Building Physics-Informed Neural Networks from scratch

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Abstract

A physics-informed neural network (PINN in short) is an artificial neural network that learns the function from mathematical constraints that govern the underlying physics to be modelled. In this work, a PINN was built from scratch using Python programming language with fundamental libraries as numpy, pandas and matplotlib. Aim of the present work is to get fundamental understanding on how a PINN works from the mathematical and programming points of view. Here, the classical fully connectected neural networks was constructed and tested by approximating a simple parabola plot data. Further, the built network was developed to be physics-informed and validated by solving the ODE governing the exponential velocity decay of fluid due to viscosity. The understanding gained will be extended in further scientific computing using NNs.

1 Introduction to neural networks

Machine learning is a branch of mathematics and computer science that develops mathematical models that learn and mimic the human behavior. Deep learning is a subset of machine learning that deals with artificial neural networks.

A neuron is a mathematical function that takes in multiple weighted inputs and returns a single output. It is similar to a biological neuron in terms of connectivity and activation. Mathematically, it is represented as below.

$$f_{neuron} = \sigma\left(\boldsymbol{w}^T.\boldsymbol{x} + b\right)$$

Here, $\boldsymbol{x}$ is the input vector to the neuron and $\boldsymbol{w}$ is its corresponding weights vector. b is the bias of the neuron and σ is the activation function.

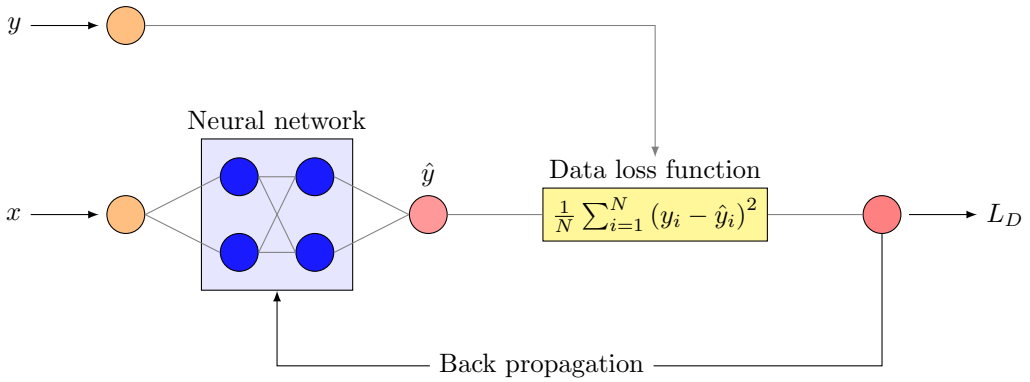


Figure 1: Example network

A Neural network is a set of inter-connected mathematically modelled neurons that can work as a function approximator. It based on the universal approximation theorm [1] which states as, any mathematically represented function $f(x)$ can be approximated by a neural network $G(x)$ of sufficiently wide and deep to the tolerance ϵ. Mathematically,

$$|G(x) - f(x)| < \epsilon$$

Today, neural networks are of many types, but the fundamental ones are of three: fully connected network, convolutional neural network, and reccurrent neural network, with each serving a specific purpose. Fully connected network, also called as dense network, is a set of layers of neurons in which each neuron on each layer will be connected to all other neurons on nearby layers. They are good in approximating the functions that invovle scalar IO variables. Convolutional neural networks are best for the field data IOs, and the reccurrent type networks are suitable for data that are of sequencial type.

In the present work, the fully connected neural network is developed from scratch and later it was turned into physics informed network. The mathematical background, and the problems solved with the developed network were discussed in the upcoming sections.

2 Mathematical view on network training

Consider an example network shown in fig. 1. Here, the input data x is fed to a fully connected network that estimates the output data $\hat{y}$, which then compared with the expected output data y through loss function.

Weights and biases of the example network were then optimized with loss as objective function, minimizing it to match the expected output values through an algorithm called back propagation. The main reference for this back propagation equations for a fully connected network is [2].

