Bayesian Fourier Neural Operators

Nicholas Betters[1], Connor Krill[2], Michael Shields[2]
[1]Ralph O'Connor Sustainable Energy Institute, [2]Department of Civil and Systems Engineering
Johns Hopkins University

Abstract

Many engineers subscribe to the belief that "all models are wrong, but some are useful." Over the last few decades, machine learning models have improved dramatically, but even when they are accurate, they have limitations in their usefulness. One shortcoming of deterministic models is their fixed outcomes. When data sets are messy and outcomes are unclear, the most useful model doesn't make a single prediction but rather provides a range of probable outcomes.
We apply this thinking to the study of neural operators and introduce Bayesian Fourier Neural Operators to predict a distribution of functions output by a neural operator.

What is a Bayesian Fourier Neural Operator?

It's a mouthful, but once you understand Bayesian, Fourier, and Neural Operator separately, it's not such a hard pill to swallow. Machine learning teaches computers to recognize patterns and make decisions based on data, similar to training a dog to fetch a ball. Our work focuses on neural networks, which learn patterns from various data types, like earthquake measurements or wind storm simulations.

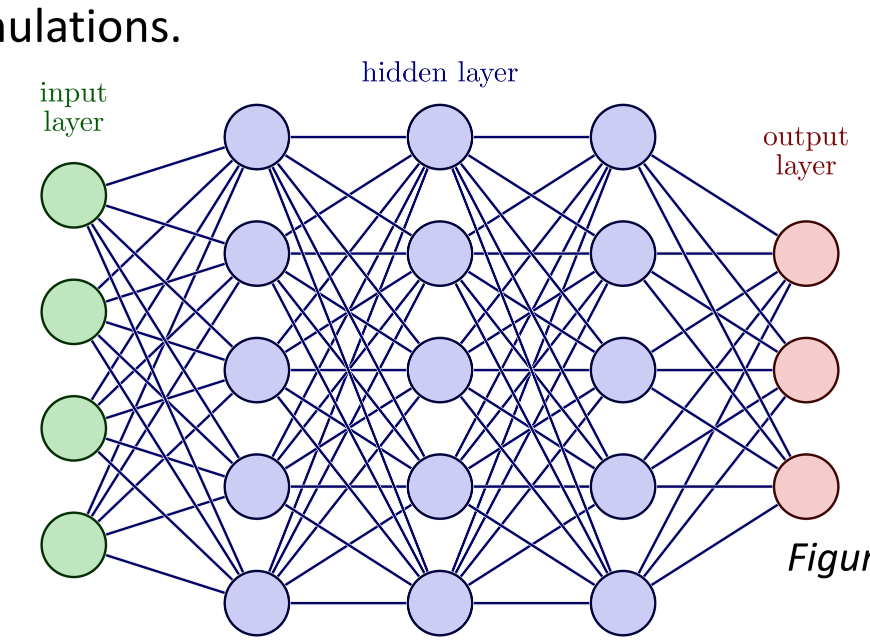
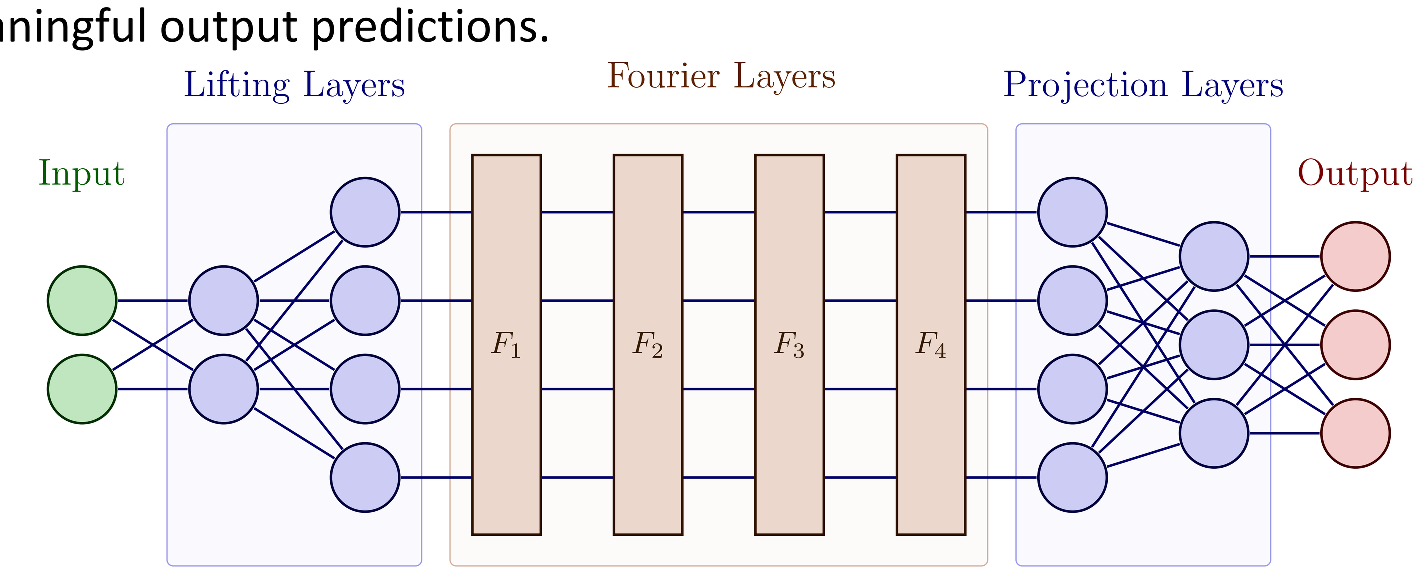


