Using Neural Networks to Solve Differential Equations in Classical Mechanics

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MICHIGAN STATE UNIVERSITY

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

Outline of Presentation

- Introduction to the Module Topic
- Overview of the Module Contents
- How can this module be worked into a classical mechanics course?
- Conclusions and Future Works

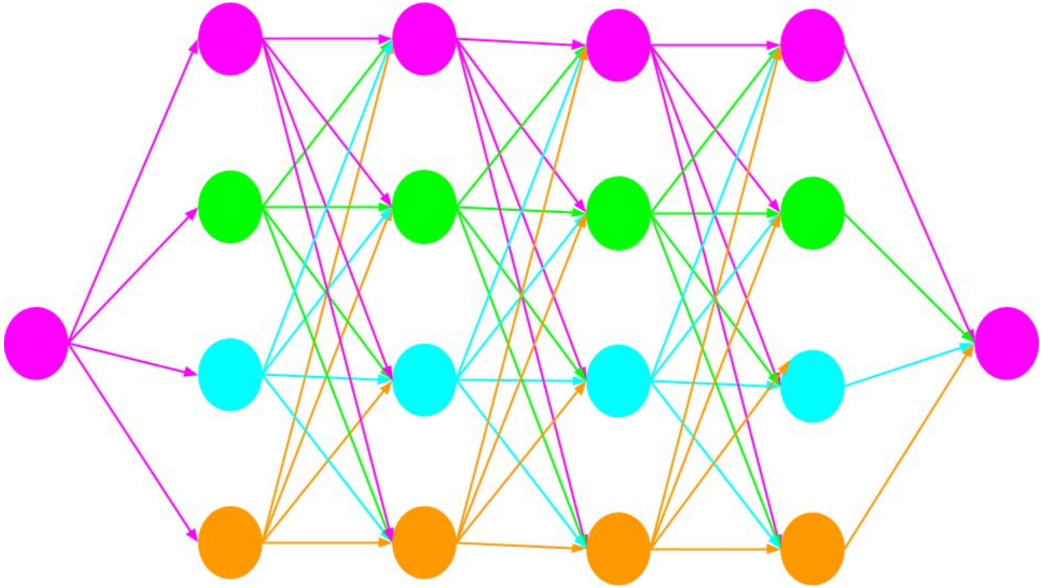
Introduction to the Module Topic

Why Incorporate Machine Learning in Classical Mechanics?

- Programming and machine learning are becoming increasingly integrated in many areas of physics
  - Important for undergraduates studying physics to be exposed to these areas
- Students in Classical Mechanics
  - Typically sophomores or juniors
  - Typically a physics majors only class

What is a Neural Network?

- Computational system that learns to match inputs to outputs by tuning a set of weights



Solving Differential Equations Numerically

- Method to solve second order differential equations by discretizing the inputs
    - Acceleration and position
- Euler's Method, Euler-Cromer Method, Velocity-Verlet Method

$$v_{i+1} = v_i + a_i \Delta t$$

$$y_{i+1} = y_i + v_{i+1} \Delta t$$

Solving Differential Equations with Neural Networks

- Assume we are given the acceleration for an object, want to model its position using a neural network

$$y_{trial}(t) = A + Bt + t^2 NN(W, t)$$
$$\mathrm{y}(0) = \mathrm{A},\ \mathrm{v}(0) = \mathrm{B}$$

- Requires taking derivatives of the neural network--automatic differentiation library called JAX

Overview of the Module Contents

Outline of Module

1. Solving Differential Equations Numerically
2. What is a Neural Network?
3. Solving Differential Equations with Neural Networks
4. Further Problems

Prerequisites:

- Python programming including NumPy and Matplotlib
- Newton's second law and related
- Derivatives, integrals, matrix-vector math

