PERFORMANCE AND SCALABILITY OF DEEP LEARNING MODELS TRAINED ON A HYBRID SUPERCOMPUTER: APPLICATION IN THE PREDICTION OF THE SHEAR STRENGTH OF SLENDER RC BEAMS

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Abstract. *Data-driven models employing artificial intelligence approaches have been increasingly utilized in structural analysis and design problems over the past two decades. The main applications involve the processing of datasets, which are gathered from experimentally derived records or obtained numerically, in order to develop closed-form formulae or numerical tools predicting quantities related to structural response and mechanical behaviour. Given that datasets are difficult to assemble due to the limited available information and the high cost entailed to enrich them, exhaustively processing the available data to produce the best possible prediction models is an essential task of particular interest. For specific applications, this exhaustive computing task involves large numbers of iterations performed to train detailed prediction models with large numbers of parameters. Despite the intense computational demands of such problems, limited research work exists on the scaling-up of the utilized algorithms on supercomputers. In this work, a distributed training and hyperparameter tuning algorithm is proposed for the modelling of the shear strength of slender beams without stirrups. The training dataset comprises results obtained from the detailed modelling and analysis of several beams with non-linear finite elements using the Reconan software. The results presented in this research work highlight the importance of optimally utilizing computational power for the solution of such problems. The developed computer code is available on GitHub.*

1 INTRODUCTION

Artificial intelligence techniques have emerged over the last decades as an effective and efficient tool to predict analysis outputs for computationally demanding engineering problems. Application areas requiring multiple analysis runs (design optimization, structural reliability, etc.) have largely benefited from various computational approaches eliminating the need for performing actual analyses by providing adequate estimations for the outputs of interest (e.g. $[1, 2, 3, 4]$.

The training process of an Artificial Intelligence model is itself a demanding task in terms of computational resources. Particularly, an Artificial Neural Network can comprise millions of parameters to train via iterative procedures, such as the stochastic gradient descent algorithm. These algorithms yield data structures that frequently cannot fit in the GPU (graphics processing unit) accelerators' RAM; hence parallelization is vital for the accomplishment of the training task, and obtaining accurate results. The optimization algorithms employed during the training process of a deep network can be parallelized by following either of two main routes. The first one is data parallelism $[5, 6, 7]$, which foresees the splitting of the "batch of samples" (utilized in each iteration) into a number of smaller mini-batches, which are processed in parallel, depending on the number of available resources (GPUs). Alternatively, we may use model parallelism [8], by partitioning the deep learning model on distributed GPUs.

Despite the fast-pacing growth of deep learning, along with the vast need for computational resources, there are rather limited relevant engineering applications reported in the literature [9, 10, 11, 12, 13], none of which concerns reinforced concrete (RC) structures or slender beams. The purpose of this work is to investigate deep-learning algorithms for the prediction of the shear strength of RC beams. For the needs of this research work, detailed 3D finite element (FE) modelling of RC structures is adopted [14, 15, 16, 17, 18], in order to develop a large database of results on slender RC beams without stirrups. The numerically generated data set is then used to train models to predict the beams' shear strength. A new algorithm is designed and programmed, in order to be able to develop multiple input files (FE models) and efficiently analyze them through the use of the software Reconan FEA [19]. The newly developed algorithm (Reconan Multirun) and Reconan FEA were used to generate and analyse approximately 36,000 slender RC beams without stirrups; the obtained results were used for the training of the predictive models.

2 DATABASE ASSEMBLY

For each beam considered, 10 independent variables (input) and one dependent variable, which is the load corresponding to the ultimate strength (output), are varied. Particularly, the basic geometric variables are varied for each beam: the net span L (mm), the width b (mm), and the effective depth d (mm) of the beam. Apart from these variables that affect the FE meshing of the beams, strength and material related variables are also varied, and, particularly, f_c (uniaxial compressive strength of a cylindrical specimen in MPa), E_c (concrete Young modulus in MPa), f_t (concrete tensile strength ratio), β (remaining shear capacity strength factor), E_s (steel Young modulus in MPa), f_y (steel yielding stress in MPa), and ρ (tensile longitudinal reinforcement ratio).

Sampling for the 10 independent variables was performed uniformly as per Table 1, with the variables' coefficient of variation $c_v = \frac{\sigma}{m}$ (standard deviation over mean) being kept within the range 0.2 to 0.5 [20]. Hence, for each group of beams, different values for geometric and strength variables were generated, and the overall database is finally constituted of 35,849

		$d \qquad b$	f_c E_c f_t β		E_{s}	ρ
					Minimum 1500.0 260.0 200.0 20.0 25000.0 0.020 0.020 1.90×10^5 400.0 0.0010	
					Maximum 8700.0 1310.0 600.0 60.0 35000.0 0.100 0.050 2.10×10^5 600.0 0.0200	
C_{η}					0.416 0.406 0.228 0.305 0.097 0.404 0.252 0.029 0.115 0.627	

Table 1: Statistical metrics of independent variables.

observations in total. Out of the total database population, 85% was used as a training set and the remaining 15% was used for testing.

