2019-2020 Grand Challenge Award Final Report

Awardee: **Tan Bui-Thanh, Associate Professor**
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Research Award Title: **Advanced deep learning strategies for forward and inverse problems**

Research Summary

The field of Machine Learning (ML) refers to computational and statistical methods for automated detection of meaningful patterns in data. Deep learning (DL), a subset of machine learning, learns data representations using artificial neural networks (NNs). While deep learning approaches have proved to be state-of-the-art methods in the fields of computer vision, speech recognition, natural language processing, etc, its success is limited in the scientific computing community. Unlike numerical methods, such as finite element methods, in which solution accuracy and reliability are guaranteed under regularity conditions, DL results are often far from providing reasonably accurate results. The reason is that though approximation capability of NNs is as good as classical methods in approximation theory, NN accuracy is not attainable in general due to limitation in training. It has been shown that the training problem is highly nonlinear and non-convex. Moreover, the gradient of loss functions can explode or vanish, thus preventing any gradient-based optimization methods, e.g. stochastic gradient descent, from converging to a minimizer. The recent ICERM Scientific Machine Learning workshop January 2019 showed that though the past decade has seen tremendous advances in both theories and computational algorithms for machine learning, training NN remains a grand challenging problem facing the machine learning community. Thus, there is a critical need to develop advanced strategies to tackle this crucial challenge in order to enable the potential of deep NNs for computational sciences and engineering applications.

Major accomplishments under the Moncrief Grand Challenge Award

- We have developed a model-constrained variational auto-encoder approach to solve Bayesian inverse problem. We have demonstrated the validity and the efficiency of the method on inverse problems governed by elliptic partial differential equations (PDEs). In addition, various theoretical results were developed to justify the approach. Our paper is in the second round of the review.

- We have been developing ROM-ML approach in which we develop a projection-based reduced- order model (ROM) to capture essential physics and then enhance the resulting ROM with a deep NN to learn the discrepancy between the full and reduced quantities of interest. We have demonstrated the accuracy and efficiency of the approach for inverse problems governed by both elliptic and convection-diffusion PDEs. We are in the final stage of finishing the paper and we expect to have it done soon.

- We have developed a CNN-autoencoder approach for data dimensionality reduction to speed up solutions of big-data inverse problem. Our approach has shown promising results for inverse problems governed by the elastic-acoustic wave equation. We currently develop approaches to further reduce the training data and the number of hyper-parameters. This is ongoing and we expect the work will be done at the end of Summer 2021.

The above major research work, when published, will acknowledge the support of the Moncrief Grand Challenge Award.