Physics Informed Neural Networks for solving Partial Differential Equations

Diganta Samanta(21PH40020)
Under Guidance of
Dr. Vishwanath Shukla
Indian Institute of Technology Kharagpur

MSc Project
Monday 28th November, 2022

Contents

Introduction

- **Machine Learning(ML)** is a sub-field of Artificial Intelligence.
- ML has a goal to develop algorithms that can learn from data automatically.
- **Artificial Neural Network(ANN), Neural Network(NN), or Neural Net** is a model of Machine Learning which is inspired by **neurons in the human brain**.
- **PINN** is an application of ANN for solving Problems in physics.

Artificial Neural Network

- The primary component of an ANN is **'stylized neurons'**.
- A neuron consists of a **linear transformation** followed by a **non-linear activation function**. There are different types of Non -linear activation functions like Perceptrons, Sigmoid, Tanh, ReLU, ELU, etc.
- ANN consists of such neurons stacked in layers. A deep Neural Network(DNN) has more than two hidden layers.

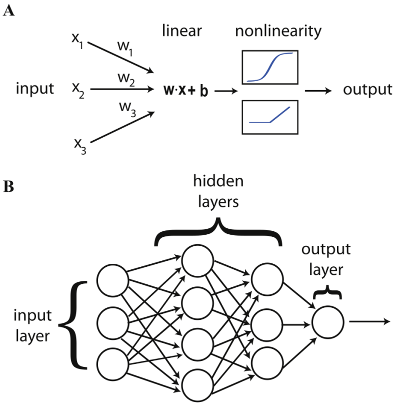


Figure: structure of Neural Network (Source: P. Mehta, M. Bukov, C.-H. Wang et al. / Physics Reports 810 (2019) 1–124)

Artificial Neural Network

- **Universal Approximation Theorem:** A neural network with single hidden layer can approximate any continuous, multi-input/multi-output function with arbitrary accuracy.

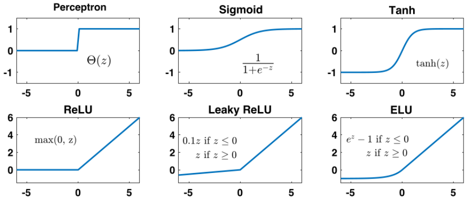


Figure: Some None Linear Activation Functions (Source: P. Mehta, M. Bukov, C.-H. Wang et al. / Physics Reports 810 (2019) 1–124)

Physics Informed Neural Network

- **Physics Informed Neural Network(PINN)** is a technique which uses Neural Network as a solution of a Partial Differential Equation.
- PINN approximates PDE solutions by minimizing a loss function that reflects the PDE, Boundary condition, Initial Condition, constraints etc.
- PINN has four parts
  1. Neural Network Architecture
  2. Auto Differentiation
  3. Loss Function
  4. Optimizer

PINN Building Blocks

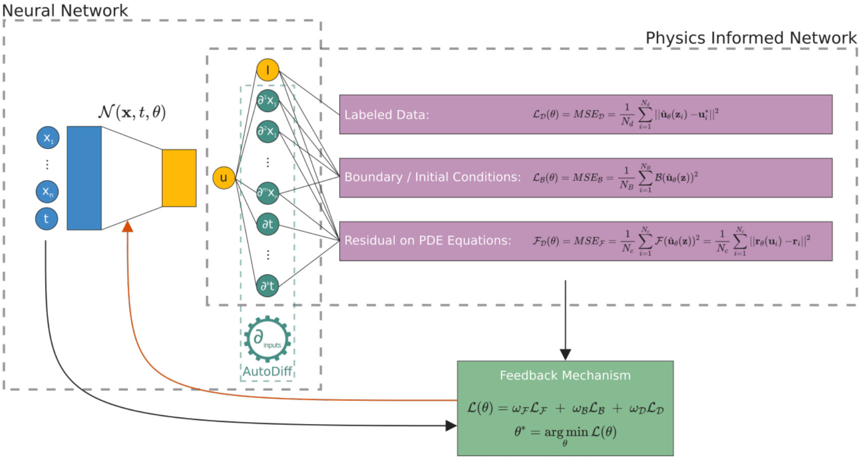


Figure: Building Block of PINN (source:Scientific Machine Learning through Physics-Informed Neural Networks,S Cuomo, V S di Cola, F Giampaolo, G Rozza, M Raissi, F Piccialli arXiv:2201.05624)

