AI in the Sciences and Engineering   **Spring Semester 2024**

Student: Carla Judith López Zurita

Project 2   Due date: Monday 20 May 2024, 23:59

The main objective of the project is to apply the concepts learned in class related to Neural Operators. The first task consists in making future (or out of samples) predictions of the fluid and solid temperature of a thermal storage system. The second task is to model the water flow on the sphere using a Spherical Fourier Neural Operator (SFNO) and compare the results with the ones obtained by a baseline neural operator. The project also includes an optional task to test the universal approximation property of the Convolutional Neural Operator (CNO). My attempt at solving each of the mentioned tasks will be described in detail below.

1. Time Series Forecasting with Neural Operators

The first task is based on the mathematical model of a thermal storage system described by the following PDEs:

$$\epsilon \rho_f C_f \frac{\partial T_f}{\partial t} + \epsilon \rho_f C_f u_f(t) \frac{\partial T_f}{\partial x} = \lambda_f \frac{\partial^2 T_f}{\partial x^2} - h_v(T_f - T_s) \quad \text{for} \quad x \in [0, L], \quad t \in [0, T], \qquad (1)$$

$$(1 - \epsilon) \rho_s C_s \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial x^2} + h_v(T_f - T_s) \quad \text{for} \quad x \in [0, L], \quad t \in [0, T], \qquad (2)$$

with ρ being the density of the phases, C the specific heat, λ the diffusivity, ϵ the solid porosity, u_f the fluid velocity entering the thermal storage and h_v the heat exchange coefficient between solid and fluid. The system is also defined with appropriate boundary conditions defined in the project description. The goal is to predict the fluid and solid temperature at future time steps using a Neural Operator. One of the main challenges of this task was to arrange the data in the correct format to feed it to the network, namely the data had to be arranged in a series of windows. I used a window generator to create the windows with a length of 34 for both inputs and outputs, which was chosem because it is the size of the final prediction we have to make. The outputs were taken from the provided measurements, but corresponding to the next 34 time steps. Fig. 1 shows an example of a window with prediction.

The data was normalized using the MinMaxScaler from the sklearn library. The data was split into training and validation sets with a ratio of 80% and 20% respectively. I chose to use a Fourier Neural Operator (FNO) to solve this task. I used a single network to predict both the fluid (T_f) and solid temperature (T_s), so that it had three channels as input (T_f, T_s and time) and two channels as output (T_f and T_s). The network consisted of 3 layers with 3 Fourier features each. It was trained using the Adam optimizer with an initial learning rate of 10^{-3} and a batch size of 10. The loss function used was the L2 norm. The network was trained for 500 epochs. The loss function of the model during training is shown in Fig. 2.

The model was evaluated on the test set and the predictions were compared with the ground truth. Fig. 3 shows the predictions of the model taken from various windows in the test set. The dashed lines represent the predicted values, while the solid lines depict the ground truth. The model seems to be able to capture the general trend of the data, and predict very close values.

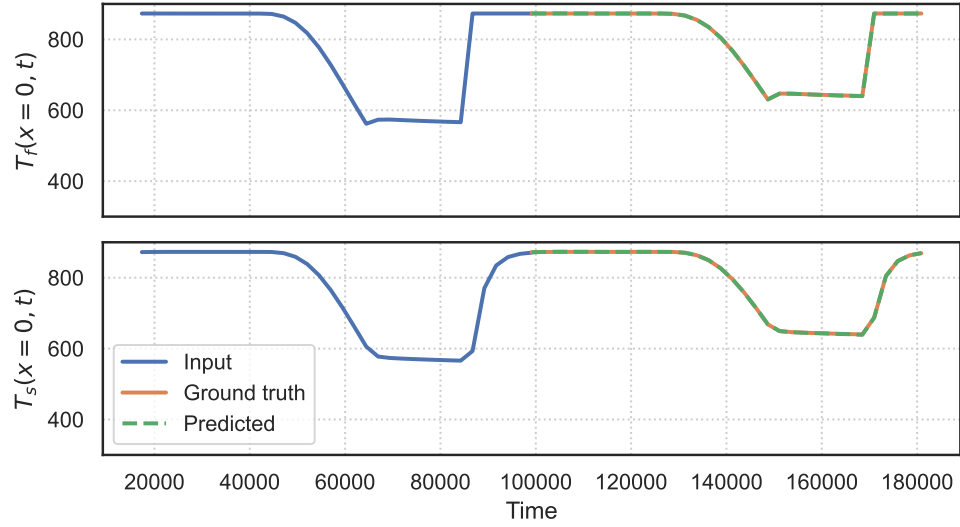Finally, we show the future predictions of the fluid and solid temperature in Fig. 4.

