Machine Learning and Computational Physics
Fall 2021

Assignment 3

Due: Oct. 4th 2021, 11:59:59 PM PDT

Physics informed neural networks (PINNs)

In this assignment, you will use feed-forward networks to solve the nonlinear diffusion-advection-reaction equation

? $u \cdot (1-u)$ in class?

$$\mathcal{L}u \equiv u''(x) - Peu'(x) + Dau(1-u) = 0 \qquad x \in (0,1) \tag{1}$$

$$u(0) = 0 \tag{2}$$

$$u(1) = 1. \tag{3}$$

100 input, 100 output

In this equation, the non-dimensional number P_e is the Peclet number; it measures the strength of advection relative to diffusion. Da is the Damkohler number, which measures the strength of reaction to diffusion.

1. Write a function that creates a feed-forward network of width=20, depth=5 with input and output dimensions 1. This will be used to represent the function $u = u(x; \boldsymbol{\theta})$. The weights and biases ($\boldsymbol{\theta}$) should initialized using `RandomNormal` distribution. All hidden layers should make use of a sine activation function, `tf.math.sin` while no activation should be used in the output layer. Use l_2 regularization in all layers with a parameter 1.0e-7.

2. Create an array of $N = 100$ uniformly spaced points in $[0, 1]$. Train a neural network with the following loss function

   (output)?

$$\Pi(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\left(\underline{\mathcal{L}u(x_i; \boldsymbol{\theta})}\right)^2 + \lambda_b(u(0; \boldsymbol{\theta})^2 + (u(1; \boldsymbol{\theta}) - 1)^2)$$

   which is the sum of the interior residual and a scaled boundary residual. Use $\lambda_b = 10$ for the training. Consider four different sets of values for the non-dimensional parameters:

   - $P_e = 0.1, Da = 0.1$ (diffusion dominates).
   - $P_e = 10, Da = 0.1$ (advection dominates).
   - $P_e = 0.1, Da = 10$ (reaction dominates).
   - $P_e = 10, Da = 10$ (advection and reaction dominate).

3. For each of the four parameter values, try three different initializations, and train the network for 8,000 epochs. Save the history of the interior loss, boundary loss, total loss, and the final predicted solution in arrays/lists. Out of these select the one that has smallest final total loss as the "best" network for each set of parameter values.

4. For each set of parameter values generate a plot of the interior, boundary and total loss as a function of epoch for the "best" network. Create another plot of the predicted solution and the benchmark solution provided to you. Which set(s) of parameter values does not yield a satisfactory solution?

5. For the set(s) of parameter values that do not yield a satisfactory solution, repeat the previous step with $\lambda_b = 1000$. What do you observe?

6. If you wanted to improve the accuracy of your solution, what would you do?

Instructions:

- At the very beginning of your notebook insert a text cell and write your name and **USC email address**.

- You need to submit your work as a single notebook saved as `A1_FirstName_LastName.ipnyb` (for example `A1_Tommy_Trojan.ipnyb`). You can create this notebook locally (on your computer using Jupyter notebook) or on cloud using Google Colab (which we recommend). If you are using Google Colab, then please make sure that you are signed in to your USC Google account before starting. This will make sharing your saved work little easier.

- For questions requiring descriptive output (such as question 5 in this assignment) use individual text cell.

- Make sure that your entire notebook runs successfully on Google Colab before submitting it. It is your responsibility to ensure this.

- Once you finish the assignment save it and share it with `hramaswa@usc.edu`. (If you are using Google Colab, then the notebook will automatically be saved to your Google Drive. Once you locate it in your Google Drive, right click on it and share it with `hramaswa@usc.edu`). While sharing make sure that you enable "editor" option, so that we can run your notebook on our end while grading it.