Solving Burgers' Equation

- I have solved **Burgers' Equation**

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \qquad x \in [-1, 1], \quad t \in [0, 1]$$

- Dirichlet boundary conditions and initial conditions are

$$u(-1, t) = u(1, t) = 0, \quad u(x, 0) = -\sin \pi x.$$

- I have solved for four values of viscosity $(\nu = 0.1, 0.01, 0.001, 0.0001)$

Results for Burgers' Equation

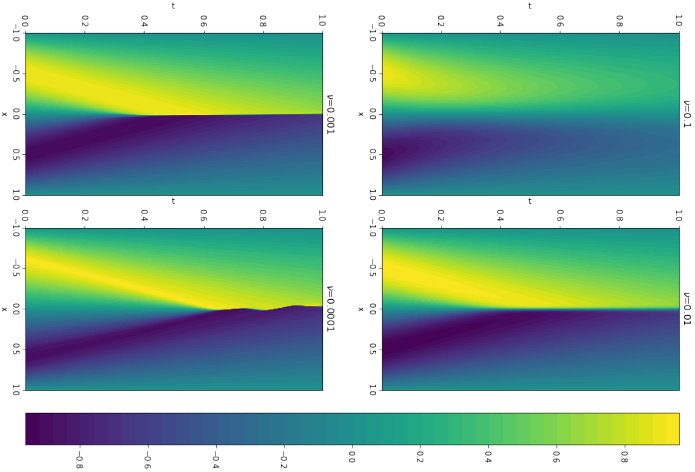


Figure: Solution plots of Burgers' Equation

Solving Heat Equation

- I have solved **1d Heat Equation**

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in [0, 1], \quad t \in [0, 1]$$

- Dirichlet boundary conditions:

$$u(0, t) = u(1, t) = 0$$

- I have solved for two initial conditions
  - Sinusoidal initial condition(taking $\alpha = 0.4$)

$$u(x, 0) = \sin \pi x$$

  - Dirac Delta initial condition(taking $\alpha = 0.008$)

$$u(x, 0) = \delta(x - \frac{L}{2})$$

    Where length of the rod = L = 1. I have generated Dirac function by using Gaussian distribution with variance very less than one.

Results for Heat Equation

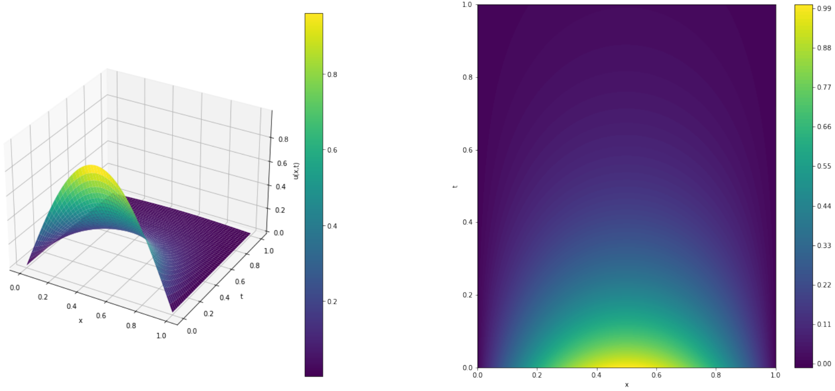
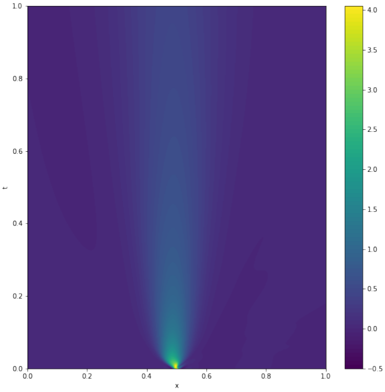