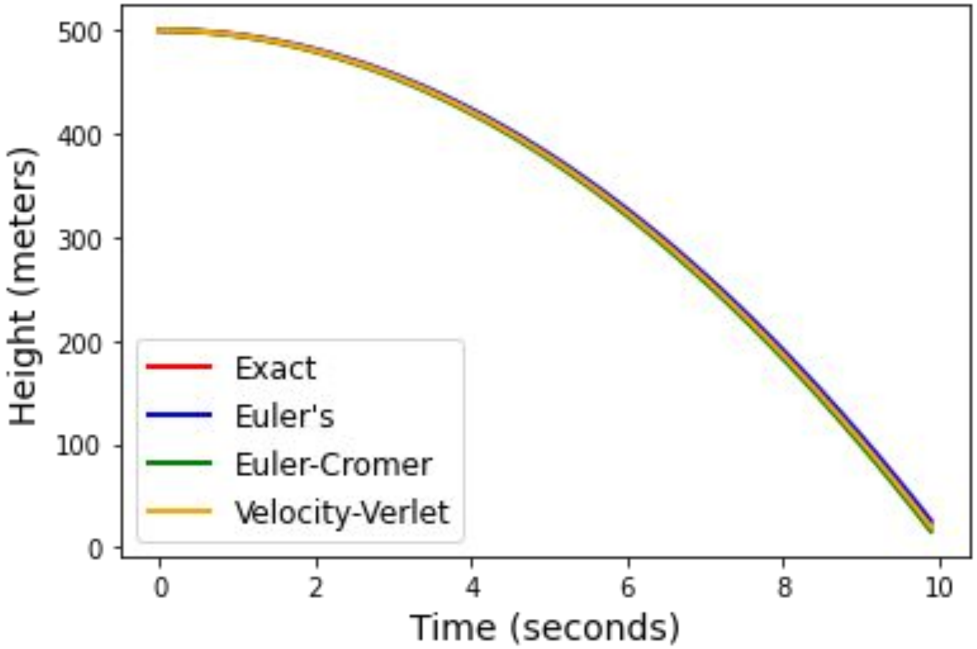
Overview of Each Notebook Contents

- Introduction to the topic containing text and equations
- Python code broken into small pieces with text explanation and comments
- Short exercises scattered throughout the notebook
- Longer “Practice What You Have Learned” at the end

```python
def neural_network(W, x):
    """
        Inputs:
            W (a list of length 2): the weights of the neural
                network
            x (a float): the input value of the neural network
        Returns:
            Unnamed (a float): The output of the neural network
        Defines a neural network with one hidden layer.  The
        number of neurons in the hidden layer is the length of
        W[0]. The activation function is the sigmoid function
        on the hidden layer an none on the output layer.
    """
    # Calculate the output for the neurons in the hidden layer
    hidden_neuron = sigmoid(jnp.dot(x, W[0]))
    # Calculate the result for the output neuron
    return jnp.dot(hidden_neuron, W[1])
```

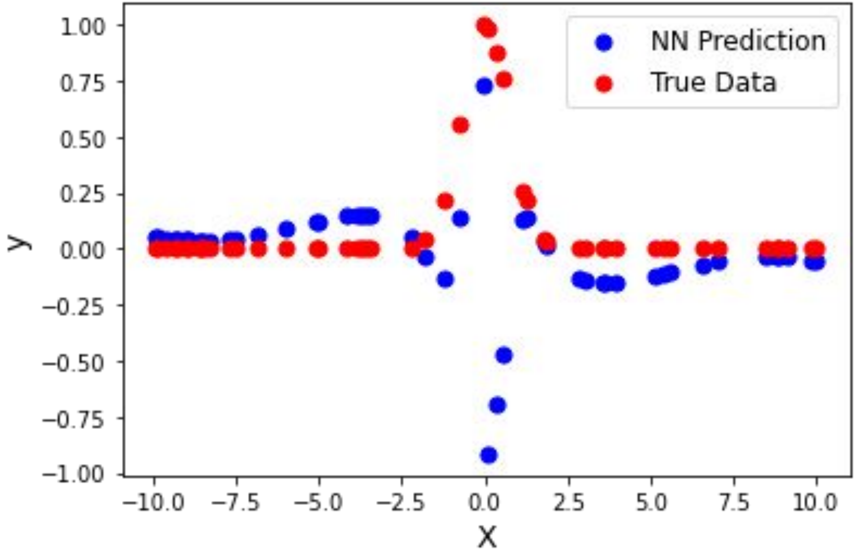
Notebook 1: Solving Differential Equations Numerically

