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# Prediction Of Nuclear Material Properties Under Uncertainty

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The nuclear sector is facing increasing pressure related to the economic sustainability and safety of the civil use of nuclear energy (Horvath and Rachlew, 2016). In fact, new nuclear reactors are still quite expensive due to the necessity to guarantee the highest level of safety. This in turn, requires demonstrating the performance of materials under new environmental conditions that it is often based on expensive material characterization where a single fracture test on a material can amount to £15000 per test (Tang et al. 2022). Therefore, there is the necessity to develop robust predictive models for nuclear materials. Recently, deep learning tools such as neural networks have started to become reliable predictive tools able at capturing the relation between inputs and output (Lye et al., 2022a), and therefore they may be become useful at predicting the nature of nuclear material as well.

Current available tools are still suffering some limitations such as the necessity to be training on a large data set, the limited capabilities of dealing with uncertainty and to capture the physics relationship between such material inputs and outputs (Boehnlein, et al., 2022). To overcome some of such limitation, a feasibility project named PROMAP project was recently carried out (Larracy et al., 2021). A database of the material properties for 58 different steel types were analysed to predict the creep-rupture properties, and tensile properties. Inputs features contain material code (represent different materials), cast code (represent different batches), temperature and composition of 19 elements; the target features contain fracture time, elongation, reduction of area, ultimate tensile strength, 0.2 % Proof Stress (PS02). It is not difficult to see there are potential physical relationships existing between the output features. To address the problem of limited training data set, the use of argumented training data set was proposed and constructed based by perturbating the values in the dataset while satisfying the covariance matrix of the original dataset (Lye et al., 2022a, 2022b). Although the approach demonstrated the possibility to enhance probabilistically the training data set and generating model predictions with confidence bounds, the approach suffers from several limitations: a very small subsection of inputs features was included, correlation and dependencies among data outputs not accounted for, and no physical constraint used to analysis the dataset. In the earliest stages of the research, attempts were made to use all the features to individually predict a single output, but this approach led to overfitting. The model had more parameters than available data points, a common issue when using a single-output network for limited data predictions (Bejani and Ghatee, 2021).

To overcome the aforementioned limitations, different methodological strategies were examined. For instance, the analysis of the behaviour of different batches, as well as the physical dependencies among outputs, and even similarities with other materials are offering alternative routes to solve inadequacies in the data set as shown schematically in Figure 1 (a). For instance, neural networks can be pre-training using secondary datasets (i.e. experimental dataset of similar material type) to pre-capture and learn a rich set of feature representations. Then, the model is fine-tuned using the limited available data, in our case specific for each material type and cask code. In other words, the learning efficiency and predictive performance are improved by using knowledge learned from similar tasks. This methodology can be seen as a type of transfer learning (Rocchetta et al. 2019). Clearly this required the collection of additional datasets that are relevant for solving the original problem.

On the other hand, by introducing physical rules as constraints as seen in the physics-informed neural networks (PINN) (Cuomo et al. 2022.), it is possible to significantly reduce the size of the training space while assuring compliance with known physical relationships. The introduction of physical constraints also prevents models from learning erroneous data relationships that are inconsistent with the rules of the actual physical world. Based on physical correlations present in the predicted output features, e.g., area vs elongation, the training dataset can be used to predict one output at the time while using the error of predicting other related physical quantities as a penalty function in the objective function.

It is also known that realistic dataset contains errors, and they are affected by uncertainty (i.e. reported values might represent realisation of underlying stochastic process, or imprecision to the actual value might be associated to the experimental and numerical accuracy). To handle the embedded uncertainty in the data set and provide prediction with associate level of confidence, Bayesian Neural Network (BNN) has been adopted in this research (Mohebali et al., 2020). Some preliminary results about the use of BNN, the pre-training, and physical constraint are shown in Figure 1 (b). These preliminary results which compares the BNN predictions under three different settings, only consider a limited number of input features and a single output and a predefined network architecture. The first BNN has been training adopting strategy of leave-one-out, the second BNN has been pretrained using dataset from NRIM Creep Data Sheet No. 38A (National Research Institute for Metals, 1991) showing a slightly improvements. The third BNN has been training adding physical constraints base on the Larson-Miller Parameter (LMP). Unfortunately, the chosen physical constrain produces a slightly decrease on the performance. Further research activities will be focusing on understanding the effect of the network architecture on the predictive performance, investigating new physical constrains and using all the features available in the original dataset of nuclear material.

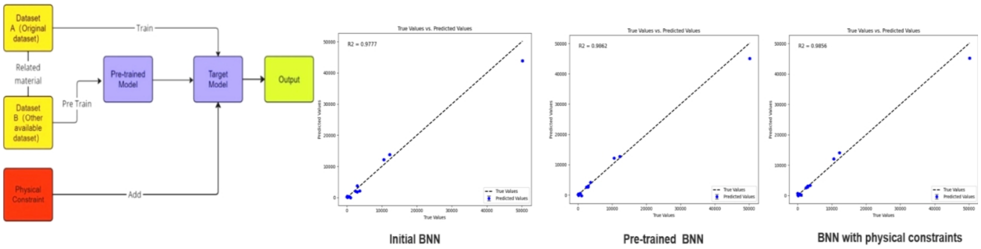


Fig. 1. (a) Strategies proposed to handle limited training datasets; (b) Preliminary results of the use of BNN model.

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