Figure 1: Neural Network from TikZ.net

Figure 1 shows a simple neural network with input, hidden, and output layers. Each neuron processes data through connections that adjust during learning to improve accuracy, with biases—additive factors that help make better predictions. Similar to a neural network, a neural operator processes data but is designed for more complex tasks, predicting entire functions instead of single values.
Bayesian methods incorporate uncertainty into predictions, providing a range of possible outcomes rather than a single estimate. **Fourier Transforms** convert complex signals into simpler sinusoidal components, like breaking down a chord into individual notes. A **Neural Operator** learns and predicts functions, handling complex data patterns.
Combining these, a BFNO uses Fourier transforms to handle complex data, neural operators to learn patterns, and Bayesian methods to visualize uncertainty. This results in a powerful tool for making robust and reliable predictions. Figure 2 illustrates the architecture of a BFNO, which consists of lifting, Fourier, and projection layers. Together they transform input data into meaningful output predictions.



$$F_i = \mathcal{F}^{-1}(R_i(\mathcal{F}x)) + W_i$$

Figure 2: BFNO architecture

Architecture of the Fourier Neural Operator

(a) The Full Architecture of Neural Operator:
1. Start with the input $a(x)$. **2**. Use a neural network P to lift the input to a higher-dimensional space. **3**. Apply consecutive Fourier layers with non-linear activation functions in between. **4**. Use another neural network Q to project back to the target dimension. **5**. The output is $u(x)$.
(b) Fourier Layers:
1. Start with the input function $v(x)$. **2**. On the top path: *a.* Apply the Fourier transform $\mathcal{F}$. *b.* (Optional) Remove higher modes. *c.* Perform a linear transformation R on the Fourier modes. *d.* Apply the inverse Fourier transform $\mathcal{F}^{-1}$. **3**. On the bottom path: *a.* Apply the convolution W. **4**. Sum the results of the top path (spectral convolution) and bottom path (regular convolution)

