CSCI 4962 Project Report
Siddha Kilaru

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, and 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. Furthermore, the neural network used throughout the project is a simple feed forward network with three dense layers. Initially, the activation functions were all ReLU; however, since the second order differential equations requires second order differentiation, I changed the activations to tanh. In the sections below, I experiment with different differential equations and their corresponding error functions.

Data Exploration and Usage

In a standard machine learning project with supervised learning, it would be typical to research for quality data sources, analyze/explore the data, and perform necessary modifications to get ready for training. However, as mentioned in the previous section, this project is focused on unsupervised learning. Additionally, I am only focused on exploiting the powerful approximation powers of neural networks to fitting analytically defined mathematical functions in $\mathbb{R}^n$. Because of this, most of the steps mentioned are unnecessary and counterproductive: it does not make sense to research for real-world data sets. I need fine control over the data I generate because it can drastically affect the neural network's performance (numerical methods resort to discretized vectors because it is impossible to have continuous variables due to memory and processing constraints).

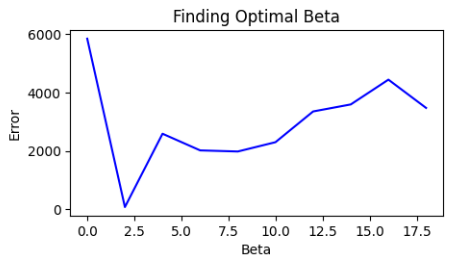
Not much preprocessing was required to generate data in one dimension ($\mathbb{R}^1$). However, generating data for two dimensions ($\mathbb{R}^2$) required a non-trivial amount of preprocessing. For $\mathbb{R}^1$, it was sufficient to decide on a range $x \in [a, b]$ and the number of points N then use `torch.linspace(a, b, N)` as needed. In contrast, for $\mathbb{R}^2$, the generated vectors need to span a whole plane. It is not sufficient to just do $x \in [a, b]$ and $y \in [c, d]$, rather we need $A = \{(x, y) \mid x, y \in \mathbb{R}; a \leq x \leq b, c \leq y \leq d\}$. This requires a lot more computational power: if $N = 500$, then the input vector will contain 500^2 elements. Fortunately, the NumPy library has a method `numpy.meshgrid` that efficiently implements part of this process.

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:

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

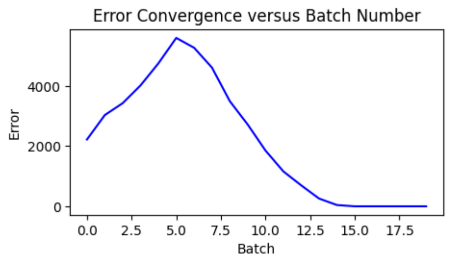
To find the optimal β, I fix $\alpha = 1$, $d = 20$, and do a search with $\beta \in [0, 20]$. The results of the grid search are shown in the plot below.



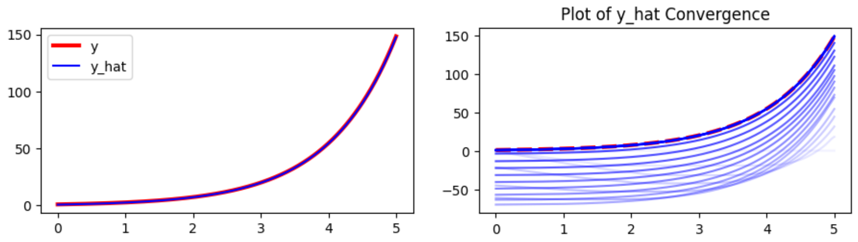
In the plot, the x-axis represents the different β, and the y-axis is the error defined as

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

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



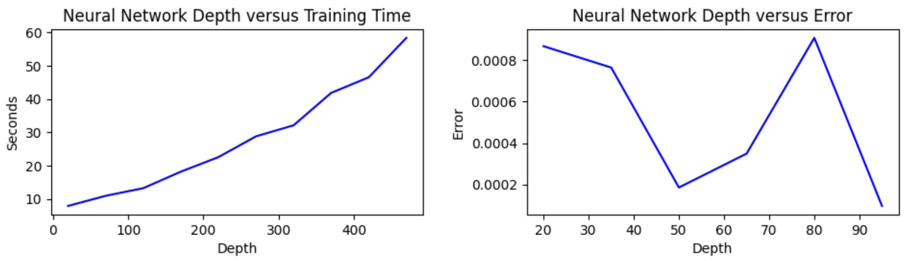
As you can see in the plot above, the error started to decrease rapidly just after a few batches. Also, looking at the plots below, the approximate solution very closely matches the exact solution.



