Reimplementation of the Classical Neural Ordinary Differential Equation Using Modern Computational Tools

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1. Introduction

Residual Neural Networks (RNN) provided a significant improvement on performance regarding deep layered neural networks. The performance gains were obtained from introducing residual elements applied to the ReLu operations within the hidden layer. This introduced robustness against the vanishing/exploding gradient problem that most classical neural networks face (Shorten, 2019).

However, there are some application of RNNs that still did not provide the ideal flexibility, in terms of training models for data involving time-series data. Since RNNs have discrete hidden layers and residual components to the ReLu operations performed to the hidden layers, it can interfere with learning dependencies which are sensitive to time (Walther et al., 2023).

A different class of neural networks look to satisfy the drawbacks that the previously mentioned network contain: Neural Ordinary Differential Equations (NeuralODE). The prime benefit that NeuralODEs provide is it is naturally suited for modelling continuos time data. In addition, it can provide computational flexibility in terms of configurability in forward-pass and backpropagation.

This paper's objective is to provide a brief literature review into works that have enabled the use of NeuralODEs and discuss the advantages and disadvantages related to the use of NeuralODEs. As many pieces of work focus on performance of NeuralODEs on time-series datasets, a short experiment involving the classification of the MNIST dataset using a proof-of-concept NeuralODE model is presented along with comparisons of performance with a typical proof-of-concept implementation of a residual neural network.

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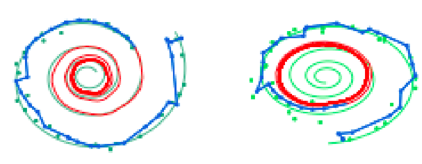
2. Related Works

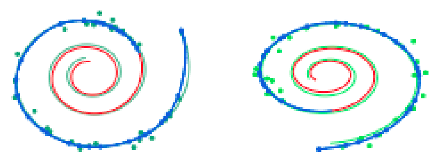
2.1. Article: Neural Ordinary Differential Equations

The concept of NeuralODEs have been discussed before the prescribed implementation by the paper *Neural Ordinary Differential Equations*. However, the primitive approach to the implementation of NeuralODEs had very large computational resource consumption, to the point where training the model on a substantial scale was not feasable. Since the NeuralODE consist of one continous layer with specific time steps for numerical integration (Derivation of Neural ODE vs. Classical NN is explained further below), performing backpropagation on NeuralODEs would be taking the gradient across each of the time steps. Since solving ODEs require small timesteps for accurate representation of the dynamics that is being learned, ordinary back-propagation become as resource dependant as a ResNet with hundreds of layers.

The major contribution for the respective paper is the adjoint sensitvity method, which allows for the back-propagation of NeuralODE block at near constant space-complexity (He et al., 2015). A comparison between a Recurrent Neural Network with 25 hidden-layers and the proposed NeuralODE architecture was presented with time-series data.



(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation

Figure 1. Comparison Between Recurrent Neural Network and NeuralODE on Time-Series Data (He et al., 2015)

2.2. Article: Augmented Neural ODE

The family of NeuralODEs have been extended from the previous contribution to make it more generalizable for existing framworks. The paper *Augmented Neural ODEs* proposes several postulates. The first assertion is that the classical implementation of NeuralODEs with the use of adjoint sensitivity method has limitations regarding representation of functions containing intersecting vector flows. The second assertion involves the existance of output space being rigid to the input space. The proposed solution to the problem was to introduce higher-dimensionality to the output space. This allows the ODE learning algorithm to lift points into additional dimension without having differential collisions (Dupont et al., 2019). The higher dimensionality mapping allowed for functions that were not representable by the classical NeuralODEs, available for training.

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\mathbf{h}(t)\\ \mathbf{a}(t)\end{bmatrix} = \mathbf{f}(\begin{bmatrix}\mathbf{h}(t)\\ \mathbf{a}(t)\end{bmatrix}, t), \qquad \begin{bmatrix}\mathbf{h}(0)\\ \mathbf{a}(0)\end{bmatrix} = \begin{bmatrix}\mathbf{x}\\ \mathbf{0}\end{bmatrix}$$

Figure 2. Activation Function Augmented with Higher Dimensionality (Dupont et al., 2019)

2.3. Article: How to Train Your Neural ODE

Beside the adjoint sensitivity method, developed by the authors of the paper *Neural Ordinary Differential Equations*, parallel efforts were also taken to address concerns of high resource usage of back-propagation of NeuralODEs. The paper *How To Train Your Neural ODE* proposes a method to reduce the computational complexity of back-propagation in time-series data predictions, by introducing regularization terms to the loss-function (Finlay et al., 2020). This allows for simpler solutions that can be sufficient while limiting NFEs (Number of Function Evaluation) to a reasonable number. The first regularization term penalty enourages particles to travel with one-dimensional translation by using optimal transport mapping, while the second regularization term enforces limitations of the vector-field Jacobian to provide force experienced to be as constant as possible. Such constraint of dynamics allow for simpler solutions with less computational complexities (Finlay et al., 2020).

2.4. A Comparative Derivation of Neural ODE

Conceptially, NeuralODEs are an extension of Residual Neural Networks. As mentioned previously, the difference between the respective family of neural networks is the continuos nature of NeuralODEs vs. the discrete nature of Residual Neural Networks. To show the difference, we will go from one forward-pass calculation of a Residual Neural Network to a NeuralODE.

Residual Neural Network

$$h_{t+1} = ReLu(W_t h_t + b_t) + h_t$$

The additional hidden layer term added after the activation function is the residual component of the Residual Neural Network.