- Introduction to differential equations
- Euler's Method
- Euler-Cromer Method
- Velocity-Verlet Method
- Walkthrough Example
  - Freefall in the presence of linear drag
- Practice What You Have Learned
  - Simple harmonic oscillator



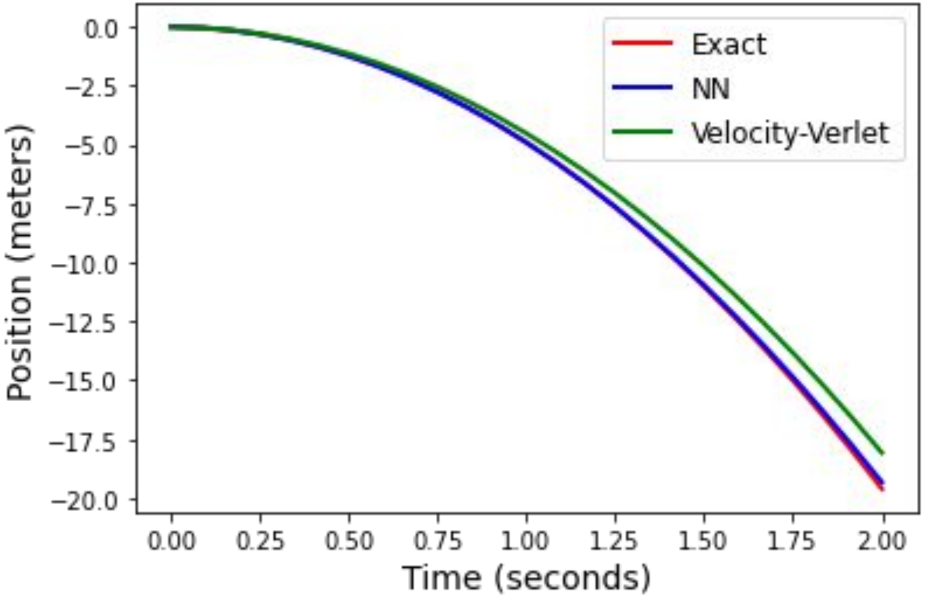
Notebook 2: What is a Neural Network?

- What is a neural network?
- Creating a neural network from scratch using JAX
- Creating neural networks with popular Python libraries
- Practice What You Have Learned
    - Optimizing the from scratch neural network



Notebook 3: Solving Differential Equations with Neural Networks

- How to solve differential equations with neural networks
- Setting up a neural network to solve for position given acceleration
  - Freefall with linear drag
- Improving the results
  - Hyperparameter Tuning and Step Size
- Practice What You Have Learned
  - Sliding with friction



How can this module be worked into a classical mechanics course?

When?

- Most advanced physics topic covered is the exact solution for freefall with linear drag
  - Sections 2.1-2.2 in *Classical Mechanics* by John Taylor
- Could be added anywhere in a classical mechanics class
- Post-exam break from learning new material or in place of instruction if professor is absent

How to Incorporate it In Class

Each Notebook Contains:

- Walkthrough of the module containing text and code
- Short exercises problems dispersed through the text
- "Practice What You Learned" problem at the end

Option 1: All Three Notebooks in Class

- Out of class time: ~3hr
- In class time: ~3hr

Option 2: Only Notebook 3 In Class

- Out of class time: ~5hr
- In class time: ~1hr

Option 3: Self-Study

- Out of class time: ~6hr
- In class time: 0hr

Conclusion and Future Works

Conclusions and Future Works

- This module introduces neural networks to students using simple physics models so the machine learning takes center stage
- The knowledge given in this module should allow students to investigate further uses of neural networks on their own