Mathematically, a single layer l is represented as given below.

$$\boldsymbol{x}^{[l]} = \sigma\left(\boldsymbol{z}^{[l]}\right)$$

where,

$$\boldsymbol{z}^{[l]} = \boldsymbol{W}^{[l]} \cdot \boldsymbol{x}^{[l-1]} + \boldsymbol{b}^{[l]}$$

Here, $\boldsymbol{W}^{[l]}$ is the weight matrix and $\boldsymbol{b}^{[l]}$ is the bias vector of layer l. $\boldsymbol{x}^{[l-1]}$ is the activated output of the previous layer $l-1$, and σ is the activation function. Let, L be the loss function evaluated at the end of last layer. Then, the gradient of loss function with respect to the unactivated output of last layer $z^{[l]}$ is given as below.

$$\frac{\partial L}{\partial \boldsymbol{z}^{[l-1]}} = \left[\boldsymbol{W}^{[l]}\right]^T \cdot \frac{\partial L}{\partial \boldsymbol{z}^{[l]}} * \left.\frac{\partial \sigma}{\partial \boldsymbol{z}}\right|_{[l-1]} \tag{1}$$

Equation (1) is called as the error of a layer. The error is back propagated from layer l to the previous layer $l-1$ by the above equation. Here, $*$ is the element-wise multiplication. To begin this back propagation, we need the above error derivative $\partial L/\partial z$ for the last layer in the network.

The computation of error for the last layer will involve the differentiation of loss function L with respect to the estimated output $\hat{y}$. Let the last layer be described as given below.

$$\hat{\boldsymbol{y}} = \sigma(\boldsymbol{z})$$

And, let the loss function be the classical mean squared error as given below.

$$L = \frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2$$

Then, the error for the last layer is calculated as shown below.

$$\left.\frac{\partial L}{\partial \boldsymbol{z}}\right|_{[l]} = \frac{\partial L}{\partial \hat{\boldsymbol{y}}} \cdot \frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{z}} = \frac{\partial L}{\partial \hat{\boldsymbol{y}}} \cdot \frac{\partial \sigma}{\partial \boldsymbol{z}} = \left(\frac{2}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)\right) \left.\frac{\partial \sigma}{\partial \boldsymbol{z}}\right|_{[l]}$$

Hence, the above equation completes the error computation for all the layers, next we have to compute the derivatives of loss with respect to weights and biases of all the layers using these error vectors. The gradients of loss with respect to weights and biases are computed using the error vector for each layer as shown below.

$$\frac{\partial L}{\partial \boldsymbol{W}^{[l]}} = \frac{\partial L}{\partial \boldsymbol{z}^{[l]}} \cdot \left[\boldsymbol{x}^{[l-1]}\right]^T \tag{2}$$

$$\frac{\partial L}{\partial \boldsymbol{b}^{[l]}} = \frac{\partial L}{\partial \boldsymbol{z}^{[l]}} \tag{3}$$

So, with the above gradient equations eqs. (1) to (3), the weights and biases of all the layers can be computed and optimized with aim of minimizing the loss function. An example problem with data-driven network is given below that was solved with the neural network built using above equations.

3 Validating neural network code

A couple of datasets were chosen for validating the developed neural network code. First is a simple parabola curve data that the network has to approximate and the second one will be a normalized flight velocity profile data which the network code has also to approximate. Each problem was explained in detail as below.

3.1 Parabola problem

The problem framed was to approximate the parabola curve defined with equation $y = x^2$ with $x \in [0, 0.5]$.

A network with three layers and single neuron on each layer, i.e. two hidden layers and one output layer, was built for this problem. The tanh() is used as the activation function for all the layers and mse is used as the loss function for the network. The schematic of network for this problem is given in fig. 2.

Training was performed on the generated data, and the resulting estimated vs exact profiles were shown in fig. 3. It can be seen that the estimated result is accurate enough to approximate the $y = x^2$ equation within the range $x, y \in [0, 0.5]$. Accuracy analysis were not performed as the motive is to check if the network code works.

