single shooting: $\mathcal{O}(W^2L)$ variables
  - Multiple shooting: $\mathcal{O}(W^2L + WLN)$ variables
- Exploration of the multiple shooting approach
  - Implemented in MATLAB
  - Constrained NLP solved by `fmincon`
  - Comparison with `nntoolbox`
  - Training algorithm is `traingd`

	tanh		ReLU	
Algorithm	avg tr MSE	avg run time	avg tr MSE	avg run time
Gradient Descent	0.0299	1.577s	0.0274	1.480s
Multiple Shooting	0.2350	23.82s	0.2111	115.8s

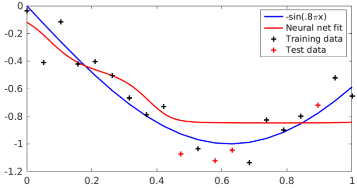
2 Gradient Descent vs Multiple Shooting



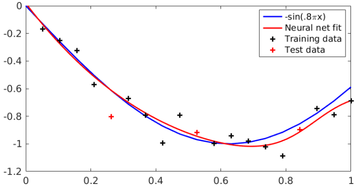
Gradient Descent Training History



Multiple Shooting Training History



NN fit with Gradient Descent



NN fit with Multiple Shooting

3 Outline

3 Augmented Lagrangian Method

- `fmincon` not well suited for this problem
  - $\Rightarrow$ implement specialized algorithm
  - exploit structure in problem
- Augmented Lagrangian Method
  - Algorithmic framework for constrained NLP
  - Similar to penalty method
- Constrained NLP:

$$\begin{aligned} \min_{u} \quad & f(u) \\ \text{s.t.} \quad & h(u) = 0 \end{aligned}$$

3 Classical Augmented Lagrangian Method

- β-augmented Lagrangian:

$$\min_u \max_\lambda \mathcal{L}_\beta(u, \lambda) = f(u) + \langle \lambda, h(u) \rangle + \frac{\beta}{2} ||h(u)||_2^2$$

- Converges to local minimizer of constrained problem if
  - β is large
  - λ is close to λ^*
- Algorithm solves series of unconstrained problems

$$u_{k+1} = \operatorname*{argmin}_u \mathcal{L}_{\beta_k}(u, \lambda_k)$$
$$\lambda_{k+1} = \lambda_k + \sigma_k h(u_{k+1})$$

3 Classical Augmented Lagrangian Method

- Penalty parameter increases or is kept the same in each iteration
  - depends on constraint violation
- Stopping criterion:

$$||h(u_k)|| \leq \tau_1 \text{ and } ||\nabla_u \mathcal{L}_{\beta_k}(u_k, \lambda_k)|| \leq \tau_2$$

- NN training has nonconvex f with nonlinear constraints, inexact solution to inner problem
- Textbook theory requires strong assumptions, exact solution
- Sahin et al. (2019) proposes alternative framework:
  - Promises $\tilde{\mathcal{O}}(1/\epsilon^3)$ calls to first-order solver
  - Theoretical estimates on convergence

3 β-Augmented Lagrangian

$$\begin{aligned} \underset{W,z}{\text{minimize}} \quad & \sum_{j=0}^{n} ||\sigma_L(W_L z_L) - y_j||_2^2 & & \min_u \quad \frac{1}{2}||F(u)||_2^2 \\ \text{subject to} \quad & z_{1,j} = \sigma_0(W_0, x_j) & \Leftrightarrow \quad & \text{s. t.} \quad h(u) = 0 \\ & z_{k+1,j} = \sigma_k(W_k z_{k,j}) & & \end{aligned}$$

- $u = \{W, z\}$ collects weight and state variables in single vector
- minimizing β-Augmented Lagrangian is LS problem

$$\begin{aligned} \underset{u}{\text{argmin}} \quad \mathcal{L}_\beta(u, \lambda) &= \frac{1}{2}||F(u)||_2^2 + \langle \lambda, h(u) \rangle + \frac{\beta}{2}||h(u)||_2^2 \\ &= \frac{\beta}{2} \left|\left| \begin{bmatrix} F(u)/\sqrt{\beta} \\ h(u) + \lambda/\beta \end{bmatrix} \right|\right|_2^2 \end{aligned} \tag{1}$$

3 Applied Augmented Lagrangian Method

Input: Initial weights vector W, penalty parameter β, stopping tolerance τ, input-target pairs $(x_i, y_i), i = 1, \ldots, n$