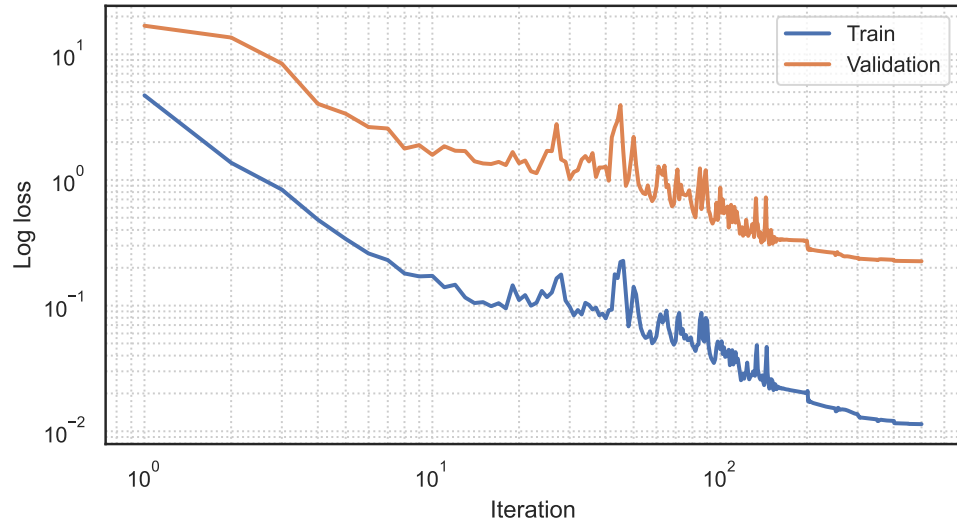Figure 1: Example of a window with prediction.

Figure 2: Loss function of the FNO model during training.

2. Modeling Water Flow on the Sphere with FNO

The next task consists in modeling the water flow on the sphere using a Spherical Fourier Neural Operator (SFNO) and comparing the results with the ones obtained by a baseline neural operator.

3. Universal Approximation for CNO (Optional)
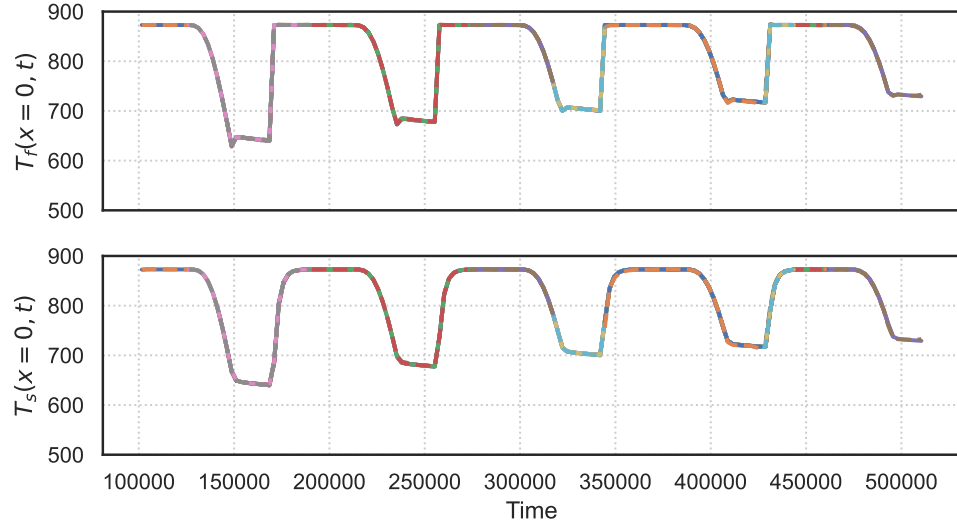
References

Figure 3: Predictions of the FNO model taken from various windows in the test set. Dashed lines represent the predicted values, solid lines depict ground truth.
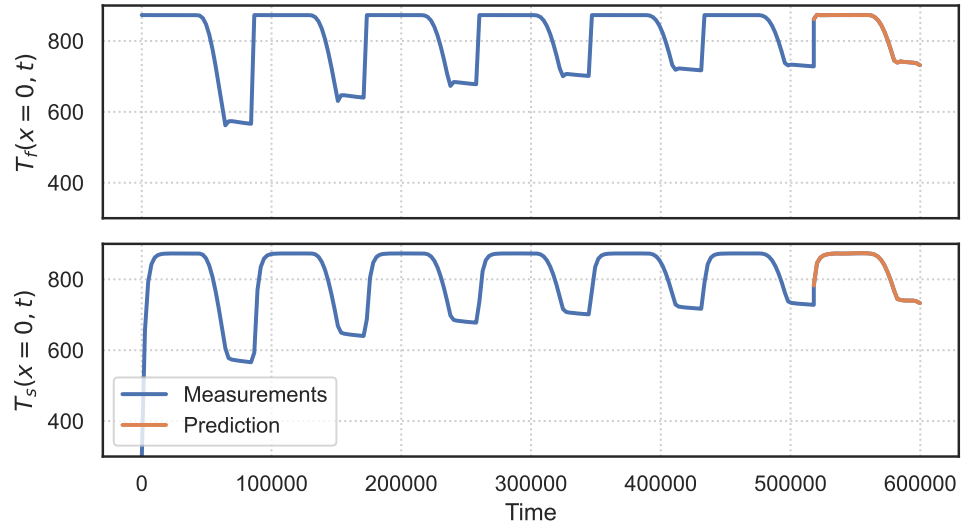

Figure 4: Future predictions of the fluid and solid temperature.