CSCI 4962 Project Report
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Neural Networks as Numeric Solvers

Introduction

The goal of this project is to explore how neural networks can be used to approximate solutions to differential equations. The paper "Physics Informed Deep Learning" by Maziar Raissi, Paris Perdikaris, George Em Karniadakis is the inspiration for this project. The paper introduces the concept of physics-informed neural networks and uses it to find solutions to nonlinear partial differential equations. In this project, I use the methods detailed in the paper but with simpler differential equations. Specifically, I focus on first-order and second-order ordinary differential equations (ODE), which have analytical solutions. In reality, there is no use in approximating a differential equation with an analytical solution; however, for the purposes of this project, I want to compute the accuracy of the approximated solution. In addition to using the methods outlined in the paper, I also experiment with different model hyperparameters and see how it affects the runtime and accuracy. Finally, I compare approximate solutions derived from neural networks with traditional methods such as Euler's and higher-order Runge-Kutta methods.

Unsupervised Approach

Consider the simple differential equation $y' = x$ with initial condition $y(0) = 1$. Also, assume we use a neural network to approximate the solution in a supervised learning setting. The set of features would be the x points, but the set of labels is not immediately obvious. One could say the set of labels is a finite set of y points. There are a couple of problems, however. First, if the differential equation has no solution, then the labels are unattainable. Secondly, if we use real-world, observed data, it might be too granular and contain too much noise. As a result, a supervised learning model is not completely appropriate for this task. The paper mentioned above uses an alternative method that makes use of unsupervised learning. The main idea is for the neural networks to learn the gradient of the differential equation. Moreover, for a given set of labels containing x points, each x point replicates the gradient described by the differential equation. In the case of $y' = x$, the gradient at each point should be equal to x. One way to do this is by devising an error function as follows:

$$\alpha\Big(\sum_{i-0}^{n}(\hat{y}_i' - x_i)^2\Big)^{1/2} + \beta(\hat{y}_0 - 1).$$

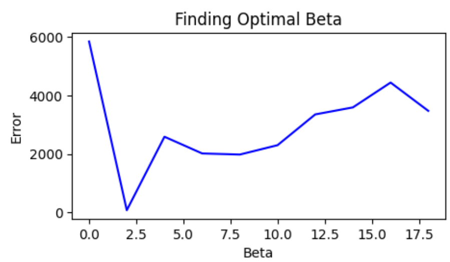
Above, α and β are hyperparameters. The first term in the sum enforces the ODE constraint, and the second term enforces the initial condition. A neural network can use this error function to find an approximate solution. I experiment with different differential equations and their corresponding error functions in the sections below.

Approximating First Order ODEs

First, let us consider the differential equation $y' = e^x$ with initial condition $y(0) = 1$. Trivially, the solution can be analytically determined to be $y = e^x$. To approximate the solution, a neural network with three hidden layers will be used. One of the hyperparameters for the model is the depth of each hidden layer, d. The other two hyperparameters α and β are part of the loss function:

$$\alpha\Big(\sum_{i-0}^{n}(\hat{y}_i' - e^{x_i})^2\Big)^{1/2} + \beta(\hat{y}_0 - 1).$$

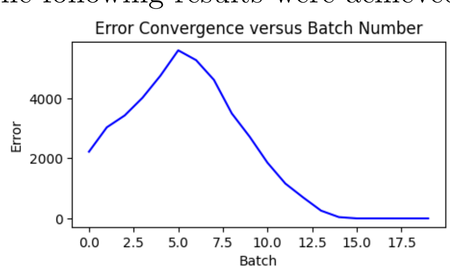
To find the optimal β, I fix $\alpha = 1$, $d = 20$, and do a search with $\beta \in [0, 20]$. The results of the grid search are shown in the plot below.



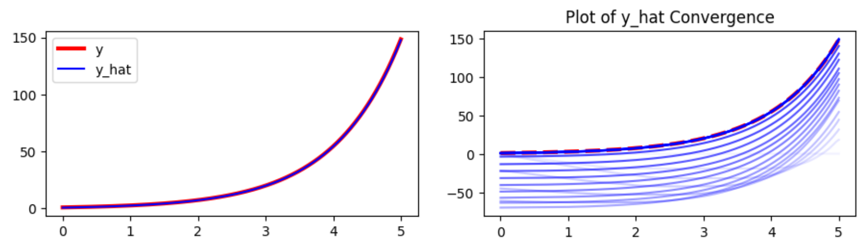
In the plot, the x-axis represents the different β, and the y-axis is the error defined as

$$\frac{1}{n}\sum_{i=0}^{n}(\hat{y}_i - y_i)^2.$$

The minimum error occurs when $\beta = 2$, which is the estimated optimal value. Next, after training the model, the following results were achieved:



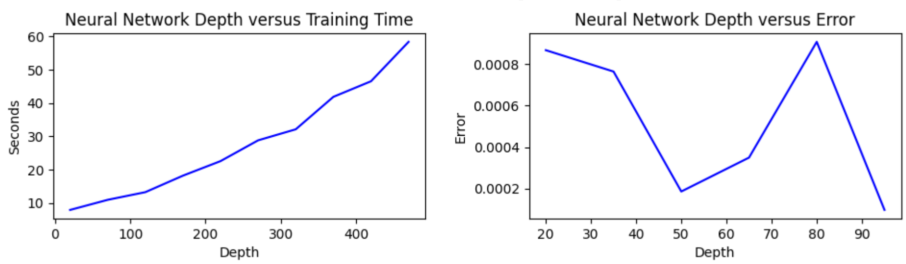
As you can see in the plot above, the error started to decrease rapidly just after a few batches. Also, looking at the plots below, the approximate solution very closely matches the exact solution.



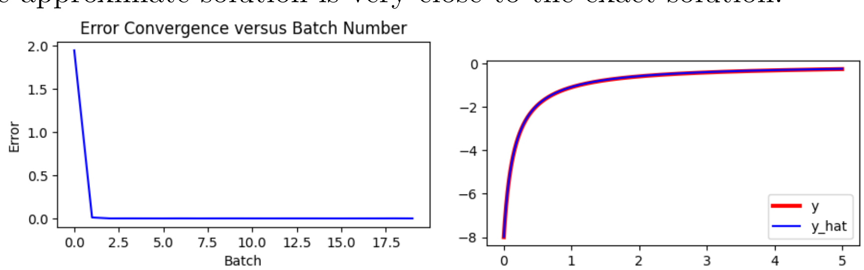
Moving on, we now focus on the differential equation $5y' - 4y^2 = 0$ with initial condition $y(0) = -8$; the exact solution is $-\frac{40}{32x+5}$. The loss function is

$$\alpha\Big(\sum_{i-0}^{n}(5\hat{y}_i' - 4\hat{y}_i^2)^2\Big)^{1/2} + \beta(\hat{y}_0 + 8).$$

I find the optimal $\beta = 11$ and $\alpha = 1$. Now, I focus on how the depth of the neural network affects accuracy and runtime. For $d \in [20, 500]$, I get the plot below.



Looking at the plot, there is a clear relationship between depth and training time: as the depth increases, the training time increases. The relationship appears linear in the plot; however, more investigation is needed to determine if that is actually the case. According to the second plot, the optimal depth is 95; however, 50 also yields a very low error. If we also consider the run time in choosing the optimal depth, then perhaps 50 is better because of its shorter runtime. Finally, looking at the plots below, we can see that the approximate solution is very close to the exact solution.

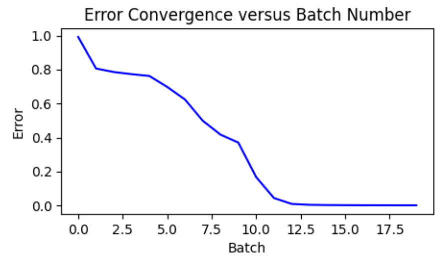


Approximating Second Order ODEs

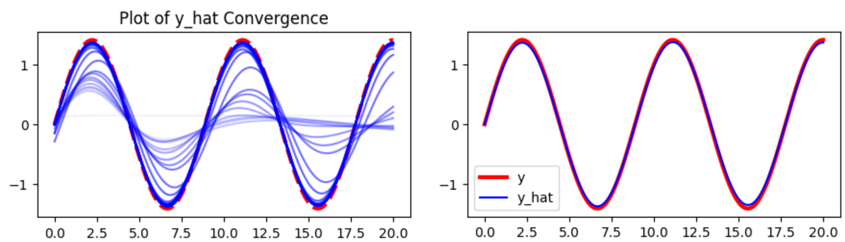
Now, let us experiment with the second order differential equation $10y'' + 5y = 0$ with initial conditions $y(0) = 0$ and $y'(0) = 1$; the exact solution is $\sqrt{2}\sin(\frac{x}{\sqrt{2}})$. The loss function is

$$\alpha\Big(\sum_{i-0}^{n}(10\hat{y}_i'' + 5\hat{y}_i)^2\Big)^{1/2} + \beta(\hat{y}_0) + \gamma(\hat{y}_0' - 1).$$

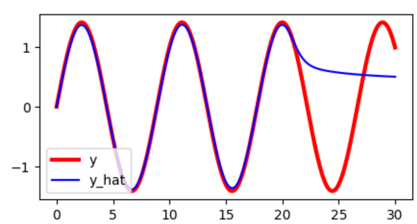
Note that compared to the first order, there is an extra term due to the added initial condition. Moving on, I find the optimal $\alpha = 1$, $\beta = 1$, and $\gamma = 500$ using the same method. These are the results for $x \in [0, 20]$:



As you can see above, the error decreases significantly towards zero. Moreover, looking at the plots below, the approximate solution matches the exact solution very closely.