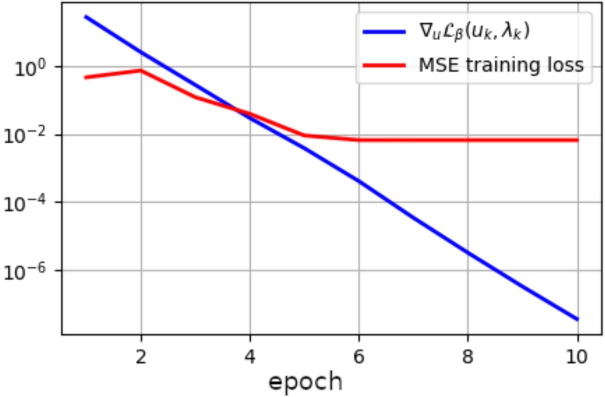
Initialization $u_0 = \{W, f_W(x)\}, \lambda_0 \in \mathcal{N}(0,1)$; *Initialize state*

for $k = 0,1,\ldots$ **do**

- $\eta_k = 1/\beta^k$; *Update tolerance*
- find u_{k+1} such that
  - $||\nabla_{u_k} \mathcal{L}_{\beta^k}(u_k, \lambda_k)|| \leq \eta_k$; *Approx. primal solution*
- $\sigma_{k+1} = \min\left(\frac{||h(u_0)|| \log^2 2}{||h(u_{k+1})|| k \log^2(k+1)}, 1\right)$; *Update dual step size*
- $\lambda_{k+1} = \lambda_k + \sigma_{k+1} h(u_{k+1})$; *Update dual variables*
- If $||\nabla_{u_{k+1}} \mathcal{L}_{\beta^k}(u_{k+1}, \lambda_k)|| + ||h(u_{k+1})|| < \tau$:
  - break ; *Stopping Criterion*

end

3 Convergence



Typical convergence behaviour of Algorithm 1

3 Jacobian

- Inner problem is nonlinear least squares
  - Solved using Trust Region Reflective method
  - `scipy.optimize.least_squares`
  - Works best with analytical solution for Jacobian matrix
- Jacobian matrix
  - Dimension $\approx (DWN \times DW(N+W))$
  - Sparse, banded structure
- Numerical Verification
  - Automatic differentiation
  - `AlgoPy` library
  - Confirms correctness of analytical solution

3 Jacobian Derivation

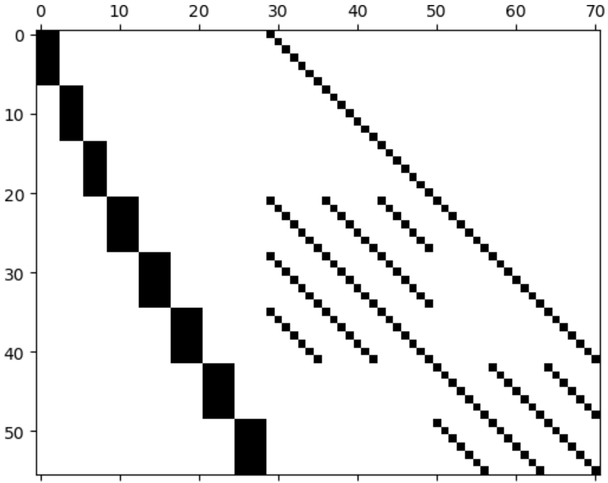
$$M_\beta(u,\lambda) := \begin{bmatrix} F(u)/\sqrt{\beta} \\ h(u)+\lambda/\beta \end{bmatrix}, J_{M_\beta} := \begin{bmatrix} \frac{\partial M_\beta}{\partial u_1} & \frac{\partial M_\beta}{\partial u_2} & \dots & \frac{\partial M_\beta}{\partial u_n} \end{bmatrix}$$

$$\frac{\partial M_\beta}{\partial W_k} = -z_{k,j}\sigma_k'(W_k z_{k,j}) \qquad , j=1,\dots,n, k=0,\dots,L$$

$$\frac{\partial M_\beta}{\partial z_k} = \begin{bmatrix} 1 \\ -W_k\sigma_k'(W_k z_k) \end{bmatrix} \qquad , k=1,\dots,L$$

- W_k, z_k are matrices $\rightarrow$ derivatives are tensors
- W_k, z_k vectorized $\rightarrow$ derivatives are block matrices

3 Visualisation of Jacobian



Network has 2 layers, 3 nodes/layer, 2 inputs, 2 outputs and 7 datapoints.