- Add more problems with different types to Notebook 4: Further Problems
  - Exam questions, clicker questions

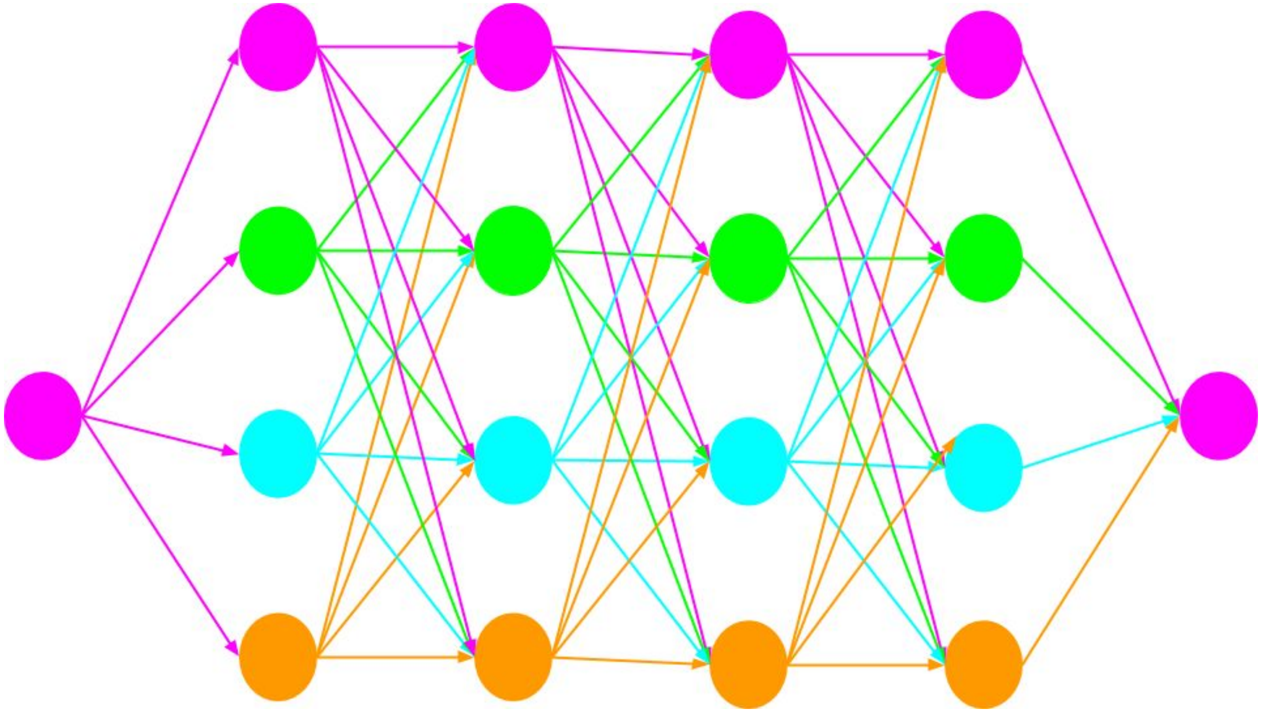
Thank You!

GitHub:

Module Feedback:

Extra Slides

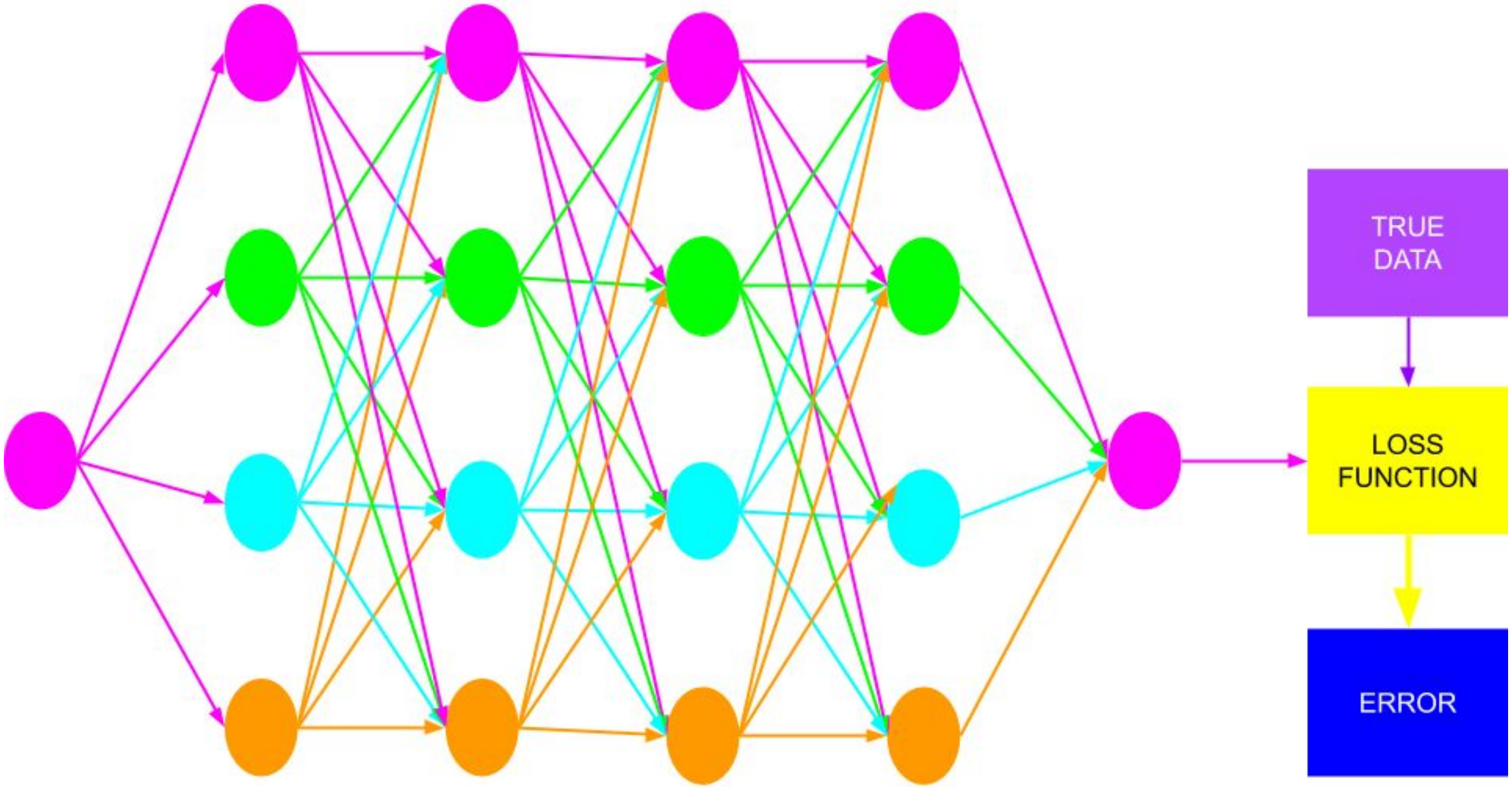
What is a Neural Network?



