Master's Thesis 2026

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Title

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Title

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Abstract

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Keywords: *Physics Informed Neural Network, ..., ...*

Acknowledgements

List of Acronyms

EV electric vehicle. 1

FE finite element. 1

Li lithium. 1, 2

LiB lithium-ion battery. 1

NN neural network. 1, 2

PINN physics-informed neural network. 1

RMSE root-mean-squared error. 3

Contents

1 Introduction

1.1 Background

With an ever growing demand for convenient energy storage, the use of lithium-ion batteries (LiBs) in portable devices have skyrocketed over the last 30 years.

physics-informed neural network (PINN), electric vehicle (EV), lithium (Li)

Contents

- Why batteries? (Nobel prize 2019, a game changer in our modern lives, necessary for climate change)
- However, there are still problems, and the hunt for even more energy efficient batteries requires models to describe the physical properties of batteries.
- While models based on finite element (FE) can be used to simulate such systems to a high accuracy, they are often computationally costly[1]. Au contraire, data-driven models such as neural networks (NNs) are generally computationally cheap once trained, but could require large dataset to reach a satisfying accuracy.
- To address this, PINN offers a middle-ground approach, where physical knowledge of the system can be combined with the data-driven approach of NNs. Specifically, in PINNs solutions outside of the physically viable domain are heavily penalized,hopefully reducing the NN output close to the true solution. Although first introduced during the 90s, PINNs have gained popularity with the rise of modern computational power.

1.2 Aim and Scope

2
Theory

2.1 Overview of Batteries

- A battery's parts, anode, cathode, electrolyte. Why use Li in the first place?
- The general working principle: charging and discharging. Potential negative effects that need to be considered. Heat development, or other factors affecting performance of the cell.
- What equations are governing? (Thermodynamics, Mechanics, electric, chemical)
- The different scales: cell vs. module vs. pack. What can be inferred from the different scales? How does microscopic properties influence macroscopic ones and vice versa.
-

2.2 Neural Networks

- General overview of neural networks. Explain neurons, weights, bias, loss function, different types of NNs. RNN??
- Motivate the use of NNs w/ the Universal Approximation Theorem, i.e., the fact that a single layer perceptron NN can achieve universallity. Put differently, any continuous function can be modelled to the desired degree of accuracy with a NN (wiki-link).

2.3 Physics Informed Neural Networks

- Generally describe the setup we're dealing with Eq. 2.1 to 2.3.
- How to make NNs PINNs? Regularization term in the loss function that penalizes NN solutions that aren't physically viable.

$$f\left(\boldsymbol{x}, t, \frac{\partial u}{\partial \boldsymbol{x}}, \frac{\partial u}{\partial t}, \boldsymbol{\lambda}\right) = 0, \quad \boldsymbol{x} \in \Omega, t \in [0, \tau], \tag{2.1}$$

$$u(\boldsymbol{x},0) = h(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{2.2}$$

$$u(\boldsymbol{x},t) = g(\boldsymbol{x},t), \quad \boldsymbol{x} \in \partial\Omega, t \in [0, \tau]. \tag{2.3}$$

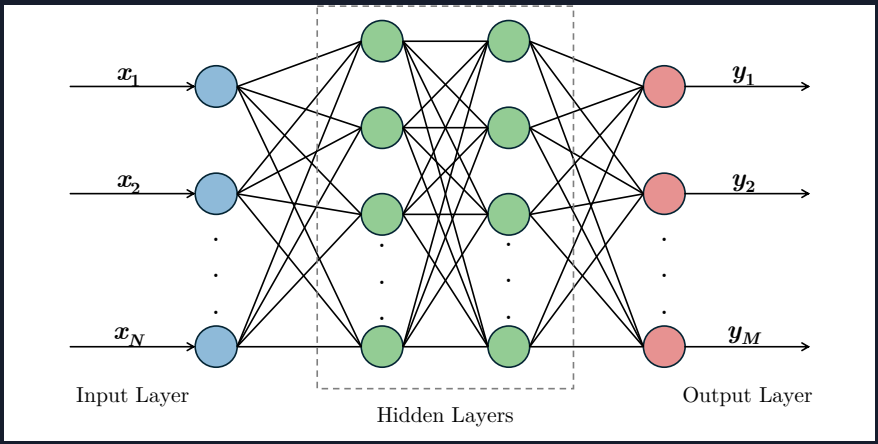

Fig 2.1: Schematic view of a neural network where each circle represents a single neuron. An input signal $\boldsymbol{X} = \{\boldsymbol{x}_i\}_{i=0}^{N}$ enters the model in the input layer, proceeds through the hidden layers, and exits from the output layer. This process produces an output $\boldsymbol{Y} = \{\boldsymbol{y}_i\}_{i=0}^{M}$, which can be interpreted as a prediction based on the input data.

Loss function, such as root-mean-squared error (RMSE).

3
Method

Here's the method

4
Results and Discussion

Here are the results

5
Conclusion

Here's the conclusion

Bibliography

[1] A. Asheri, M. Fathidoost, V. Glavas, S. Rezaei, and B.-X. Xu, "Data-driven multiscale simulation of solid-state batteries via machine learning," *Computational Materials Science*, vol. 226, p. 112 186, 2023, ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2023.112186. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0927025623001805.

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Appendix A: Extra Stuff

In Fig. A.1, ...

Fig A.1: hej