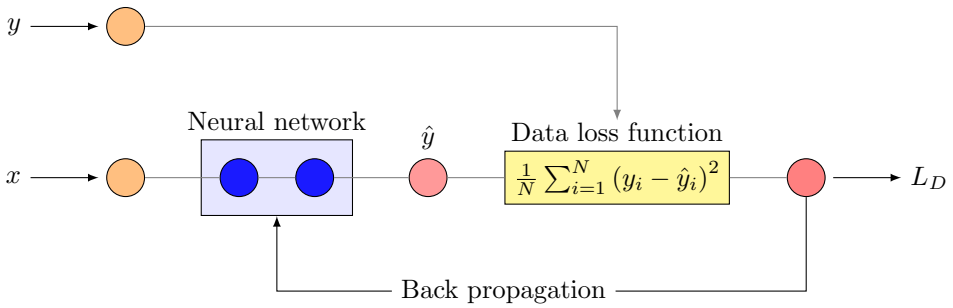


Figure 2: Neural network schematic for parabola problem

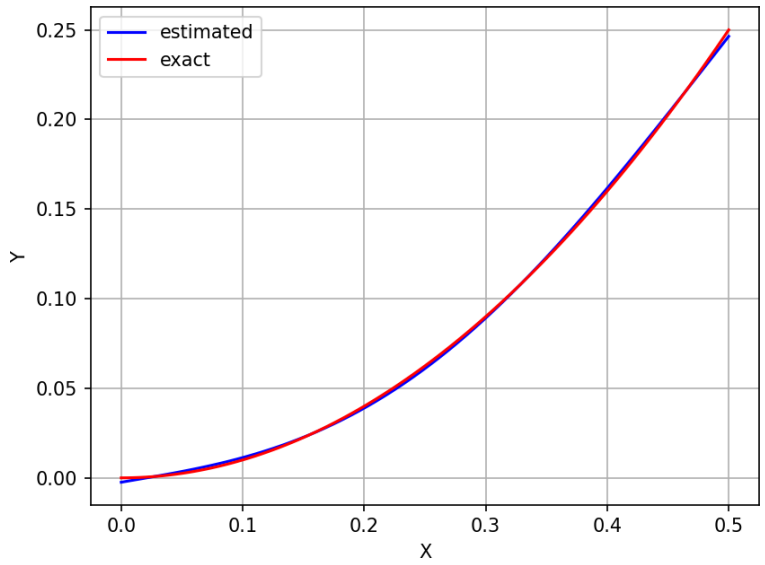


Figure 3: Estimated vs exact parabola profile by the built neural network

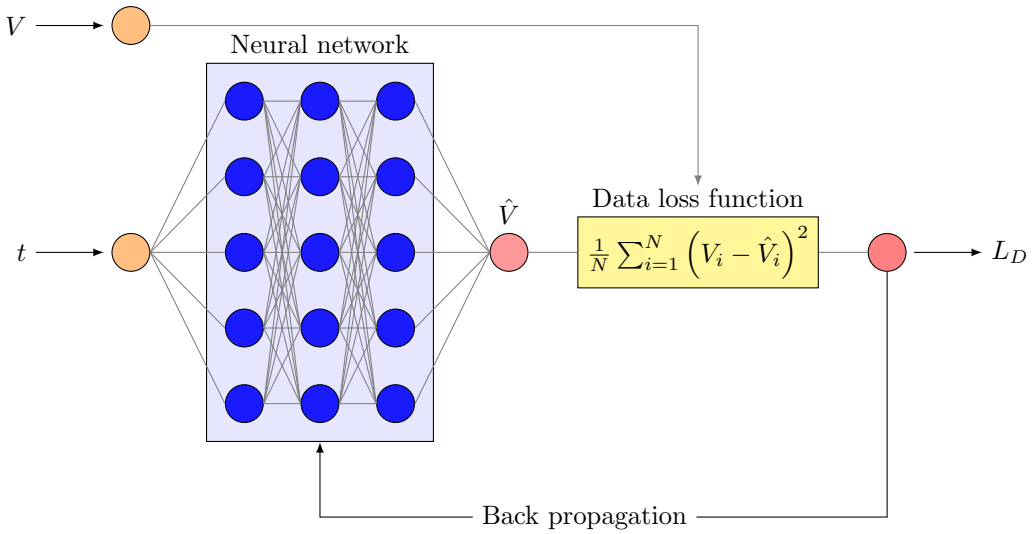


Figure 4: Neural network schematic of flight velocity profile problem

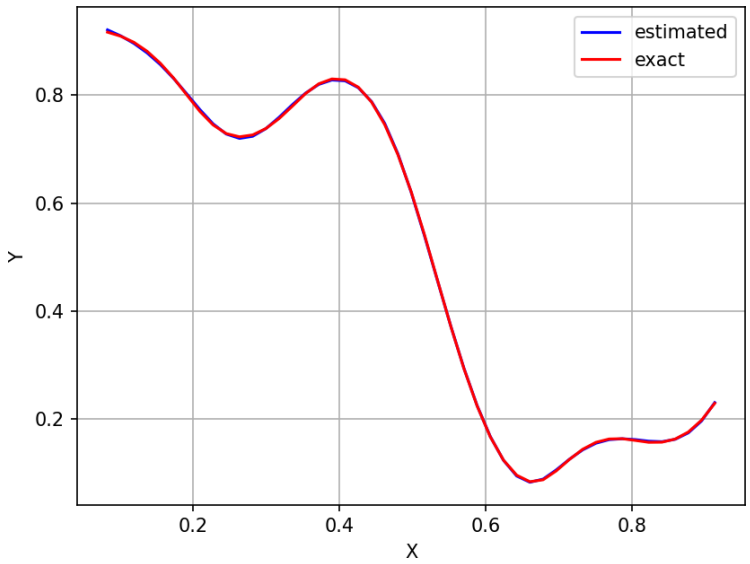


Figure 5: Estimated vs exact flight velocity profiles, here X is t and Y is V

3.2 Flight velocity profile

Second validation was performed using a flight velocity profile that was obtained from the flight dynamics simulation done for an academics assignment work. The profile was smooth and have both positive and negative curvatures, hence chosen for the work.

Schematic of the neural network built for this approximation was shown in fig. 4. The network has 5 neurons with 3 hidden layers and 1 neuron for the output. Same $tanh()$ activation function was used in all the layers.

The estimated vs exact flight velocity profiles were given in fig. 5. It can be seen that the estimation matches pretty well with the exact velocity profile, proving that the network code is correct. Thus, the next step of enhancing the code to include physics information was performed.

4 Enhancing network with physics information

The already developed neural network code was validated against two dataset, and now the code has to be enhanced to include physics information in the form of mathematical constraints.

For each problem to be solved with this network code, the code has to be modified to include the mathematical constraints in the last layer or so. The mathematical constraints can be of two types, either algebraic or differential equations. Algebraic equations involving output and input variables can be directly coded, but, coding the differential equations will require the derivatives to be computed using automatic differentiation in the network which was accomplished as explained below.

4.1 Computing derivatives output w.r.t input

The differential equations (ODEs and PDEs) will involve the derivatives of dependent variables w.r.t. independent variables. In the network terms, the dependent variables are the output variables and the independent ones are the input variables. Thus, as similar to the loss derivative equations, an equation for computing derivative of a layer output w.r.t. its input was derived.

Keeping backpropagation equations as base idea, the matrix equation for $\partial\sigma/\partial x$ of a layer was propertly derived and is given below as.

$$\left[\frac{\partial\sigma}{\partial \boldsymbol{x}}\right] = [\boldsymbol{W}]^T \cdot diag\left(\frac{\partial\sigma}{\partial \boldsymbol{z}}\right) \tag{4}$$

Here, $\partial\sigma/\partial x$ is a vector of the layer and $diag\,(\partial\sigma/\partial x)$ is a diagonal matrix with those vector elements on the diagonal.$\left[\frac{\partial\sigma}{\partial \boldsymbol{x}}\right]$ is a mtrix of same size as of $[\boldsymbol{W}]^T$.

It has to be noted that the eq. (4) gives derivative of output with respect to input of a single layer only. The chain rule in differential calculus has to be used to get the derivative of overall output of the network to its actual input.

4.2 Validating the gradient equation

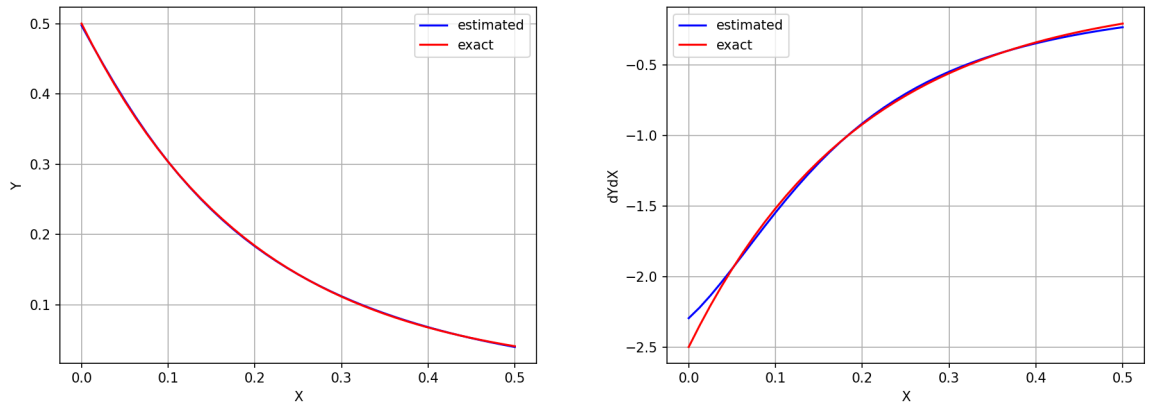
The matrix equation eq. (4) was validated for it working by testing it on the network that was trained based on pure data. A network was built and trained using a synthetic data of fluid velocity decay at a point in flow due to fluid viscosity. The synthetic data was generated using below equation with $k = 5.0$ and $V_0 = 1$.