4 Outline

4 Test setup

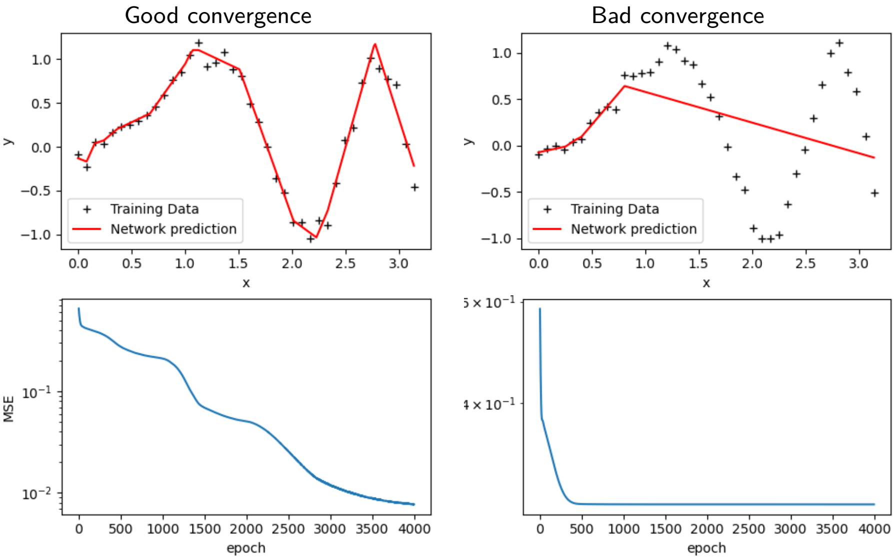
- Regression problem
  - Approximate:
$$y = \sin(x^2), x \in [0, \pi]$$
  - Using fully connected feedforward network
- ADAM optimizer for comparison
  - ADaptive Moment Estimation
  - Robust, industry standard optimizer
  - Stochastic gradient descent with adaptive learning rate
- 20 training runs per test configuration
  - Same initial conditions each run
  - Same data, noise, weight initialization
  - Gradient estimation over full dataset in each epoch
- Intel® Core™ i5-7300HQ CPU 2.50GHz with 8Gi RAM

4 Halting criterion

- Nonconvex Optimization
  - Local minimizer of cost function: small gradient
- Machine Learning
  - "Early Stopping"
  - Based on performance metric on validation set
- Time based, epoch based halting
- Goal of thesis: local minima $\Rightarrow$ Halt at local minimum
  - ADAM: 10 epochs without any improvement to cost function
  - ALM: 1 epoch without significant improvement:

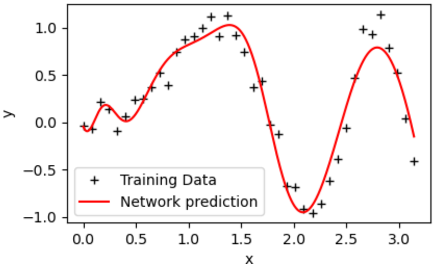
$$(1+\epsilon)C(W_{k+1}) > C(W_k)$$

  - Halting based on gradient
  - Discards influence of states, constraint violation

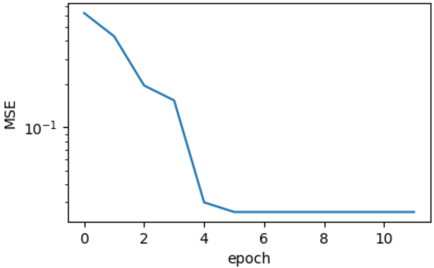


Examples of convergence behaviour of ADAM optimizer for a network using ReLU activation and 40 data points. The network has 2 hidden layers of 16 nodes.

Good convergence

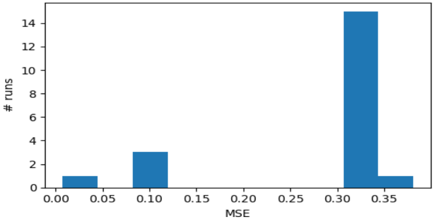


Convergence History

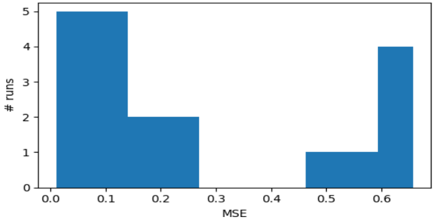


Example of convergence behaviour of ALM optimizer for network using $tanh$ activation and 40 data points. The network has 2 hidden layers of 8 nodes.