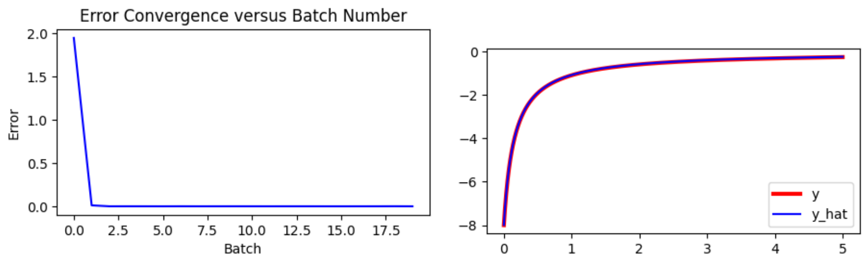
Moving on, we now focus on the differential equation $5y' - 4y^2 = 0$ with initial condition $y(0) = -8$; the exact solution is $-\frac{40}{32x+5}$. The loss function is

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

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.

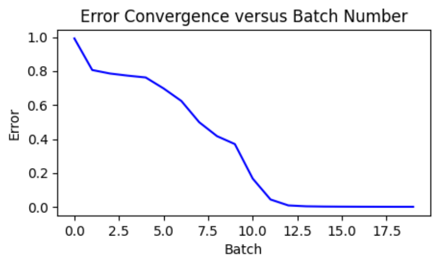


Approximating Second Order ODEs

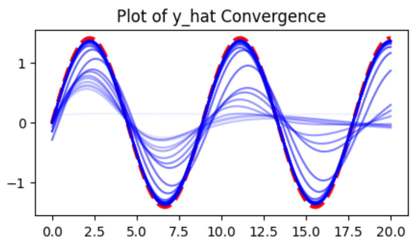
Now, let us experiment with the second-order differential equation $10y'' + 5y = 0$ with initial conditions $y(0) = 0$ and $y'(0) = 1$; the exact solution is $\sqrt{2}\sin(\frac{x}{\sqrt{2}})$. The loss function is

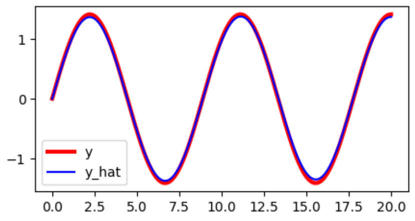
$$\alpha\Big(\sum_{i=0}^{n}(10\hat{y}_i'' + 5\hat{y}_i)^2\Big)^{1/2} + \beta(\hat{y}_0) + \gamma(\hat{y}_0' - 1).$$

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 $x \in [0, 20]$:

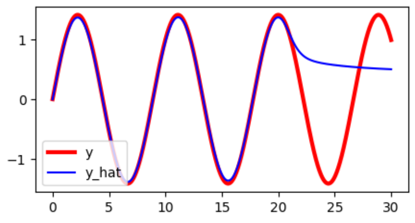


As you can see above, the error decreases significantly toward zero. Moreover, looking at the plots below, the approximate solution matches the exact solution very closely.





The results shown above are auspicious; 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.



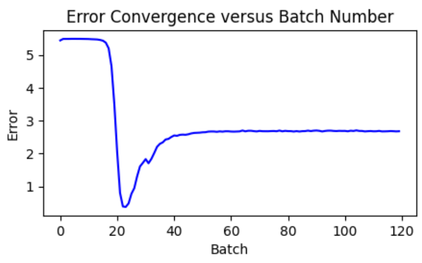
Similar to the last differential equation, consider $my'' + by' + ky = 0$. In physics, this equation models damped oscillatory behavior, or in other words, a damped spring. Let us set $m = 10$, $b = 2$, and $k = 2$. Here the mass is 2, damping constant is 2, and spring constant is 2. Also, let the initial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

