NP-ODE: Neural Process Aided Ordinary Differential Equations for Uncertainty Quantification of Finite Element Analysis

Yinan Wang[1], Kaiwen Wang[2], Wenjun Cai[2], and Xiaowei Yue[2]
[1]Rensselaer Polytechnic Institute, Troy, NY, USA
[2]Virginia Tech, Blacksburg, VA, USA

1. Research Overview

Dr. Yinan Wang and his research group focuses engineering-driven machine learning for complex physical systems. This research overview will present one of their works on the physics-informed stochastic process for uncertainty quantification of finite element analysis. This research was awarded the Best Paper Award in the 2022 IISE Transactions with Focus Issue on Design and Manufacturing and selected as the Finalist in 2021 INFORMS Quality, Statistics and Reliability (QSR) Best Student Paper Competition.

2. Introduction

Finite element analysis (FEA) is a powerful tool in modeling complex nonlinear systems and has been applied to many fields, including advanced manufacturing, new material design, solid/fluid mechanics, and multiphysics systems. Despite the strength of the FEA method in accurately analyzing complex systems, its application is hindered by two limitations: (1) the high-fidelity FEA simulation usually requires a high computational cost; (2) FEA is a deterministic simulation without explicitly considering the system uncertainties. In most systems with complicated nonlinear behaviors, it is challenging to obtain deterministic and accurate measurements of the parameters when building up the FEA so that uncertainty quantification (UQ) is highly demanded in FEA. To tackle the aforementioned limitations of FEA, stochastic surrogates, such as Gaussian Process (GP), Bayesian Neural Network (BNN), and Neural Network with Dropout (NN with Dropout), are built on the simulations of FEA to approximate and replace the FEA in system modeling, which both improve the computational efficiency and conduct UQ. However, the performances of these stochastic surrogates are highly related to the choice of hyper-parameters. Furthermore, their learning process is prohibited on the large and complex dataset. Following the idea of GP, Neural Processes (NPs) are proposed to learn distributions over functions between the input and output based on given observations, which uses the Neural Network (NN) to approximate the covariance function and has the strength in modeling large and complex dataset. However, it is still a purely data-driven method, which lacks the physical insights in replacing FEA to model systems governed by differential equations.

To strengthen Deep Neural Network (DNN) in modeling the real engineering system, most recent research works explored the interesting connections among DNN, Ordinary Different Equation (ODE), and GP. It has been shown that the output of DNN with the infinite number of residual blocks (infinite-depth) mathematically converges to the solution of ODE using Euler's method (Neural-ODE), and the infinite-width random DNN is theoretically equivalent to the GP. These two important mathematical connections inspire us to propose the new idea to design a physics-informed stochastic data-driven surrogate for the FEA by fusing the features from DNN, ODE, and GP. Motivated by the gap between properties of the FEA and existing surrogates, we propose Neural Process Aided Ordinary Differential Equations (NP-ODE) by incorporating Neural-ODE as basis modules into NPs. To this extent, both the

FEA and our proposed NP-ODE are built to approximate solutions for systems with underlying differential equations. Furthermore, the structure of stochastic processes enables the NP-ODE to conduct UQ on the predicted output. Lastly, the NP-ODE has the mathematical connections and convergent property with infinite-depth and infinite-width NN by making full use of the merits of neural networks, differential equations, and Gaussian processes.

As shown in Fig. 1, NP-ODE mainly follows the encoder-decoder structure. The deterministic encoder is followed by an attention module and its role is to take the weighted aggregation of the deterministic representations $(\mathbf{d}_{1:n})$ based on the similarity of observed inputs $(\mathbf{x}_{1:n})$ and the queried (unobserved) input $\mathbf{x}_{n+1}$. Similarly, the $\mathbf{s}_c$ is generated by the mean aggregation of stochastic representations $(\mathbf{s}_{1:n})$. The NP-ODE is built to incorporate the Neural-ODE as the decoder. As shown in Fig. 1, in Neural-ODE, the ODE network along with the ODE solver (e.g. Euler method) can approximate the continuous transformation $\mathbf{f}_{NODE}(D)$ of the input representations, and a smaller step size ΔD can give a better approximation accuracy of FEA simulations. $h_1(.)$ and $h_2(.)$ represent two FC layers used to map the output features from Neural-ODE to predicted mean $\bar{\mathbf{y}}_{n+1}$ and standard deviation $\boldsymbol{\sigma}_{n+1}$, $\hat{\mathbf{f}}_{NODE}(D_i)$ represents the dynamic feature transformations modeled by Neural-ODE, $\mathbf{d}_C$ and $\mathbf{z}$ are the deterministic and latent representations of observed data, respectively. To learn the parameters of NP-ODE, the loss function is to maximize the evidence lower bound (ELBO) based on the observed data points $(\mathbf{x}_{1:n}, \mathbf{y}_{1:n})$ and unobserved target data points $(\mathbf{x}_{n+1:n+T}, \mathbf{y}_{n+1:n+T})$.

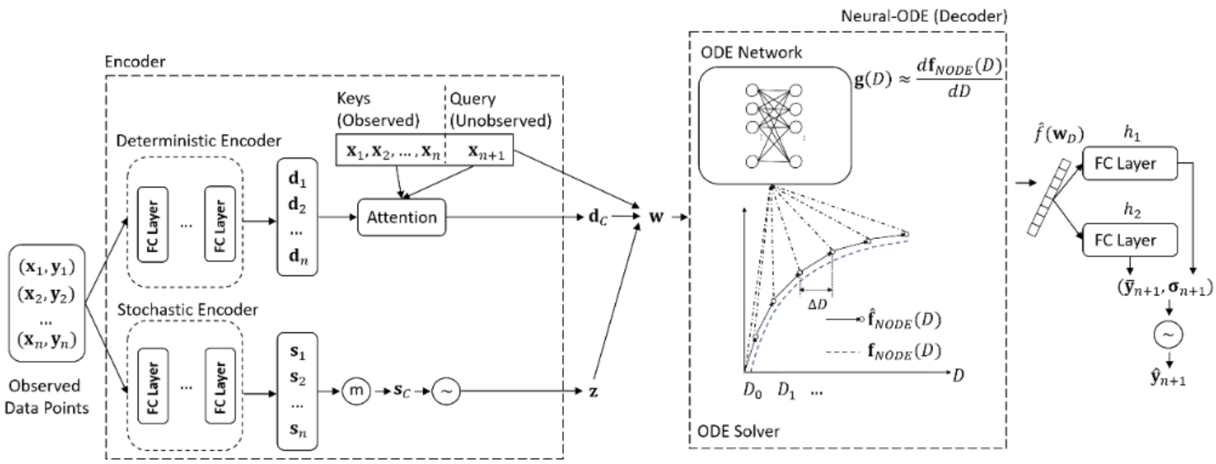

Figure 1. Structure of NP-ODE

The advantages of our proposed NP-ODE can be summarized into several aspects: (a) compared with the Gaussian process and its variants, our proposed NP-ODE shows a better ability in exploring limited training samples and has a robust performance in both predictive error and UQ when decreasing the training samples; (b) compared with original NPs, the incorporation of Neural-ODE reduces the number of model parameters and enables our proposed NP-ODE to better model FEA simulations; (c) the proposed NP-ODE solves differential equations in its decoders, so it is more physically close to the mechanism of original FEA. The codes and dataset for this paper are available in this link https://github.com/wyn430/NP_ODE. The full version of this work can also refer to https://doi.org/10.1080/24725854.2021.1891485.