Containing the activation function with standard notations, we can rewrite the equation as:

$$h_t = f(h_t, \theta_t) + h_t$$

We can convert the following equation to its differential form by expressing it in terms of its limits

$$h_{t+1} - h_t = f(h_t, \theta_t)$$

If we reduce the change between one hidden layer to the next to be infinitesimally small, we can express the equation as:

$$\frac{h_{t+\delta} - h_t}{\delta} = f(h_t, \theta_t)$$

Taking the limit of δ and setting it to zero provides us with the differential form of the equation:

$$\lim_{\delta \to 0} \frac{h_{t+\delta} - h_t}{\delta} = f(h_t, \theta_t)$$

$$\frac{\mathbf{dh_t}}{\mathbf{dt}} = \mathbf{f}(\mathbf{h_t}, \theta_\mathbf{t})$$

- Legend:
  - h_t: Hidden Layer t
  - W_t: Weight Matrix t
  - b_t: Bias Vector t
  - θ_t: Layer Parameters t
  - δ: Change in Hidden Layer (Infinitesimally Small)

3. Experiment

3.1. Defining the Experiment

An implementation of the Proof-of-Concept NeuralODE is developed. The workflow is modified from a typical NeuralODE implementation to accomodate visual classification of the MNIST dataset

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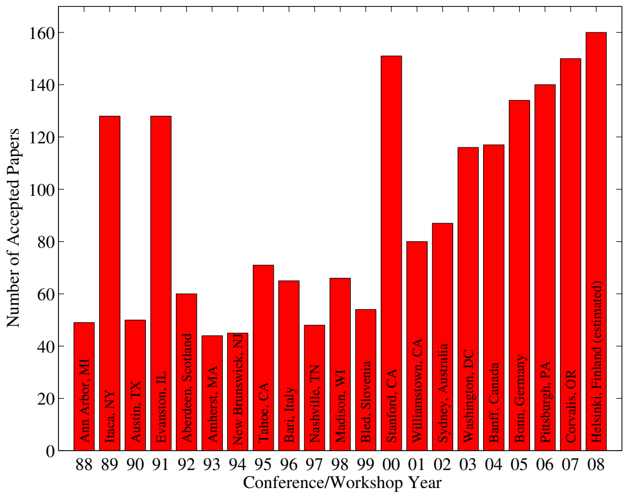

Figure 3. Historical locations and number of accepted papers for International Machine Learning Conferences (ICML 1993 – ICML 2008) and International Workshops on Machine Learning (ML 1988 – ML 1992). At the time this figure was produced, the number of accepted papers for ICML 2008 was unknown and instead estimated.

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[1] Footnotes should be complete sentences.

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Algorithm 1 Bubble Sort

Input: data x_i, size m
repeat
  Initialize $noChange = true$.
  for $i = 1$ **to** $m - 1$ **do**
    if $x_i > x_{i+1}$ **then**
      Swap x_i and x_{i+1}
      $noChange = false$
    end if
  end for
until $noChange$ is $true$

Table 1. Classification accuracies for naive Bayes and flexible Bayes on various data sets.

Data set	Naive	Flexible	Better?
Breast	95.9± 0.2	96.7± 0.2	$\surd$
Cleveland	83.3± 0.6	80.0± 0.6	$\times$
Glass2	61.9± 1.4	83.8± 0.7	$\surd$
Credit	74.8± 0.5	78.3± 0.6	
Horse	73.3± 0.9	69.7± 1.0	$\times$
Meta	67.1± 0.6	76.5± 0.5	$\surd$
Pima	75.1± 0.6	73.9± 0.5	
Vehicle	44.9± 0.6	61.5± 0.4	$\surd$

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References

Author, N. N. Suppressed for anonymity, 2021.

Duda, R. O., Hart, P. E., and Stork, D. G. *Pattern Classification*. John Wiley and Sons, 2nd edition, 2000.

Dupont, E., Doucet, A., and Teh, W. Y. Augmented neural odes. Number 32, 2019.

Finlay, C., Jacobsen, J.-H., Nurbekyan, L., and Oberman, A. M. How to train your neural ode. 2020.

He, K., Zhang, X., Ren, S., and Sun, J. Deep residual learning for image recognition. pp. 770–778. IEEE, 2015.

Kearns, M. J. *Computational Complexity of Machine Learning*. PhD thesis, Department of Computer Science, Harvard University, 1989.

Langley, P. Crafting papers on machine learning. In Langley, P. (ed.), *Proceedings of the 17th International Conference on Machine Learning (ICML 2000)*, pp. 1207–1216, Stanford, CA, 2000. Morgan Kaufmann.

Michalski, R. S., Carbonell, J. G., and Mitchell, T. M. (eds.). *Machine Learning: An Artificial Intelligence Approach, Vol. I*. Tioga, Palo Alto, CA, 1983.

Mitchell, T. M. The need for biases in learning generalizations. Technical report, Computer Science Department, Rutgers University, New Brunswick, MA, 1980.

Newell, A. and Rosenbloom, P. S. Mechanisms of skill acquisition and the law of practice. In Anderson, J. R. (ed.), *Cognitive Skills and Their Acquisition*, chapter 1, pp. 1–51. Lawrence Erlbaum Associates, Inc., Hillsdale, NJ, 1981.

Samuel, A. L. Some studies in machine learning using the game of checkers. *IBM Journal of Research and Development*, 3(3):211–229, 1959.

Shorten, C. Introduction to resnets, 2019. URL https://towardsdatascience.com/introduction-to-resnets-c0a830a288a4. Accessed: April 10th, 2023.

Walther, D., Viehweg, J., Haueisen, J., and Mader, P. A systematic comparison of deep learning methods for eeg time series analysis. *Frontiers in Neuroinformatics*, 17, 2023.

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