Seattle SciML Summer School: Case Study One
An introduction to PINNs

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1 Introduction

This study will give you an introductions to PINNS [RPK19] and to PyTorch. It will (i) give you an example of the use of PINNS to solve simple BVP and IVP differential equations in one-dimension (ii) study questions of the convergence and stability of the PINNS solver as a function of the architecture of the neural net and the location of the collocation points.

2 Solving a linear BVP

1. Open a **Colab notebook** session. Check that it is working by asking a simple question such as what is $1 + 1$.

2. Copy the code aengus.py in the Python_Examples Git-Hub folder into the Colab notebook.

3. The code uses a simple 3-layer PINN to solve the linear BVP

   $$-u''(x) = f(x), \quad u(-1) = \alpha, u(1) = \beta. \tag{1}$$

   In the code $f(x), \alpha$ and β are chosen so that (1) has the *exact solution*

   $$u(x) = \tanh(x).$$

   The PINN is trained to minimise the residual

   $$r(x) = (-u'' - f(x))^2$$

   evaluated at, and summed over, a set of collocation points x_i combined with the boundary conditions. The ADAM optimiser is used in training. It is then compared to the exact solution. Read through the code to make sure that you understand how it works.

4. Run to code as given to check that it gives a sensible answer.

5. Now modify the code so that the equation (1) has the exact solution $u(x) = \tanh(ax)$ for varying values of a. Run this modified code to see how the PINN performs as the value of a is increased.

6. Experiment with changing the width of the PINN and the number of collocation points to see how the solution converges (or not) to the exact solution, and how this convergence rate depends on the value of a

3 Solving a linear IVP

We will now use a PINN to solve the linear second order initial value problem

$$u'' + \omega^2 u = 0, x \in [0,1] \quad u(0) = 0, u'(0) = 1. \tag{2}$$

- Modify the previous example to solve this IVP for $x \in [0,1]$. Compare your solution with the exact solution for the case of $\omega = 5$. Investigate how the convergence depends on ω the number of collocation points etc.
- Using the PINN trained over the interval $[0,1]$ as above, apply it to solve (2) for $x \in [0,10]$. Comment on your answer.
- If you wish you can experiment with the related nonlinear equation

  $$u'' + \omega^2 \sin(u), \quad u(0) = 0, u'(0) = v$$

  for varying values of $v > 0$ and $\omega > 0$. Note that theoretically there is a change in the qualitative behaviour of the solution to this equation as v increases through $v = 2\omega$. Does the PINNS solution capture this?

4 Solving a nonlinear IVP

We will finally use a PINN to solve the nonlinear first order initial value problem

$$u' = u^2, x \in [0,1] \quad u(0) = \gamma.$$

- Modify the previous example to solve this IVP for $x \in [0,1]$. Compare your solution with the exact solution for the case of $\gamma = 1/2$.
- Now set $\gamma = 2$. What is the exact solution in this case? What does the PINN give? Does this depend on the parameters of the PINN?

References

[RPK19] M. Raissia, P. Perdikarisb, and G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comp. Phys.*, 2019.