The results shown above are very promising however, what does the approximate solution look like outside the domain $x \in [0, 20]$ of which the neural network was trained on? Looking at the plot below, we can see that approximate solution starts to diverge away from the exact solution. This kind of behavior is expected because since we only train the neural network on a specific range of x values, only those values should have the correct gradient. In other words, the model does not prioritize generalization at all; instead, the model focuses on approximating as close as possible to the desired solution.



Similar to the last differential equation consider $my'' + by' + ky = 0$. In physics, this equation models damped oscillatory behavior, or in other words, a damped spring. Let us set $m = 10$, $b = 2$, and $k = 2$. Here the mass is 2, damping constant is 2, and spring constant is 2. Also, let the initial conditions be $y(0) = -10$ and $y(0)' = 0$.

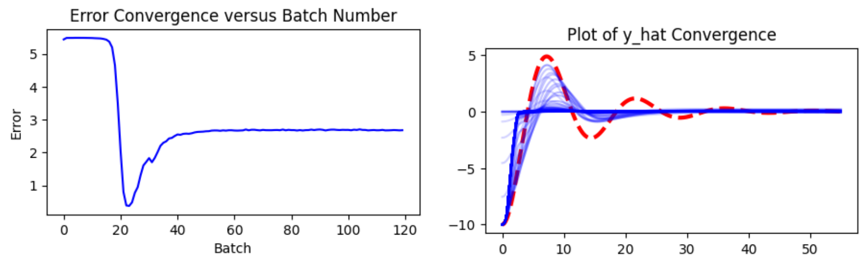
These conditions state that the object starts at position -10 with 0 initial velocity. The exact solution to this is

$$y(x) = -\frac{10}{19}e^{-\frac{x}{10}}(\sqrt{19}\sin(\sqrt{19}x/10) + 19\cos(\sqrt{19}x/10)),$$

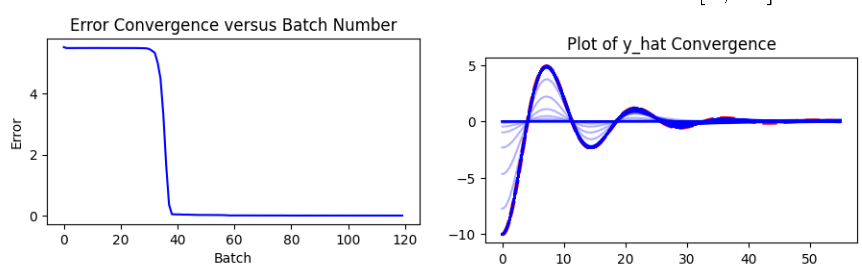
and the loss function is

$$\alpha\Big(\sum_{i-0}^{n}(10\hat{y}_i'' + 2\hat{y}_i' + 2\hat{y}_i)^2\Big)^{1/2} + \beta(\hat{y}_0 + 10) + \gamma(\hat{y}_0').$$

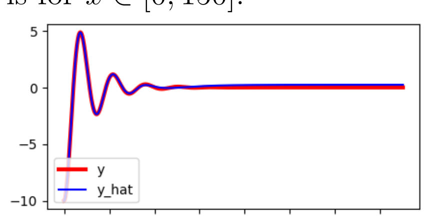
Training the neural network with $x \in [0, 55]$ with 50 points yields the results below.



Interestingly, the error rapidly decreases then starts to increase. This is also represented in the second plot where it first starts to properly fit, then starts reverting into a worse approximation. I theorize this is due to the fact that 50 points in the range 0 to 55 is not enough. The fewer points cause a single point to appease to contrasting gradients. Below are the results for the neural network trained with $x \in [0, 55]$ with 300 points.



Now, the error function is monotonically decreasing, and the approximate solution is very close to the exact solution. Another interesting thing about this solution in particular is that it decays, or in other words the derivative flattens as x increases. A consequence of this is that unlike the previous equation where the approximate solution deviates away from the exact solution, the approximate solution will continue to follow the exact solution. This can be seen in the plot below. The network was only trained for $x \in [0, 50]$, but the plot is for $x \in [0, 150]$.



Comparison to Traditional Methods