3 BASELINE AND MACHINE LEARNING MODELS

The predictive modelling of the database was implemented by utilizing four machine learning (ML) methods, and in particular Linear Regression (LR), Non Linear - higher order Regression (NLR) [21], Random Forests (RF) [22] as implemented in [23], and Gradient Boosting $[24]$ (GB) as implemented in $[25]$. The performance of each ML method varies, and the Mean Absolute Percentage Error (MAPE) [26] was used as a meaningful metric for engineering applications. The MAPE in the test set for the four methods was 10.843 (RF), 12.178 (GB), 22.036 (NLR), and 32.211 (LR). Random forests exhibit the lowest MAPE for the test set, while LR the highest, which was expected as it is the simplest (linear) model used. Nonlinear regression (NLR) exhibits higher error than RF and GB, however, the NLR model is useful due to the closed-form formula that it generates. The distribution of ML models' residuals exhibited a shape close to the Gaussian, for all methods except the linear regression, which was skewed. This is due to its inability to capture the non-linear behaviour of the variables included in the model, highlighting the need for more complex ML models.

4 DISTRIBUTED DEEP LEARNING

PyTorch was used herein which is an "imperative style, high-performance deep learning library" [27], distinguished for scientific as well as industrial projects, due to a straightforward yet efficient implementation of an automatic differentiation algorithm [28]. For multi-GPU training, the Horovod [29] was implemented, a library that has been developed at Uber. Particularly, by using Horovod, one may take a single-GPU training script and efficiently scale it to run across many GPUs in parallel. With MPI commands [30], each process is initialized and is assigned its MPI rank in a straightforward manner, which is achieved with fewer code changes compared to other approaches. Ultimately, Horovod scripts can run on a single-GPU, multiple-GPUs, or even multiple hosts without any further code changes. Algorithms on various experiments were tested for the needs of this research work on the Cyclone Supercomputer¹, utilizing PyTorch for computer vision as well as regression tasks², highlighting the efficiency of data parallelism, as well as the scaling-up capabilities compared with standard ML platforms, such as Kaggle and Google Colab.

4.1 Parallel Stochastic Gradient Descent

In Stochastic Gradient Descent, at each iteration, a random data-point i is selected, the Loss Function for this data-point is differentiated, and then the weights for the entire network are

¹https://hpcf.cyi.ac.cy/

²https://github.com/CaSToRC-CyI/artificial-intelligence-hpc

updated. In mini-batch Stochastic Gradient Descent, i is the current "batch" of data, which is a subset of all dataset indices. The parallelization is performed at this point, by updating the weights for all batches in parallel. Hence, in Parallel Stochastic Gradient Descent, for each GPU (in parallel) a random data-point is selected, for which the gradient is computed and the weights are mixed. The average for the mixing of the weights can be implemented for this purpose, or other methods, such as ensembles, AdaSum, etc. Afterwards, the update of the weights for all GPUs takes place. In order to perform this operation in parallel, the utilization of MPI³ framework is required, so as to gather the results among all GPUs, reduce, and broadcast them across all available GPUs again. This algorithmic procedure is described in Figure 1.

Figure 1: Parallel Stochastic Gradient Descent.

In general, it applies that, when using larger batch sizes the procedure becomes faster, and when adopting smaller batch sizes it becomes more accurate. In any case, the batch must fit into the relevant hardware memory, so the utilization of a larger number of nodes is required when a GPU cannot handle the batch size. Furthermore, in practice, the weights' mix causes some accuracy losses. However, all these aspects regarding the computational behaviour of the Parallel Stochastic Gradient Descent procedure are not always absolutely valid, as the loss function is a highly non-linear function of the Artificial Neural Network's (ANN's) weights and depends on the dataset's particular features, thus the computational procedure's behaviour cannot be predicted. Therefore, the training of the network has to be performed by investigating a variety of architectures. In order to effectively treat this issue, hyperparameter tuning is adopted in the present work, and, ultimately, the training of a very large network on Cyclone supercomputer is attempted.

4.2 Hyperparameter tuning

In order to investigate the effect of the network's hyperparameters, the Ray-Tune⁴ module of PyTorch is implemented. Particularly, a number of ANNs are constructed by varying the batch size, the drop-out ratio, the number of Epochs and neurons, as well as the learning rate. Subsequently, the training of the networks is conducted. Accordingly, for each training example, the time for the training is recorded, while the final loss function and the ratio among the validation and train loss *Ratio V-T* are computed. The results obtained are presented in the Appendix. This

³https://mpitutorial.com/tutorials/mpi-reduce-and-allreduce/

⁴https://pytorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html

is a time-consuming procedure, therefore, it was found useful to identify an optimal drop-out region of ratios [31]. As depicted in Figure 2, it can be concluded that, for lower drop-out values, the corresponding values of the loss function are also lower. However, as will be explained below, the drop-out could not be zero.

Figure 2: Ray-Tune results.

4.3 Combination of MPI & Horovod

During the training of an ANN, the loss function is automatically recorded, as loss is the core function that is differentiated to update the weights. In engineering applications, the Mean Squared Error (MSE) does not offer meaningful information, and the MAPE is being utilized as a more practical metric. Accordingly, as the best ANN's architecture is not known in advance, and given that multiple experiments must be performed, it is necessary to record the MAPE during training in real-time. However, as the data are split and reside at many GPUs, an operator should be implemented that gathers the individual predictions to obtain an aggregated metric for the dataset as a whole.

For this purpose, a mix of Horovod with MPI is proposed. In Figure 3, three code snippets are depicted describing the implementation of such an operation. The overall operation starts with the initialisation of vector *pred* in the code at the upper right part of Figure 3, which is used later as a container of all results. The code at the upper left part imports the MPI module from mpi4py and gets the rank of each GPU. Afterwards, as shown in the code at the bottom-left part of Figure 3, after each step of the optimizer, a barrier is set to wait for all GPUs to finish with their numerical processes. Then, the responses y_{r} train pred of each GPU are stored in vector *pred_{-i}* and, with the *comm.gather* command, all results are placed in *pred_{-i}*. Finally, an additional barrier is introduced to wait for all GPUs to finish and concatenate the results in vector *pred* only for rank 0. At this stage, vector *pred* holds the concatenated predictions and can be utilized to calculate the MAPE.

Figure 3: Combination of MPI and Horovod.

4.4 Parallel training

Figure 4 demonstrates the learning curves for the model without using a drop-out and with a 10% drop-out. In the case of no drop-out (Figure 4, left), even though there is in general a decreasing tendency in MAPE with the number of epochs, a number of significant peaks are evident. This can be interpreted as an effect of the averaging of the weights in parallel, which is a source of error. However, with the utilisation of a 10% drop-out (Figure 4, right), smoother learning curves are achieved and the aforementioned phenomenon seems to be not activated. Furthermore, it should be stressed that the validation curve for 10% drop-out is lower than the training curve, which is very important for the generalisation of the results.

Figure 4: Drop-out effect on the loss function during training in parallel. The model with drop-out exhibits a validation loss history with lower values than the corresponding train curve.

It is noteworthy to state that a variety of experiments was performed to attain an optimal dropout ratio. Figure 5 presents results for a drop-out equal to 0.01. As can be seen at the right part of Figure 5, when the validation curve is higher than the training curve, it practically stabilizes around a constant value. This is helpful during training, as over-training of the network will not cause over-fitting of the derived predictive model.

Figure 5: Results for low drop-out=0.01.

5 CONCLUSIONS

The numerical experiments performed in the present work comprised networks with large numbers of neurons, and thus, weights. For example, a network with 1000 neurons per layer and 10 layers corresponds to approximately 10 million weights to be optimised. As the most suitable network architecture is not known a-priori, several experiments need to be performed towards establishing the minimum possible error. Hence, computational power is vital for the best possible accuracy of the predictions.

It was also found that using PyTorch and Horovod as a functional solution for running deeplearning models on Cyclone Supercomputer is a very efficient approach. Furthermore, according to the parametric investigation performed in this research work, deep learning exhibited high accuracy in comparison to other ML methods. The best loss attained (MAPE) was 5.94%, while with Random Forests the corresponding loss was 10.7%, with Gradient Boosting 12.7% , Non-Linear Regression 24.0%, while Linear Regression had the worst numerical response with 32.3% loss.

The dataset under study comprised values with an increment of 10 kN and an average of 98.22 kN, thus an error $\frac{10/2}{98.22} = 5.091$ inevitably occurs on average. Henceforth, any improvement of the 5.94% loss attained would be trivial. This highlights the power of deep learning on one hand, however, the computational demand for training as well as optimising the architecture of such networks is very expensive. Distributed training made these operations possible herein, achieving both efficient and accurate results.

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⁵https://hpcf.cyi.ac.cy/

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APPENDIX: HYPERPARAMETER TUNING RESULTS