$$V(t) = V_0 e^{-kt}$$

And its corresponding ODE for derivative computation is given below.

$$\frac{dV}{dt} = -kV$$

The network was trained for $X = t = [0, 0.5]$ and its corresponding velocity values. The estimated vs exact velocity decay profile is given in fig. 6a. And then, the trained layer weights were used to compute the derivative dV/dt which were compared to the exact values and given in fig. 6b. It can be seen that the derivative profiles match quite well except at the beginning which is due to limitation in approximating the velocity profile, and that was later rectified in validating the PINN network. Thus, the derivative computation is validated, and next step will be to validate the self built physics-informed neural network.



(a) Velocity profile estimated vs expected

(b) dV/dt profile estimated vs expected

Figure 6: Validation graphs for derivative computation

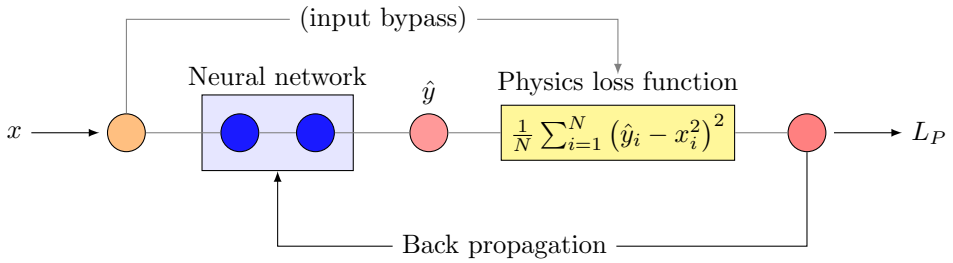


Figure 7: PINN network schematic for parabola problem

5 Validating Physics-Informed Neural Network (PINN) code

Validating the enhanced PINN code was done with two chosen problems. First one is to approximate the same parabola profile but with equation $y = x^2$ instead of y-data, and the second one is to model the fluid velocity decay profile due to fluid viscosity, which involves differential equation.

5.1 Parabola profile with equation

The problem is similar to the one used for validating the neural network code earlier, except the fact that, the y-data is made unavailable and the governing equation $y = x^2$ is given instead. The residual of the equation will be given to the loss function which has to be minimized for training the model. The network architecture is given in fig. 7. And the estimated vs expected results graph is given in fig. 8.

5.2 Exponential velocity decay due to fluid viscosity

Given a point in a free fluid flow, the velocity of fluid particles will decay at the point due to the resistance termed as fluid viscosity. This decay will be in exponential form and is governed by eq. (5), which was already discussed partially in the derivative validation section.

$$\frac{dV}{dt} = -kV \tag{5}$$

Here, k is a constant denoting fluid viscosity. The equation is of autonomous form and has analytical solution given as below.