ADAM Histogram



ALM History



MSE of batch using 40 data points and ReLU activation function

4 Results for network with $\tanh$ activation

$\sigma(\cdot) = \tanh(\cdot)$

	N	avg MSE	best MSE	time(s)	avg epochs	converging runs / 20 runs
ADAM	10	$2.09e^{-2}$	$1.20e^{-11}$	18.7	3790	17
ALM		$2.10e^{-1}$	$1.59e^{-1}$	1.85	6.38	16
ADAM	20	$1.25e^{-2}$	$9.84e^{-4}$	19.8	3960	17
ALM		$5.87e^{-2}$	$7.69e^{-3}$	8.06	7.50	20
ADAM	40	$2.56e^{-2}$	$7.58e^{-3}$	19.2	3920	15
ALM		$1.61e^{-2}$	$7.90e^{-3}$	11.6	6.90	20

Fully connected feedforward network, 2 hidden layers, 8 nodes / layer

4 Results for network with ReLU activation

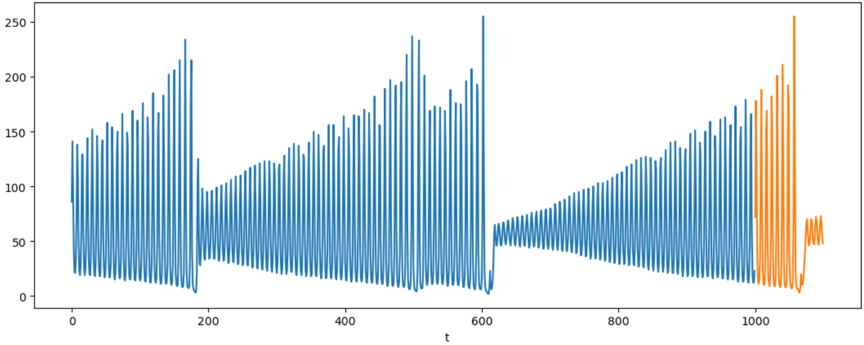
$$\sigma(\cdot) = \max(\cdot, 0)$$

	N	avg MSE	best MSE	time(s)	avg epochs	$\frac{\text{converging runs}}{\text{20 runs}}$
ADAM	20	$1.22e^{-1}$	$3.15e^{-3}$	30.3	3500	5
ALM		$1.63e^{-1}$	$1.08e^{-2}$	4.41	5.47	15
ADAM	40	$6.28e^{-2}$	$8.85e^{-3}$	22.4	2690	5
ALM		$9.89e^{-2}$	$1.37e^{-2}$	8.09	5.11	18
ADAM	80	$7.61e^{-2}$	$7.64e^{-3}$	29.9	3150	4
ALM		$1.02e^{-1}$	$1.03e^{-2}$	25.3	4.21	14

Fully connected feedforward network, 2 hidden layers, 16 nodes / layer

5 Outline

5 Santa Fe timeseries data



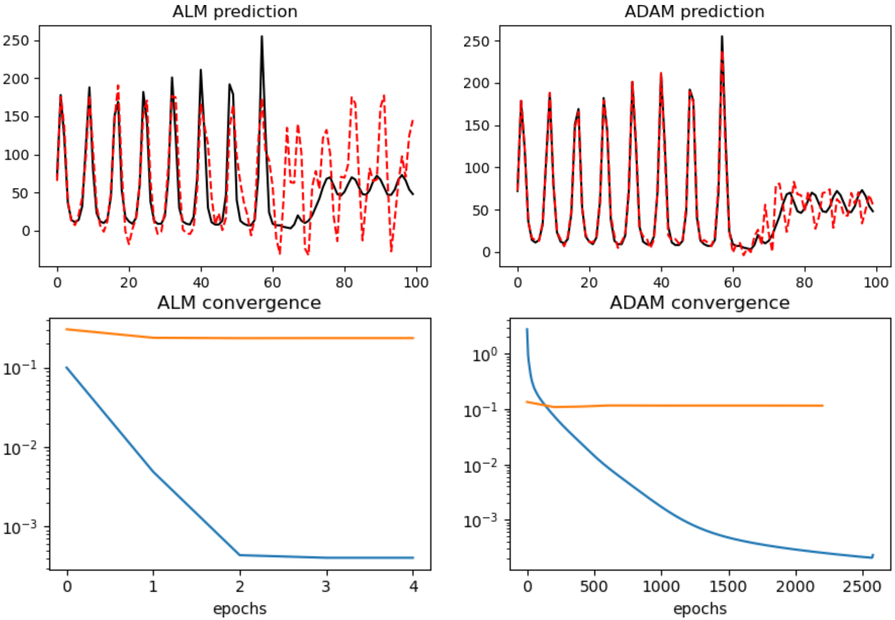
- Far-infrared laser fluctuations, coupled nonlinear ODEs
- 1000 data points training, 100 points test data

