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Evaluation of Best Theories using Neural Networks and Adaptive Sampling

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Abstract. This work presents an Adaptive Sampling-based surrogate framework for predicting the accuracy of higher-order beam theories generated within the Carrera Unified Formulation. The objective is to identify the minimal set of generalized displacement variables required to achieve a prescribed accuracy, thereby reducing the need for exhaustive high-fidelity structural analyses. Structural theories are built using Taylor-like polynomial expansions, and an Adaptive Sampling strategy based on an Extra Trees Regressor iteratively selects the most informative generalized variables by combining predicted error, uncertainty, and structural diversity. The selected dataset is then used to train a Neural Network to predict the average error in natural frequencies. The proposed strategy is evaluated using Best Theory Diagrams, which relate model accuracy to the number of degrees of freedom. Results show that Adaptive Sampling achieves accuracy comparable to, and in some cases better than, random sampling at the same sampling budget, while correctly identifying the most effective structural theories with fewer high-fidelity analyses. The framework, therefore, provides an efficient tool for data-driven selection of refined beam models.

Introduction

In structural mechanics, creating accurate reduced models is crucial to lowering the computational complexity of 3D analyses. Since they involve fewer degrees of freedom than full 3D models, 1D and 2D theories are frequently employed. However, their accuracy may vary significantly depending on the structural problem, geometry, material properties, and loading conditions. Classical theories such as the Euler–Bernoulli Beam Theory (EBBT) [1] and the Timoshenko Beam Theory (TBT) [2,3] often fail to capture complex behaviors, including material anisotropy, shear deformability, and warping effects. To overcome these limitations, higher-order theories (HOT) [4,5] have been developed to address more complex structural problems. The Carrera Unified Formulation (CUF) [6] provides a general and systematic framework for defining structural theories of any order. The Axiomatic/Asymptotic Method (AAM) [7,8] can be applied to identify the most influential generalized unknowns and to construct efficient reduced theories for a given problem. Through AAM, the Best Theory Diagrams (BTD) [7,8] can be generated, which require evaluating a large number of candidate theories, resulting in high computational costs. In recent years, Machine Learning (ML) techniques [9,10], and in particular Neural Networks (NN), have attracted increasing attention in structural mechanics and finite element analysis due to their predictive capabilities and reduced computational time. The present paper trains an NN to predict the influence of each generalized variable and to identify the best theories that achieve the highest accuracy for a given number of degrees of freedom. In previous works [11,12], the theories included in the training set were randomly selected. In the present work, the selection uses the Adaptive Sampling [13-15] strategy to identify the most informative and meaningful generalized variables for training the NN. During the selection process, an Extra Trees

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surrogate model is iteratively updated and used to guide sampling based on quality, uncertainty, and diversity criteria.

CUF and FEM Formulations

The reference system adopted for beam structures is shown in Fig. 1. Here, the x-z plane lies on the cross-section Ω. More details about the theoretical formulations are available in [6].

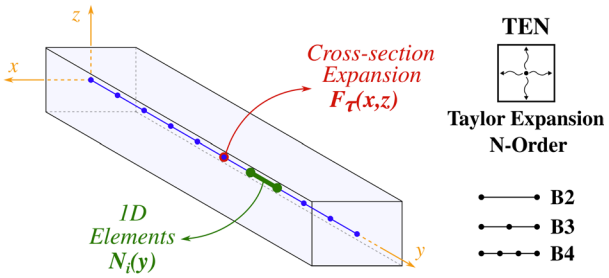


Figure 1: Reference Coordinate System for Beam Models

The displacement field for beams can be expressed as:

$$\boldsymbol{u}(x,y,z) = N_i F_\tau(x,z)\boldsymbol{u}_{\tau i} \tag{1}$$

Where F_τ is the expansion function; τ=1,…, M, and M is the number of expansion terms. N_i is the shape function; $i = 1, \ldots, N_n$, where N_n is the number of FE nodes. $\boldsymbol{u}_{\tau i}$ is the vector of the nodal unknowns. For 1D theories, the expansion function F_τ acts on the cross-section x-z, while the shape function is along the beam axis. For a complete fourth-order beam theory, the displacement field is:

$$\begin{aligned} u_x &= u_{x_1} + xu_{x_2} + zu_{x_3} + x^2u_{x_4} + xzu_{x_5} + z^2u_{x_6} + \cdots + xz^3u_{x_{14}} + z^4u_{x_{15}} \\ u_y &= u_{y_1} + xu_{y_2} + zu_{y_3} + x^2u_{y_4} + xzu_{y_5} + z^2u_{y_6} + \cdots + xz^3u_{y_{14}} + z^4u_{y_{15}} \\ u_z &= u_{z_1} + xu_{z_2} + zu_{z_3} + x^2u_{z_4} + xzu_{z_5} + z^2u_{z_6} + \cdots + xz^3u_{z_{14}} + z^4u_{z_{15}} \end{aligned} \tag{2}$$

Modal shapes and natural frequencies (ω_n) can be obtained by solving the eigenvalue problem:

$$(\boldsymbol{K} - \omega_n^2\boldsymbol{M})\boldsymbol{U} = 0 \tag{3}$$

Neural Networks and Adaptive Sampling

This work aims to train an NN to estimate the accuracy of a structural theory. NN has one input vector, each representing a structural beam theory, which is encoded as a sequence of 0s and 1s, where 1 represents an active generalized variable, e.g.,

$$u_x = u_{x_1} + xu_{x_2} + x^2u_{x_4} + z^2u_{x_6} + x^3u_{x_7} + z^4u_{x_{15}} = [1\ 1\ 0\ 1\ 0\ 1\ 0\ 0\ 0\ 0\ 0\ 1] \tag{4}$$

The resulting arrays are fed into a NN, where the labels are the average relative errors of the first 10 natural frequencies computed for each beam theory with respect to the reference complete fourth-order theory shown in Eq. (2), e.g.,

$$u_x = u_{x_1} + xu_{x_2} + x^2u_{x_4} + z^2u_{x_6} + x^3u_{x_7} + z^4u_{x_{15}} \rightarrow \%E_{AVG} = 3.26\% \tag{5}$$

The trained NN predicts the error of a beam theory for that structural case, taking as inputs the vectors of the structural theories. In previous works [11,12], the training input samples were randomly selected. In contrast, here they are selected using a multi-criteria Adaptive Sampling [13

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15] algorithm to train the NN with the most informative and meaningful samples, as shown in Fig. 2.

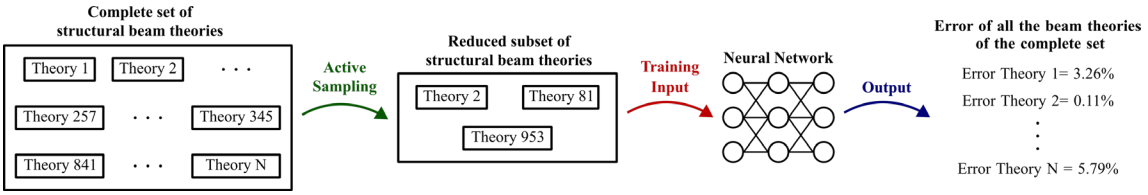


Figure 2: Workflow of the Adaptive Sampling and NN

The adaptive sampling algorithm starts from a small initial set of beam theories and progressively enriches it by selecting new candidates from the complete set. At each step, an Extra Trees surrogate model is trained on the currently selected theories to approximate the relationship between the beam theories and their errors. The trained surrogate is then used to predict the error of the unselected candidate theories. These predictions define a quality contribution, while the variability among the individual trees' predictions provides an estimate of uncertainty. A diversity contribution is also introduced to promote candidates differing from the already selected theories. The final acquisition score is computed as a weighted combination of quality ($\alpha Q(x)$), uncertainty ($\beta U(x)$), and diversity terms ($\gamma D(x)$). The acquisition function is the following:

$$f(x) = \alpha Q(x) + \beta U(x) + \gamma D(x) \tag{6}$$

The theory with the highest score is added to the selected set, and the Extra Trees surrogate is retrained on the enriched dataset. The procedure is repeated until the number of theories requested in the reduced subset is reached, and the resulting set is then used to train the NN.

Numerical Results

The results provided hereafter refer to a single structural beam case. The beam is clamped-free, with a length L of 5m. The material properties are: E=69 GPa, ν=0.33, ρ=2700 kg/m3. The cross section of the beam is shown in Fig. 3. The BTD computed by FEM, NN with random sampling, and NN with adaptive sampling are shown in Fig. 4, while Tables 1, 2, and 3 report the best theories and their accuracies, from AAM using FEM, and the two NN, respectively. In Table 1, the solid black triangle indicates that the generalized variable is active, and the empty one indicates the opposite. A solid blue triangle in Table 2 indicates that the NN predicted the presence of an inactive term in the reference AAM table; an empty blue triangle indicates the opposite. The same applies to the red triangles in Table 3.

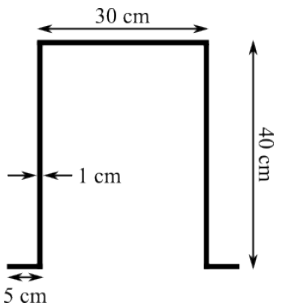


Figure 3: Omega cross-section and its dimensions

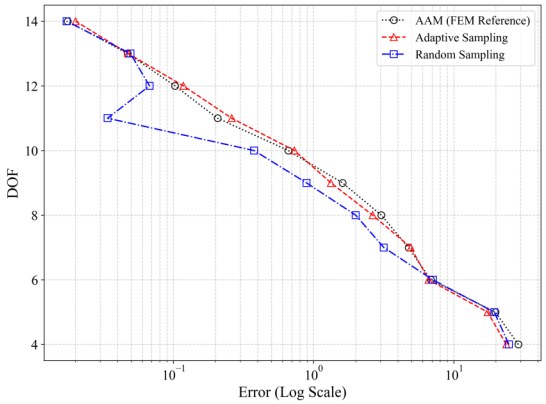


Figure 4: Best Theory Diagram computed by AAM, NN with Random Sampling, and NN with Adaptive Sampling