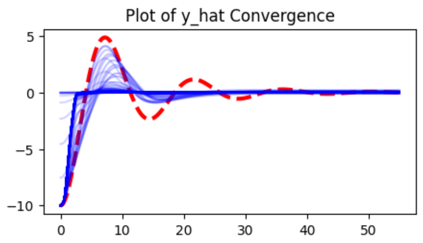
$$y(x) = -\frac{10}{19}e^{-\frac{x}{10}}(\sqrt{19}\sin(\sqrt{19}x/10) + 19\cos(\sqrt{19}x/10)),$$

and the loss function is

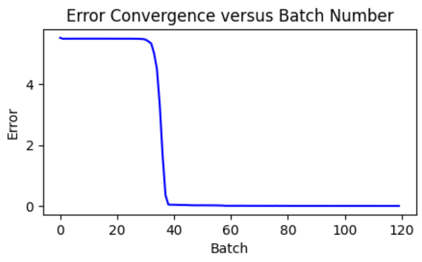
$$\alpha\left(\sum_{i=0}^{n}(10\hat{y}_i'' + 2\hat{y}_i' + 2\hat{y}_i)^2\right)^{1/2} + \beta(\hat{y}_0 + 10) + \gamma(\hat{y}_0').$$

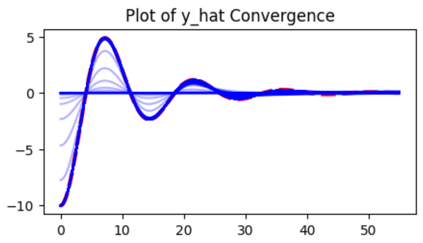
Training the neural network with $x \in [0, 55]$ with 50 points yields the results below.



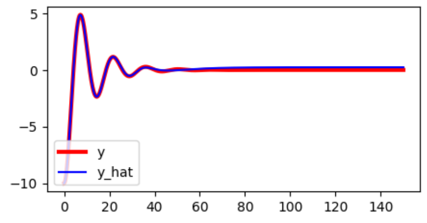


Interestingly, the error rapidly decreases and then starts to increase. This is also represented in the second plot, where it first starts to fit properly, then starts reverting to a worse approximation. I theorize this is due to the fact that 50 points in the range of 0 to 55 are not enough. The fewer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





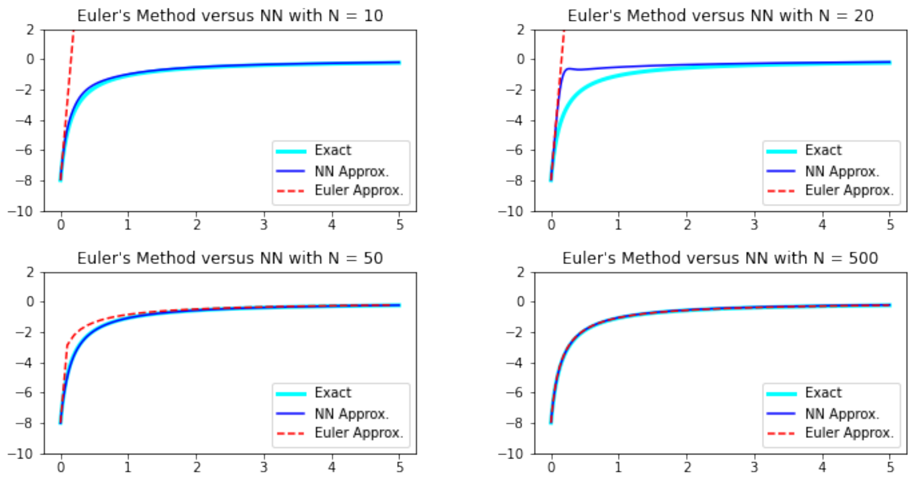
Now, the error function is monotonically decreasing, and the approximate solution is very close to the exact solution. Another interesting thing about this solution, in particular, is that it decays, or the derivative flattens as x increases. A consequence of this is that, unlike the previous equation, 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