5 Test Setup

- Approximate using recurrent neural network:

$$\hat{y}_{k+1} = f_W\left(\begin{bmatrix}\hat{y}_k & \hat{y}_{k-1} & \cdots & \hat{y}_{k-p}\end{bmatrix}^T\right)$$

- Previous predictions used to make next prediction
- $\tanh$ activation, 80 inputs, 1 layer, 48 nodes
- 920 training pairs, 600 in training set, 320 in validation set
- 4 training runs per algorithm, same initial conditions
- Intel® Core™ i5-7300HQ CPU 2.50GHz with 8Gi RAM



Test MSE in blue, Validation MSE in orange

5 Timeseries data test results

Algo	avg MSE	best MSE	avg pred MSE	best pred MSE	epochs	time
ALM	$3.712e^{-4}$	$2.779e^{-4}$	$1.070e^{0}$	$8.288e^{-1}$	5	1201s
ADAM	$2.517e^{-4}$	$2.329e^{-4}$	$2.016e^{-1}$	$9.100e^{-2}$	2353	20.9s

- ALM is very slow: 20min on avg, compared to 20s for ADAM
- Similar performance for training data, ADAM much better on test data
- Most calls to jacobian are in first epochs:

Epoch	1	2	3	4	5
#evals	42.25	12.75	17.0	3.0	2.0

Average number of Jacobian evaluations per epoch

6 Outline

6 Conclusion

- Novel perspective on neural network training using control theory
  - Single shooting: Backpropagation with Gradient Descent
  - Multiple shooting: new algorithm
  - MATLAB provides POC
- ALM framework implemented
  - Framework adapted from [Sahin et al. 2019]
  - Analytical solution for Jacobian
- Numerical Tests
  - ALM outperforms ADAM for network with many bad local minima
  - ALM becomes impractical for larger datasets
- Mini-batch approach for ALM can mitigate scaling problem
  - Cannot be easily adapted from stochastic gradient descent
  - Multiple shooting is harder to warm-start

7 References

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[5] M. F. Sahin, A. eftekhari, A. Alacaoglu, F. Latorre, and V. Cevher. An inexact augmented lagrangian framework for nonconvex optimization with nonlinear constraints. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 32. Curran Associates, Inc., 2019.

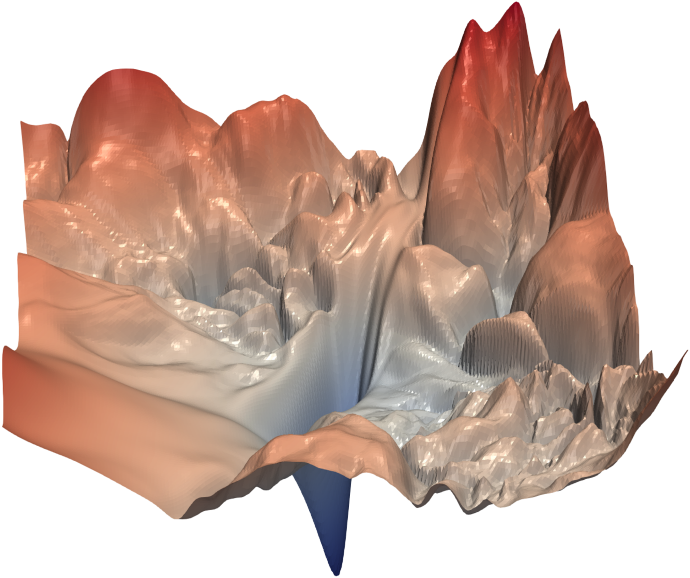
Questions

7 Comparison to Evens et al (2021)

- Different ALM framework
- Gauss-Newton approach for inner problem
- Not tested on larger datasets

7 Loss Functions

quadratic loss function	cross-entropy loss
$\|\|y^2 - \hat{y}^2\|\|$	$y\log(\hat{y}) + (1-y)\log(1-\hat{y})$
Mean Squared Error(MSE)	negative log-likelihood
Regression	Classification



Visualisation of loss surface of ResNet-56 [Li et al. 2018].