Report - Problem 2
Neural Operators in practice

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May 16, 2024

1 Task 1

The primary objective of Task 1 is to apply neural operators to a task concerning the preliminary design of a thermal energy storage system. In addressing this problem, we utilized Neural Operators to analyze the system's dynamics. We explored two main approaches: firstly, employing two neural networks, each with a single output dimension; alternatively, using a single neural network with a 2-dimensional output.

We chose the former approach, as the provided code was structured accordingly. However, it assumes independence between Tf and Ts, which isn't entirely accurate due to their mutual influence. Nevertheless, the model effectively captured the system's dynamics, benefitting from its inherent periodicity.

The utilization of tensors to mitigate rounding issues showed promise during data processing. However, it became evident that using float64 defined as Double would not align with the neural network model. After careful consideration and multiple trials, we found that employing numpy was the most suitable choice. Additionally, we utilized all available data for training, expecting that augmenting the dataset could improve the system's performance. After training, the values were

Tf	**Ts**
Epoch: 4990 Train Loss: 8.230268273716016e-06	Epoch: 4990 Train Loss: 4.108344076788247e-06

Our approach to solving the task involved the following steps:

1. Converting the files into tensors
2. Constructing the model
3. Developing two neural networks
4. Training the neural networks

5. Visualizing the results to assess performance

For the visualised final result, we obtained the following

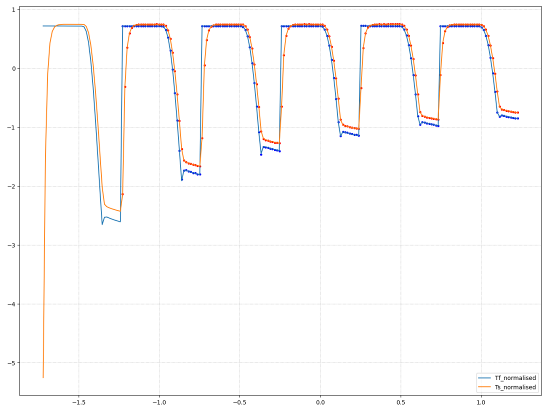

Figure 1: Plot of simulated data and the points taken into account

2 Task 2

In Task 2, the objective was to implement a Spherical Fourier Neural Operator (SFNO) from scratch. This report outlines the steps taken and the findings obtained during the implementation process.

2.1 Data Visualization and Preprocessing

The initial phase involved comprehensive data visualization and preprocessing steps. Test data were segmented into different resolutions for clarity. Visualization techniques, including Channel Visualization, Color Mapping, Histogram, and 3D Surface Plot, were employed. Additionally, a custom function named "add_spatial_information" was introduced to manipulate the data for model training. Notably, data normalization was omitted as the primary focus was on SFNO implementation rather than achieving specific metrics.

2.2 Implementation of Spherical Fourier Neural Operator

Following data visualization and preprocessing, the implementation of SFNO was undertaken. This involved utilizing key components such as SphericalSpectralConv2d and SphericalFNO2d. SphericalSpectralConv2d utilized theta and lambda as proxies for latitude or longitude, performing Spherical Harmonic Transform (SHT), linear transformation, and Inverse Spherical Harmonic Transform. The implementation closely followed the tutorial, with the exception of padding, as SphericalSpectralConv2d did not reduce the spatial dimensions of the input tensor.

2.3 Implementation of Fourier Neural Operator

Similar to SFNO, the implementation of Fourier Neural Operator (FNO) followed a comparable process. Some code snippets were borrowed from the Moodle tutorial, with differences primarily revolving around padding implementation due to unexpected dimension changes. Notably, the input and output configurations of FNO and SFNO differed, with SFNO featuring 5 input channels and 3 output channels compared to FNO's 3 input channels and 1 output channel.

2.4 Model Training

Model training utilized the Adam optimizer and StepLR scheduler. A total of 10 epochs were conducted, though it is acknowledged that training over a larger epoch range may yield lower L2 Test Norm values. Following training, SFNO exhibited a lower loss compared to FNO, indicating its superior performance in this context.

Table 1: Training Loss and Relative L2 Test Norm

Epoch	Train Loss (SFNO)	Relative L2 Test Norm (SFNO)	Train Loss (FNO)
9	0.008192814	20.132964	-
9	-	21.995300	0.009337362

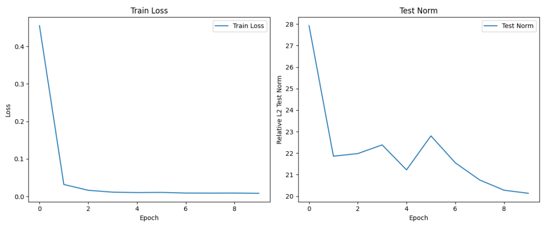

Figure 2: Training of Spherical Fourier Neural Operator

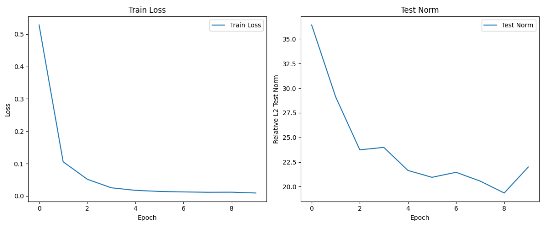

Figure 3: Training of Fourier Neural Operator

2.5 Testing the Model at Different Resolutions

Model testing was conducted at varying resolutions, specifically (32, 64) or (64, 128). Higher resolutions revealed significant discrepancies between predictions and ground truth. Notably, SFNO demonstrated better generalization capabilities compared to FNO, particularly from a visual standpoint. Plots and their comparisons were normalized to enhance visualization clarity.

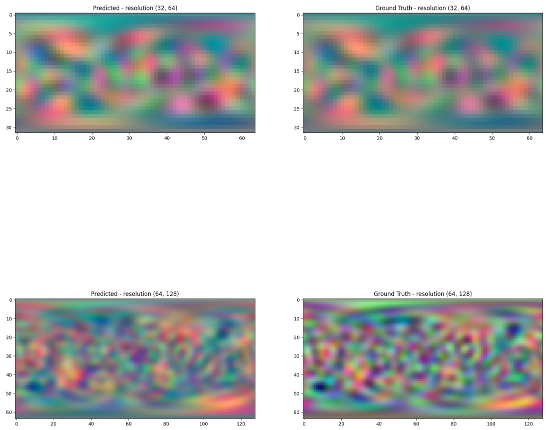

Figure 4: Plot of normalised test data at different resolutions with prediction through Spherical Fourier Neural Operator

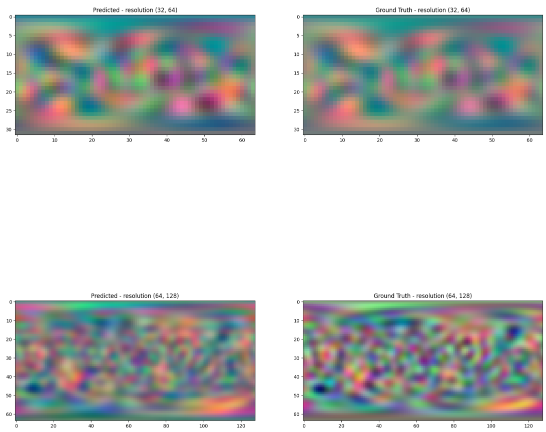

Figure 5: Plot of normalised test data at different resolutions with prediction through Fourier Neural Operator