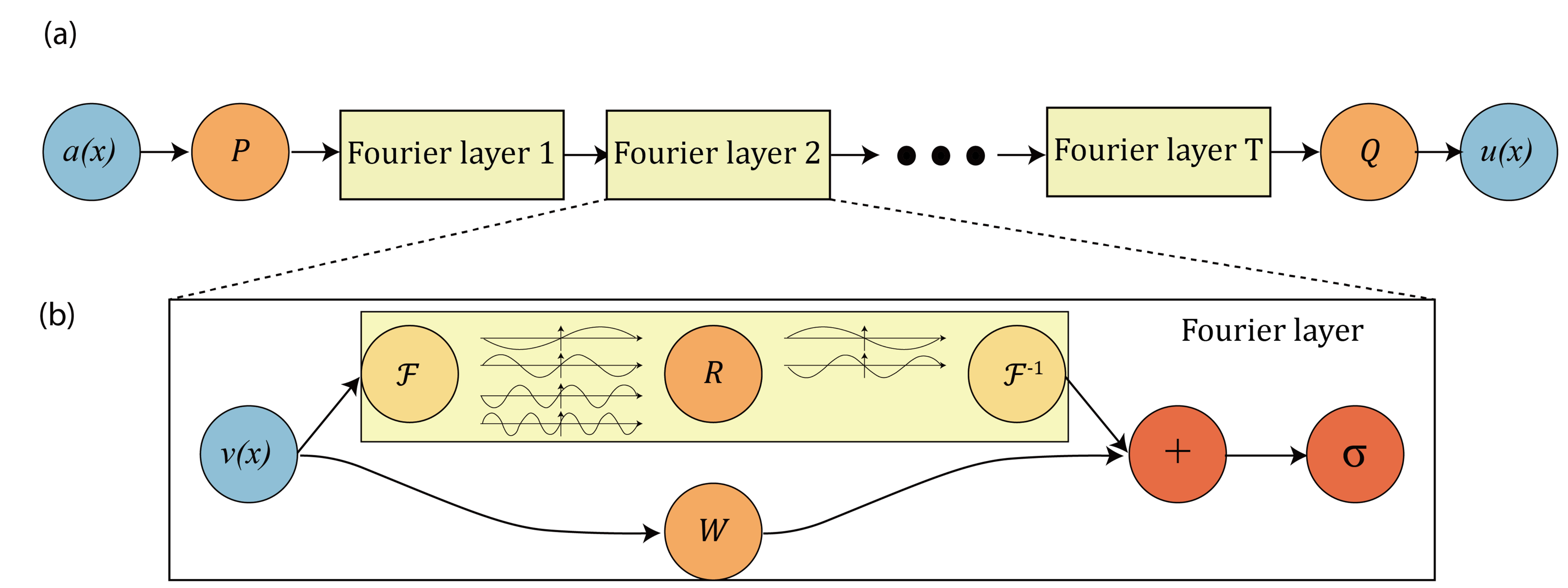


Figure 3: FNO Architecture From Li 2021

Deterministic vs. Stochastic Model

Here we compare the usefulness of deterministic and Bayesian Fourier Neural Operators (FNOs). Our results show that Bayesian FNOs achieve comparable accuracy to their deterministic counterparts but provide additional information that increases our confidence in the model.

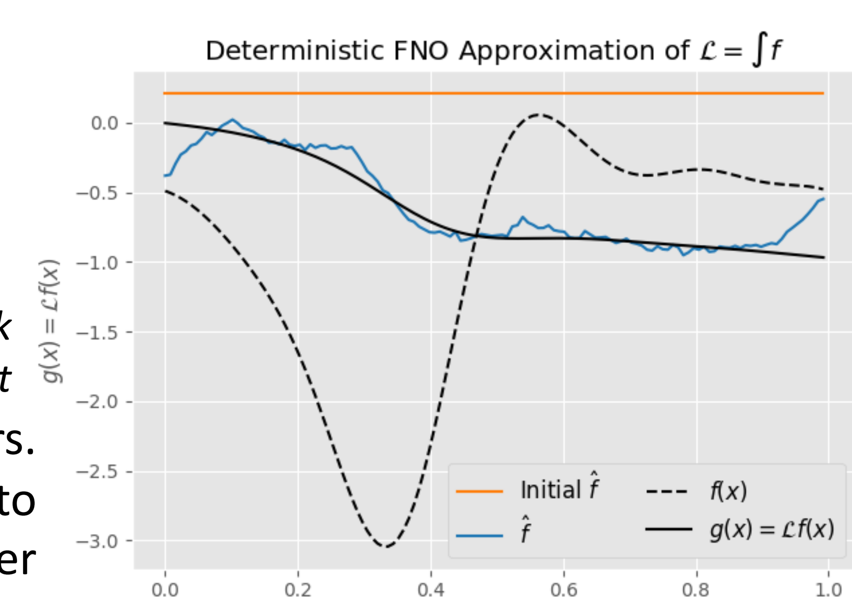


Figure 4: A deterministic FNO provides a single prediction, seen as the solid blue line.