DOF	x^2	xz	z^2	x^3	x^2z	xz^2	z^3	x^4	x^3z	x^2z^2	xz^3	z^4	$\%E_{AVG}$
14	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	▲	1.757E-02
13	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	△	4.720E-02
12	▲	▲	▲	▲	▲	▲	▲	△	▲	△	▲	△	1.027E-01
11	▲	▲	▲	▲	△	▲	▲	△	▲	△	▲	△	2.064E-01
10	▲	▲	▲	▲	△	▲	△	△	▲	△	▲	△	6.602E-01
9	▲	▲	▲	▲	△	△	△	△	▲	△	▲	△	1.608E+00
8	▲	▲	▲	▲	△	△	△	△	▲	△	△	△	3.046E+00
7	△	▲	▲	▲	△	△	△	△	▲	△	△	△	4.755E+00
6	△	▲	△	▲	△	△	△	△	▲	△	△	△	6.876E+00
5	△	▲	△	▲	△	△	△	△	△	△	△	△	1.983E+01
4	△	△	△	▲	△	△	△	△	△	△	△	△	2.889E+01

Table 1: Best theories of the omega beam computed by AAM (FEM Reference)

DOF	x^2	xz	z^2	x^3	x^2z	xz^2	z^3	x^4	x^3z	x^2z^2	xz^3	z^4	$\%E_{AVG}$
14	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	▲	1.728E-02
13	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	△	4.940E-02
12	▲	▲	▲	▲	△	▲	△	▲	▲	△	▲	▲	6.752E-02
11	△	▲	▲	▲	△	▲	▲	▲	▲	△	▲	△	3.387E-02
10	△	▲	▲	▲	△	▲	△	▲	▲	△	▲	△	3.764E-01
9	△	▲	△	▲	△	▲	△	△	▲	△	▲	▲	8.909E-01
8	△	▲	△	▲	△	▲	△	△	▲	△	▲	△	1.998E+00
7	△	▲	△	▲	△	▲	△	△	▲	△	△	△	3.172E+00
6	△	▲	△	▲	△	△	△	△	▲	△	△	△	7.095E+00
5	△	△	△	▲	△	△	△	△	▲	△	△	△	1.949E+01
4	△	△	△	▲	△	△	△	△	△	△	△	△	2.478E+01

Table 2: Best theories of the omega beam predicted by NN trained with Random Sampling

DOF	x^2	xz	z^2	x^3	x^2z	xz^2	z^3	x^4	x^3z	x^2z^2	xz^3	z^4	$\%E_{AVG}$
14	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	▲	2.009E-02
13	▲	▲	▲	▲	▲	▲	▲	▲	▲	△	▲	△	4.752E-02
12	▲	▲	▲	▲	▲	▲	▲	△	▲	△	▲	△	1.179E-01
11	▲	▲	▲	▲	△	▲	▲	△	▲	△	▲	△	2.605E-01
10	▲	▲	▲	▲	△	▲	△	△	▲	△	▲	△	7.305E-01
9	△	▲	▲	▲	△	△	△	▲	▲	△	▲	△	1.330E+00
8	△	▲	△	▲	△	△	△	▲	▲	△	▲	△	2.642E+00
7	▲	▲	△	▲	△	△	△	△	▲	△	△	△	4.941E+00
6	△	▲	△	▲	△	△	△	△	▲	△	△	△	6.628E+00
5	△	△	△	▲	△	△	△	△	▲	△	△	△	1.747E+01
4	△	△	△	▲	△	△	△	△	△	△	△	△	2.371E+01

Table 3: Best theories of the omega beam predicted by NN trained with Adaptive Sampling

Conclusions

This paper presents an improved methodology, compared with previous works, for estimating the accuracy of a beam theory and its generalized variables for a given problem. The proposed methodology uses an NN to correlate structural theories with their error and an Adaptive Sampling algorithm to select the most informative generalized variables for training the NN. The results show that the NN trained with Adaptive Sampling predicts both the error and the generalized variables of the best theories more accurately than the NN trained with random sampling. Compared with random sampling, the error prediction of the NN trained with Adaptive Sampling improves, and the NN can predict the exact formulation of the best theories with greater precision. For instance, in Table 2, the NN trained with random sampling correctly predicts 56 terms out of 66, while this number increases to 61 terms out of 66 for the NN trained with Adaptive sampling. The results are problem-dependent, since the error and the number of correctly predicted terms vary with the structural beam case. Nevertheless, a general improvement is achieved with only a minor increase in the computational cost of the Adaptive sampling algorithm.

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