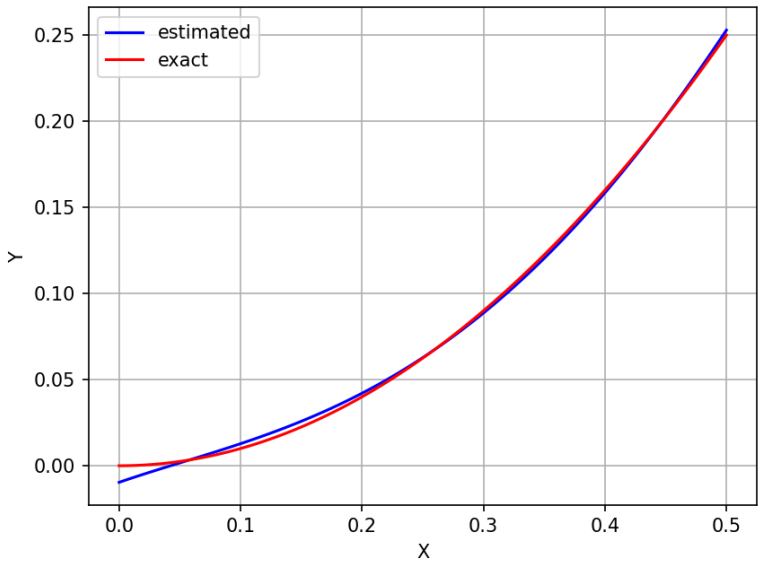


Figure 8: Parabola estimated vs exact result using PINN

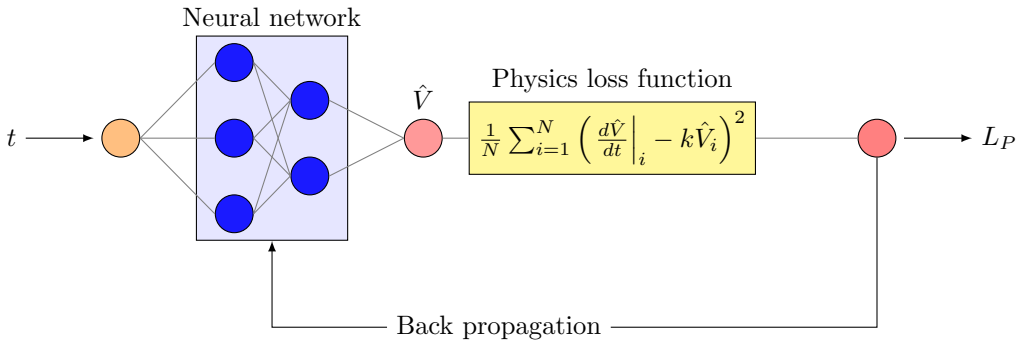


Figure 9: Velocity decay problem PINN schematic

$$V = V_0 e^{-kt}$$

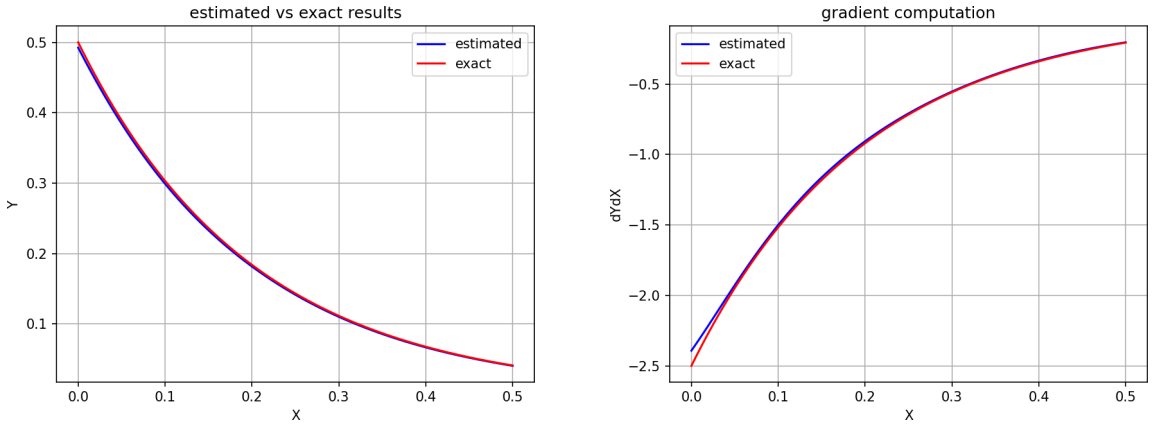
V_0 is the initial velocity of the fluid flow. Schematic of the PINN used for the problem is given in fig. 9. Here, the network has two hidden layers with 3 and 2 neurons respectively, and an output layer with 1 neuron. $tanh()$ activation function was used in all the layers.