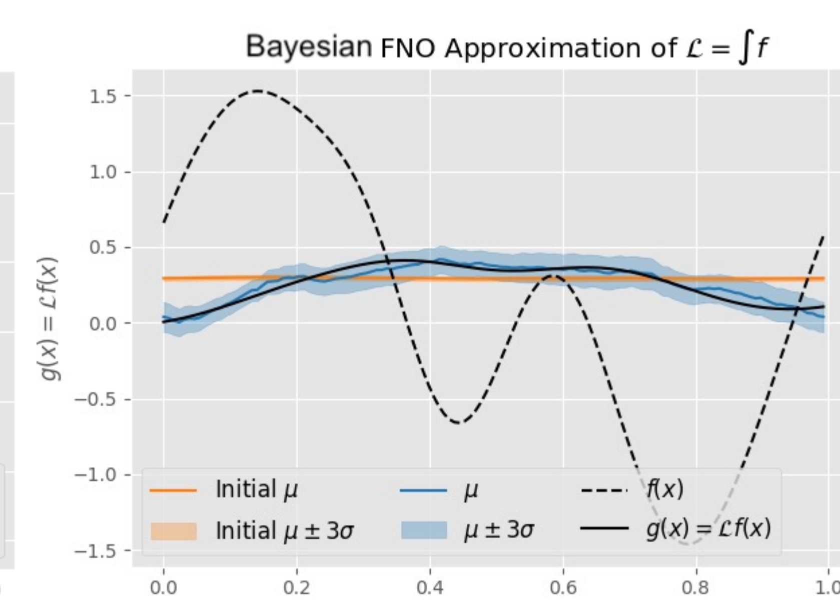
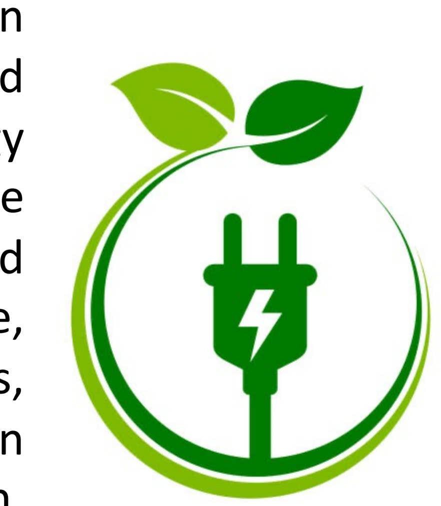


Figure 5: A Bayesian FNO provides an average, the solid blue line, and a range of predictions, shown as the shaded blue.

In the deterministic case, as seen in Figure 4, the FNO provides a reasonable approximation of the integral, with the blue line following the solid black line. Similarly, the Bayesian FNO, shown in Figure 5 approximates the integral well, with the blue line closely following the black line. The training and testing losses for both models (not shown), are similar, indicating comparable accuracy. However, the Bayesian FNO is more useful because it measures model uncertainty. Unlike deterministic FNOs, which learn static values, Bayesian FNOs learn a distribution of weights and biases. By evaluating the Bayesian FNO 1,000 times on the same input, we obtain a distribution of predictions and estimate the standard deviation, σ. The $\pm 3\sigma$ range, shown as the shaded blue region in Figure 5, represents this uncertainty.
This blue shaded region is crucial for understanding model uncertainty, achieved by introducing random variables to the network's weights and biases and learning their distributions during training.

Applications to Energy

A Bayesian Fourier Neural Operator (BFNO) offers powerful applications in the energy sector, including predictive maintenance and fault detection, optimization of energy systems, resource forecasting, climate and environmental modeling, and smart building energy management. By accurately predicting maintenance needs and faults, BFNOs enhance the reliability and efficiency of energy systems. They optimize performance, forecast resources, and model environmental impacts, aiding in the development of sustainable solutions. In smart buildings, BFNOs manage energy consumption, reducing costs and improving efficiency. These applications are just the beginning; the potential uses for BFNOs in energy are endless.



Conclusions

The Bayesian Fourier Neural Operator (BFNO) marks a significant advance in machine learning by integrating a probabilistic approach to uncertainty quantification. Building on Bayesian neural networks (Blundell 2015) and Fourier Neural Operators (Li 2021), BFNO enhances prediction accuracy and reliability through error bars. This has various applications in the energy field, such as optimizing renewable energy sources, improving grid stability, and enhancing energy consumption forecasts. Our research offers a proof of concept for BFNO's utility and a user-friendly implementation of both deterministic and Bayesian Fourier layers. We aim to create more effective models and encourage further research into innovative network architectures through our open-source contributions which will be available soon as a part of UQpy.

Acknowledgments

Thanks to ROSEI for the opportunity to participate in this Undergraduate Research Experience. I am grateful for the support and guidance of Professor Michael Shields, my student mentor Connor Krill, and the entire Shields Uncertainty Research Group. It has been an incredible opportunity to be apart of this amazing program.

For more information, contact nbetter1@jhu.edu