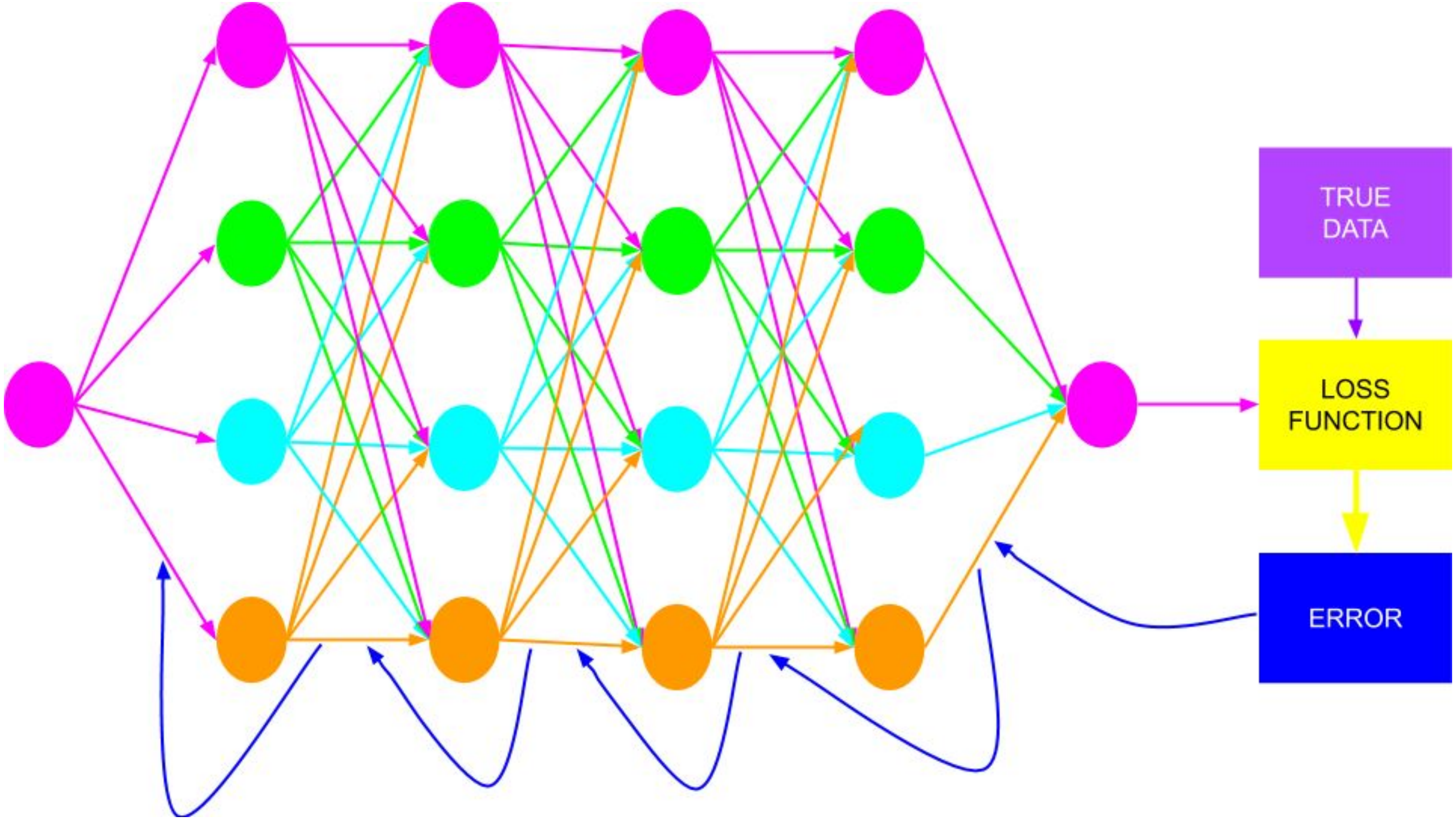
Neural Network: Computational system that is trained to match a given input to a given output

Exact mathematical form for each neuron and layer

Training a Neural Network



Training a Neural Network



Training a Neural Network: Gradient Descent

$$J(W) = \frac{1}{N} \Sigma_{i=i}^{N} (y_i - \hat{y}_i)^2$$

$$\mathrm{W} = \mathrm{W} - \mathrm{r}_l \frac{\partial J(W)}{\partial W}$$

Training a Neural Network: Many iterations of a forward pass followed by backpropagation to update the weights