The loss function of this network is made in two parts, the first part will enforce the initial condition of velocity and will be made active only at the starting of time data, it is given as below.

$$L_{IC} = \left(\hat{V}_i - V_i\right)^2\Big|_{t=0,i=0} \tag{6}$$

The second part will contain the governing equation constraint and that will be executed for all timesteps. The equation is as given below.

$$L_{ODE} = \frac{1}{N}\sum_{i=0}^{N}\left(\frac{d\hat{V}}{dt}\Big|_i - k\hat{V}_i\right)^2 \tag{7}$$



(a) Estimated vs expected velocity decay profile, (here X = t, Y = V)

(b) Estimated vs expected gradient profile, (here X = t, Y = V)

Figure 10: Exponential velocity decay due to fluid viscosity problem solution using PINNs

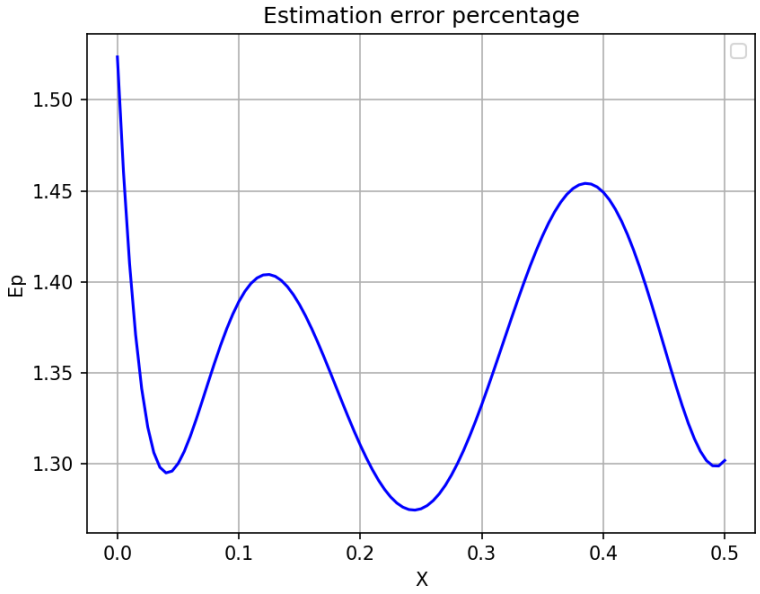


Figure 11: Error percentage of estimated vs expected velocity profiles

So, the total loss function for the network will be sum of eqs. (6) and (7), as given below.

$$L = L_{IC} + L_{ODE} = \left(\hat{V}_i - V_i\right)^2\Big|_{t=0,i=0} + \frac{1}{N}\sum_{i=0}^{N}\left(\frac{d\hat{V}}{dt}\Big|_i - k\hat{V}_i\right)^2 \tag{8}$$

Actually, to increase the weightage of initial condition as it is active only in a part of the back propagation, a factor of 10 was multiplied to its compontent and the final loss equation is given as below.

$$L = L_{IC} \times 10 + L_{ODE} \tag{9}$$

The model was trained successfully, and the estimated results of velocity profile and the derivative computation were given in fig. 10. It was found that the derivative estimated was accurate than the one shown for the validation. This is because the network that learns a function through physics constraints learn better than the network that maps the same function through data.

The error percentage graph for the estimated vs expected velocity profiles was given in fig. 11. The error percentage were in the order of 1-2%, hence this validates the PINN code developed.

6 Python code structure

In each of the source code that was provided with this documentation, there will be 3 python scripts, each handling specific part of the program. They are as listed below.

- script_main.py
- inputData.py
- customLayers.py

The *script_main.py* is the main script that constructs the network and has snippets related to physics information. *inputData.py* script contains the snippets that determine the input parameters, such as number of layers and neurons on them, whether to save/load weights and learning rate adaptation code. Finally, *customLayers.py* contains the class definition of a neural network layer that has everything related to layers such as activation function, its derivative and forward evaluation. Activation function is hard coded for now, and later may be made generalizable.

The code was made as generalizable in terms of having number of neurons/layers for now, and the code is for fully connected dense network. Later, the future work may include custom codes for other network types when the need arises.

7 Conclusion and future works

I conclude the present work by stating that a high level of understanding and knowledge gained in the perspective of mathematics and programming of neural networks, that opened gateways for other methods of using neural networks, such as optimizing input values itself based on loss to find optimal values etc... The present work is limited to the generalization code of fully connected dense network. And, this code may be extended for other scientific computation uses such as Neural ODEs.

References

[1] George Cybenko. "Approximation by superpositions of a sigmoidal function". In: *Mathematics of control, signals and systems* 2.4 (1989), pp. 303–314.

[2] *Deriving the backpropagation equations from scratch (part 1).* `https://towardsdatascience.com/deriving-the-backpropagation-equations-from-scratch-part-1-343b300c585a`. Accessed: 2024-07-01.