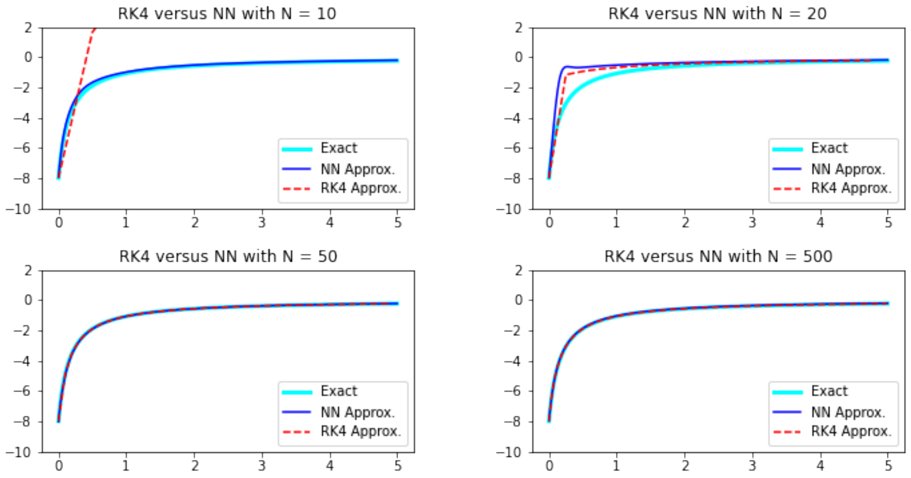
Euler's Method is one of the most popular and simplest methods for numerically solving differential equations. One important difference between Euler's Method and any finite difference method for solving differential equations are that they are iterative. Moreover, if the initial condition is at $x = 0$, and you desire a solution at $x = 100$, then you must iteratively compute the solution. So, if the spacing between each point is κ, you must do $\frac{100}{\kappa}$ computations. This can be costly because κ must be very small to approximate the solution accurately. In contrast, with a neural network, any point within the trained bounds can be instantly computed with a single feed-forward computation. Yes, the neural network requires training time which is arguably more costly; further analysis should be done to understand the tradeoff between the two methods.

Below are plots comparing Euler's Method to a neural network's approximate for a different number of points N. I use the differential equation $5y' - 4y^2 = 0$ with initial condition $y(0) = -8$.



Looking at the plots with $N = 10$ and $N = 20$, the solution created by Euler's Method ended up being highly unstable and increasing towards infinity. However, with $N = 50$ and $N = 500$, the solution was a fairly good fit. The neural network approximation was stable for all N and got better as N increased. Even with $N = 10$, the neural network approximation was fairly accurate.

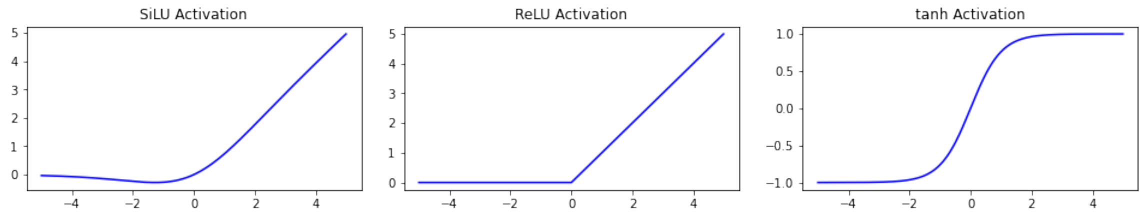
The next traditional method I would like to compare neural networks against is RK4. Compared to Euler's Method, RK4 is a lot more robust (much more stable) and better at approximating. However, it requires several more function evaluations compared to Euler's Method. Below are the plots comparing RK4 to a neural network using the same differential equation as above.



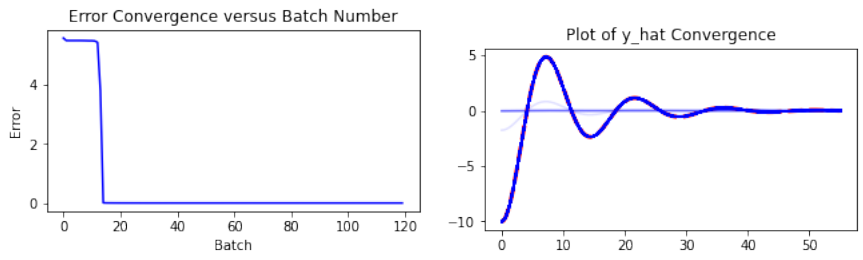
At $N = 10$, RK4 is unstable and tends toward infinity. However, at $N = 20$, unlike Euler's Method, it approximates the solution. At $N = 50$ and $N = 500$, RK4 is spot on. Comparing this to the neural network, we can see that the neural network only outperformed with $N = 10$ and $N = 20$.

Comparison of Activation Functions

As mentioned previously, any linear activation function or activation function without a second derivative is not sufficient for approximating higher order differential equations. The activation function used for all the experiments above were tanh, but in this section, I use the SiLU activation function: $x * \sigma(x)$. SiLU (swish function) is closely related to ReLU, but does allow for approximating second-order differential equations. Below is a visual comparison between the different activation functions:



The main problem with using tanh as an activation function is the vanishing gradient problem and the usual solution is to use the ReLU activation instead. However, as stated above, that will not work, so instead, I used SiLU. Below is the error convergence of the same spring damper differential equation used above:



As you can see, the error dropped to zero just before 20 batches using SiLU, but it took about 40 batches using tanh. Additionally, the approximated solution matches the exact solution much more closely.