Figure: Plots of solution of Heat equation for periodic initial function

Results for Heat Equation



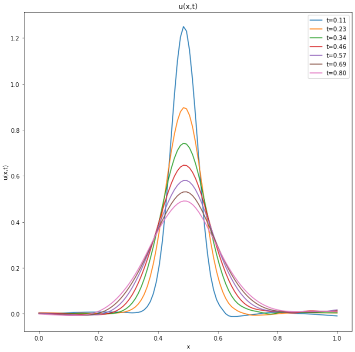


Figure: Plots of solution of Heat equation for Dirac delta initial function

Advantages of PINN

- A trained PINN can predict the values on the simulation grid of **different resolutions** without being retrained.
- A trained PINN can predict the values on the simulation grid of different resolutions without being retrained. PINN uses **automatic differentiation** to compute required derivatives which is superior to numerical or symbolical differentiation.
- Besides using experimental data, PINN uses the underlying physics during the network training. So
  - If the **size of the data is small**, it can give an accurate solution.
  - It can predict a precise value if the **boundary conditions are not provided**, and there is sufficient data.

References

1. Scientific Machine Learning through Physics-Informed Neural Networks: Where we are and What's next.-Salvatore Cuomo1 , Vincenzo Schiano Di Cola, Fabio Giampaolo , Gianluigi Rozza , Maziar Raissi and Francesco Piccialli
2. Lu, Lu and Meng, Xuhui and Mao, Zhiping and Karniadakis, George Em, DeepXDE: A deep learning library for solving differential equations
3. P. Mehta, M. Bukov, C.-H. Wang et al. / Physics Reports 810 (2019) 1–124)
4. Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations-Maziar Raissi, Paris Perdikaris and George Em Karniadakis

DeepXDE

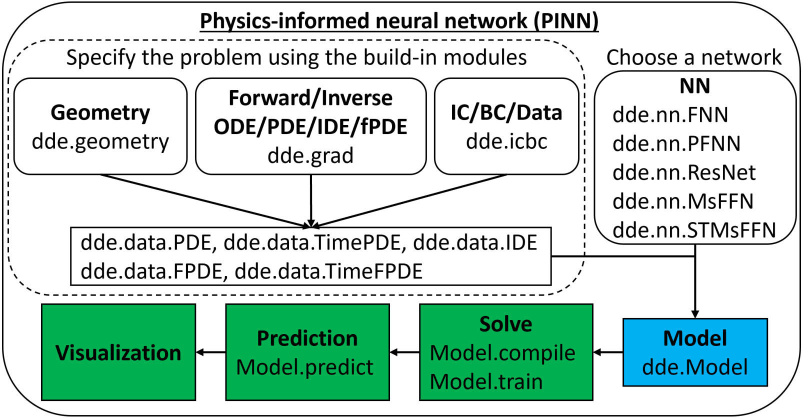


Figure: Implementation of PINN by DeepXDE (source:Lu, Lu and Meng, Xuhui and Mao, Zhiping and Karniadakis, George Em, DeepXDE: A deep learning library for solving differential equations)

Training data for Burgers' equation

ν	Optimizer	Training time (second)	final train loss
0.1	L-BFGS	128.997	2.05×10^{-06}
0.01	L-BFGS	214.848	4.50×10^{-06}
0.001	adam(lr=0.001) + L-BFGS	1417.553	2.05×10^{-06}
0.0001	adam(lr=0.001) + L-BFGS	1166.165	2.89×10^{-02}

Table: Training times and final losses for different viscosity

Training data for heat equation

Initial function	Optimizer	Training time (second)	final train loss
Periodic	adam(lr=0.001) + L-BFGS	145.807	6.72×10^{-07}
Dirac delta	adam(lr=0.001) + L-BFGS	145.332	3.60×10^{-02}

Table: Training times and final losses for different initial function

Acknowledgements

I thank Professor Vishwanath Shukla for giving me an opportunity to work, despite my lacking of the detailed theoretical nuances needed. This project helped me to practice and sharpen my skills in the field of physics and computing.

I especially thank Dr. Abhay Kumar Tiwari, a Data Scientist at More Retail Private Ltd., who has given me valuable advice in this Deep Learning field.

I was also helped by my fellow members of StatFluid Lab who have listened to my problems and helped me when I was struck. I am grateful for their generous aid.

I want to thank also my parents, friends, roommates who have continuously motivated me.

Thank You

भारतीय प्रौद्योगिकी संस्थान खड़गपुर

INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR