An Algorithm to reduce evaluation time of Interpolated Deep Material Network during Hyper parameter tuning

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I. Introduction

In recent times, availability of high resolution μ-CT images of microstructures allows for Digital Material characterization workflows to obtain virtual experimental data [1]. Calibrating the effective nonlinear material models from experimental data uses modern state-of-the-art methods [2]. There is a need to replace the forward problem in the calibration process with faster models that are not only data-driven, but incorporate more physics to ensure confidence in predictions [3]. Deep Material Network (DMN) [3] combines concepts in laminate theory and machine learning to allow predictions, that extrapolate to the nonlinear elastic domain by just training in the linear elastic domain. The training in the linear elastic case is described as offline training and nonlinear prediction is named as online prediction. It was seen that among 5 DMN's that were trained linear elastically, only one DMN worked well in the online prediction [5]. Dey et al [5], proposed to perform inelastic creep predictions of the model at intermediate epochs during the offline training to decide the stopping criteria. Adding to this, Gajek et,al [4] proposes an interpolated version of Deep Material Network which allows jointly identifying a single model for the entire fiber orientation triangle(FOT) [4]. Each point on the FOT represents a microstructure. In this work 31 points are sampled on the FOT and the online prediction for plasticity is performed over 109 points for validation. For a highly nonlinear case of the interpolated DMN, evaluating inelastic predictions like creep on many different microstructures at intermediate epochs like the one proposed by Dey [5] might be computationally expensive. Instead of a stopping criteria based approach, in this work an alternate method is proposed to choose the best model. In the proposed method, offline training is performed over a fixed number of epochs and intermediate models are stored in every few epochs. Then these models are selectively evaluated based on an adaptive threshold, thus reducing the number of evaluations. The algorithm is proved for the plasticity case and future scope for identifying an interpolated version of the DMN for the creep case is motivated.

II. Design

Training the interpolated version of Deep Material Network involves sampling and generating the microstructures [5] for each point on the FOT [4]. Material stiffnesses are sampled and linear elastic homogenization is performed to generate the training data. This way an equivalent laminate microstructure whose arrangement can be changed is obtained as shown in Figure 1. During training intermediate model states at specified epochs are stored for the online evaluation. The basic components are shown in Figure 2. The online evaluation is performed using the distillation algorithm shown in algorithm 1. Here the **state list** indicates a list of model states at chosen intervals of epoch. The **node list** is the list of all the points on which online evaluations are run in the plasticity case for validation. The goal is to identify the best model in the **state list** that gives the least **Error metric** for all the microstructures in the **node list**. The chosen **Error metric** is adaptively increased in precomputed fixed intervals until the best model is obtained. This significantly reduces the number of evaluations.

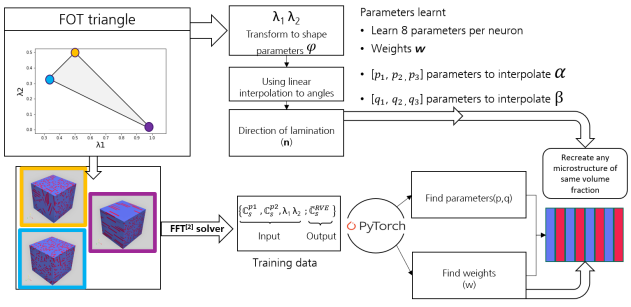

Fig. 1. The figure shows the simplified offline training procedure of an interpolated Deep Material Network

III. Evaluation

A hyperparameter set was identified and data was generated with 31 different microstructures [6]. The error metrics used for both maximum and mean values over the entire FOT is

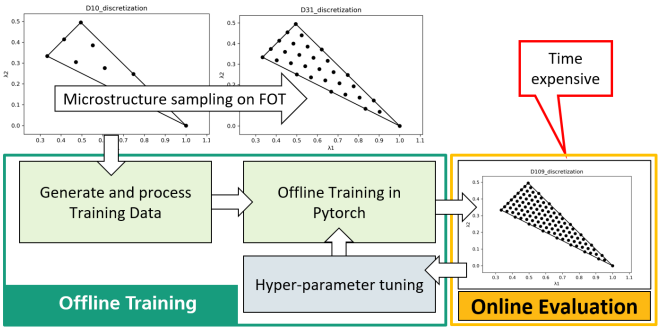

Fig. 2. The figure shows the global steps of Hyper parameter tuning in Deep Material Network. Note that retuning is required in the offline training if errors in online predictions are high. In this case: After training on 31 different microstructures and storing models at intermediate epochs. Online Evaluation with plasticity is done on 109 different microstructures resulting in huge computational bottle neck.

Algorithm 1 Selective distillation algorithm

state list : $S_1 \dots S_M$
node list : $N_1 \dots N_N$
while count != 109 **do** ▷ Until we reach bottom most filter
    count = 0 ▷ restart from initial node every time the inner loop exits
    for node in node list **do**
        if node == first node **then**
            for state in state list **do**
                E_1^{state} evaluate to list E_1^M
            end for
            Error metric = min of list E_1^M ▷ assign the threshold
            Update = $\frac{maxE_1^M - minE_1^M}{1000}$ ▷ precomputed increments
            state list : state with $E_1^{state} \leq$ Error metric
        else
            for state in state list **do**
                E_{node}^{state} evaluate to list E_{node}^m ▷ $m \leq M$ states removed
            end for
            state list : state with $E_{node}^{state} \leq$ Error metric
        end if
        Count = Count + 1
        if state list is empty **then**
            Error metric = Error metric + Update ▷ increase the threshold
            Exit for loop
        end if
    end for
end while

given by equation 1 and equation 2 respectively. The errors are calculated as the maximum over 6 loading cases and are cyclically loaded in time to cause plastic perturbation in the matrix. Further maximum error over the entire FOT is considered as the final metric. The online evaluation for the case of plasticity was performed for 109 different microstructures with the selective distillation algorithm. The time taken without the algorithm has been estimated. The table I summarizes the key results.

$$e_{max}^{\text{plast}} = \max_{i\in(1,2,3),j\in(i,3)} \max_{t\in\mathcal{T}} e_{ij,t}^{\text{plast}}. \quad (1)$$

$$e_{mean}^{\text{plast}} = \max_{i\in(1,2,3),j\in(i,3)} mean_{t\in\mathcal{T}} e_{ij,t}^{\text{plast}}. \quad (2)$$

Parameters	without distillation	with distillation
states to be evaluated	120 states	120 states
Number of nodes	109	109
Number of load cases	6 load cases	6 load cases
Full evaluation number	120 × 109 × 6 = 78480 evaluations	**800 evaluations**
Total time taken	9-14 days	approx 15 hours

TABLE I
TIME COMPARISON FOR FULL EVALUATION

Loadcase	Maximum error in %	Mean error in %	Variance of distribution
Aggregate	10.9168	7.3187	3.1287

TABLE II
ERRORS OVER THE ENTIRE FOT ACHIEVED BY THE IDENTIFIED DMN

IV. Conclusion and Future Work

Table I shows the number of evaluations for online evaluation without and with selective distillation. For the particular case, 98.9 percent of the evaluations were reduced. The algorithm can further be enhanced by introducing node ranking which places nodes with higher errors in a higher priority so that models are eliminated early on. The table II shows the maximum error obtained over the FOT is within acceptable limits.

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The work was supervised also by Dr Fabian Welschinger during the thesis work conducted at the University Of Stuttgart. The code for online evaluations was also a contribution of Dr.Welschinger.

References

[1] Dey, A. P., Welschinger, F., Schneider, M., Gajek, S., Bohlke, T. (2023). Rapid inverse calibration of a multiscale model for the viscoplastic and creep behavior of short fiber-reinforced thermoplastics based on Deep Material Networks. International Journal of Plasticity, 160, 103484.
[2] M. Kabel, A. Fink, and M. Schneider, The composite voxel technique for inelastic problems, Computer Methods in Applied Mechanics and Engineering, vol. 322, pp. 396418, 2017.
[3] Z. Liu and C. Wu, Exploring the 3d architectures of deep material network in data-driven multiscale mechanics, Journal of the Mechanics and Physics of Solids, vol. 127, pp. 2046, 2019.
[4] S. Gajek, M. Schneider, and T. Bohlke, An FEDMN method for the multiscale analysis of short fiber reinforced plastic components, Computer Methods in Applied Mechanics and Engineering, vol. 384, p. 113952, Oct. 2021.
[5] Dey, Argha , Welschinger, Fabian , Schneider, Matti , Gajek, Sebastian , Bohlke, Thomas. (2022). Training deep material networks to reproduce creep loading of short fiber-reinforced thermoplastics with an inelastically-informed strategy. Archive of Applied Mechanics.
[6] P. Bhat Keelanje Srinivas, master thesis-A data driven efficient multiscale computational tool using hybrid AI modelling framework for short fiber reinforced thermoplastics, University Of Stuttgart, 2022.