Approximating a Solution to the Heat Equation

The heat equation in one dimension is

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}.$$

The boundary conditions will be

$$u(a,t) = 0 \text{ and } u(b,t) = 0,$$

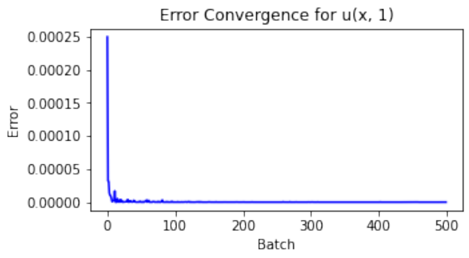
and the initial condition is

$$u(x,0) = f(x).$$

I set the initial distribution for the heat to be $f(x) = 6\sin(x\pi/b)$ and set $a = 0$, $b = 1$, and $\kappa = 1$. The exact solution is $u(x,t) = 6\sin(x\pi)e^{-t\pi^2}$. The loss function is

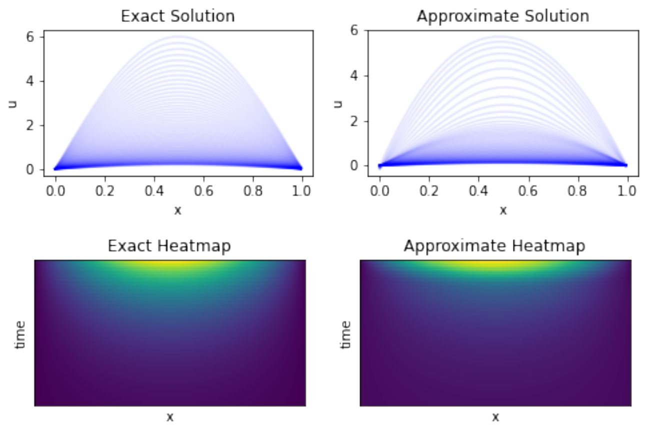
$$\alpha\left[\sum_{i=0}^{n}\left(\frac{\partial \hat{u}_i}{\partial t_i} - \frac{\partial^2 \hat{u}_i}{\partial x_i^2}\right)^2\right]^{1/2} + \beta\left(\sum_{i=0}^{n}(\hat{u(x_i,0)} - f(x_i))^2\right)^{1/2} + \kappa\left(\sum_{i=0}^{n}\hat{u(0,t_i)}^2\right)^{1/2} + \gamma\left(\sum_{i=0}^{n}\hat{u(1,t_i)}^2\right)^{1/2}.$$

Through experimentation I found the optimal hyperparameters to be $\alpha = 1, \beta = 250, \kappa = 60$, and $\gamma = 60$. Below is the error convergence for $\hat{u(x,1)}$ over 500 batches.



As shown by the plot, the error immediately drops after just a few batches and continues to decrease slowly. Training a two-dimensional function took much more time than a one-dimensional function. If n training points were used in a one-dimensional setting, then comparably, n^2 points must be used to capture all pairwise relationships. Moreover, on my setup, the training times for $n = 50$ in the one-dimensional setting was about the same as $n = 10$ in the two-dimensional setting.

The plots below are the final results produced by the trained neural network:



As you can see, the neural network approximates the solution fairly well. The two plots on top (the exact and approximate solution) represent the plots of $u(x,t)$, where the lighter lines have a t closer to 0. For the heatmaps on the bottom, a darker shade is cooler, and the time increases in the downward direction of the y-axis.

Conclusion

The results of my project illustrate that neural networks could be a viable approach to approximating differential equations. However, there are specific problems with neural networks and the unsupervised approach. First, in one of the sections above, I showed that the approximated solution becomes unreliable when the inputs used are outside the training boundaries. This is a significant drawback in simulating events when there is no clear upper bound. Though one possible exception to this is the spring damper equation with a decaying solution. Second, training times can be very long and not worth using over alternative methods. However, when compared to traditional methods, the neural network could approximate with fewer points hinting at lower runtimes. Still, more advanced numerical methods , such as the RK4 quickly caught up. In conclusion, neural networks are dope, but for now, I'd stick to the tried and tested and do more research on neural network solvers.

Notebook

The jupyter notebook for this project can be accessed here:
https://github.com/siddha20/CSCI4962/blob/master/Project/project.ipynb.