Learning Mechanically Driven Emergent Behavior with Message Passing Neural Networks

Peerasait Prachaseree
pprachas@bu.edu
Emma Lejeune
elejeune@bu.edu
Department of Mechanical Engineering, Boston University

We examined the ability of **neural message passing** to predict **mechanically driven emergent** behavior: the connection between a column's **geometric structure** and the **buckling direction**.

BOSTON UNIVERSITY

Introduction

Recently, there has been a growing interest in both using machine learning methods to approximate mechanical behavior directly from experimental data, and using machine learning methods to reduce the computational cost of physics-based simulations. Here, we are interested in machine learning methods that can be used to predict global emergent properties from complex local geometric properties. Our work addresses the following methodological gaps in training metamodels for problems in solid mechanics:

1) There is a lack of methods tailored to "true" classification problems in mechanics.
2) There are few metamodeling approaches that deal well with non-gridlike data that can't be approximated via a small number of parameters.

In this work, we introduce a novel dataset of structures with complex geometry and present methods for (1) representing these data and (2) making predictions based on these data with a machine learning model.

Asymmetric Buckling Columns "ABC" Dataset (Fig. 1)

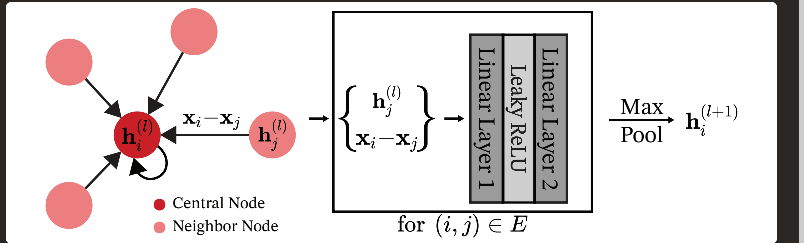
The dataset consists of compressed inhomogeneous columns with fixed-fixed boundary conditions. The columns are compressed until the onset of instability and the emergent buckling direction under compression. The dataset is split into three sub-datasets, each with varying complexity of geometric features:

1) Sub-dataset 1: Generated by stacking rectangular blocks on top of each other
2) Sub-dataset 2: Generated by intersecting rings of the same size.
3) Sub-dataset 3: Generated by overlapping and trimming rings of differing sizes

Methods (Fig. 2)

Data Representation:
To deal with complicated geometry, we convert the structure into a graph. We first convert our structure to a high resolution image. Then, by using Simple Linear Iterative Clustering (SLIC) segmentation and retaining the superpixels associated with the structure, we obtain nodes of the graph. The edges of the graph are constructed by ball query, which is a hyperparameter that can be tuned. The nodes of the graph contain features vectors consisting of centroid, area, and eccentricity of the superpixels.

Machine learning model:
To deal with graphs, and to enforce locality, we use spatial graph convolutions. The graph convolution layer we use is PointNet++. PointNet++ constructs its message function from nodal features and edge features, before passing the message into a Multilayer perceptron (MLP) to obtain the final graph embedding. Batch normalization and skip connections are employed after each convolution layer to obtain the final graph embedding, which is then passed through to a linear classifier.



Results (Fig. 3)

Data Augmentation:
We augmented our graphs by reflecting the images over the x-axis, y-axis and y=x axis. The labels are flipped for images reflected over y-axis and y=x axis. The models trained with augmented data perform significantly better than the models trained without augmented data.

Ball Query and Superpixel Density:
We systematically varied the graph construction for each dataset. Each dataset has graph variations with different node densities (Sparse, Medium, Dense) and ball queries (r = 0.2, 0.3, 0.4 of the column width). We conclude that after a certain number of edges, there is no benefit to adding more edges, either through increasing the node density or ball query radius, since doing so will not increase the accuracy significantly.

Current Best Performance:
Sub-dataset 1: With medium node density and r = 0.4, the maximum accruacy achieved is 93.5±0.4 % (95% CI)
Sub-dataset 2: With desnse node density and r = 0.3 the maximum accuracy achieved is 90±1 % (95% CI)
Sub-dataset 3: With desnse node density and r = 0.3 the maximum accuracy achieved is 84.3±0.3 % (95% CI)

Future Work

We plan to publish our ABC dataset and the associated code under a Creative Commons License and a MIT License respectively. In the short term, we are interested in using data and model visualization techniques to better interpret the trained machine learning models, and exploring alternative methods to making predictions on the ABC dataset. In the long term, we are interested in building on these approaches to investigating more complex three dimensional structures and extending this work to experimental data.

Acknowledgements

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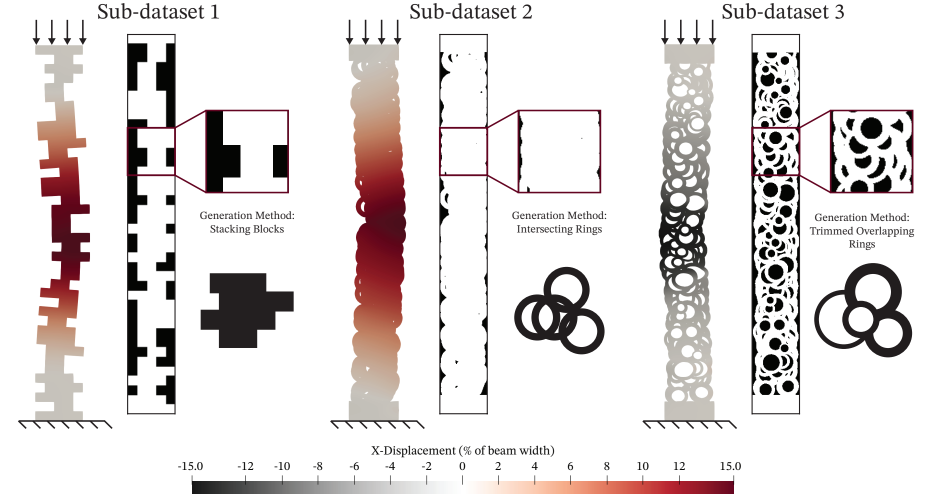
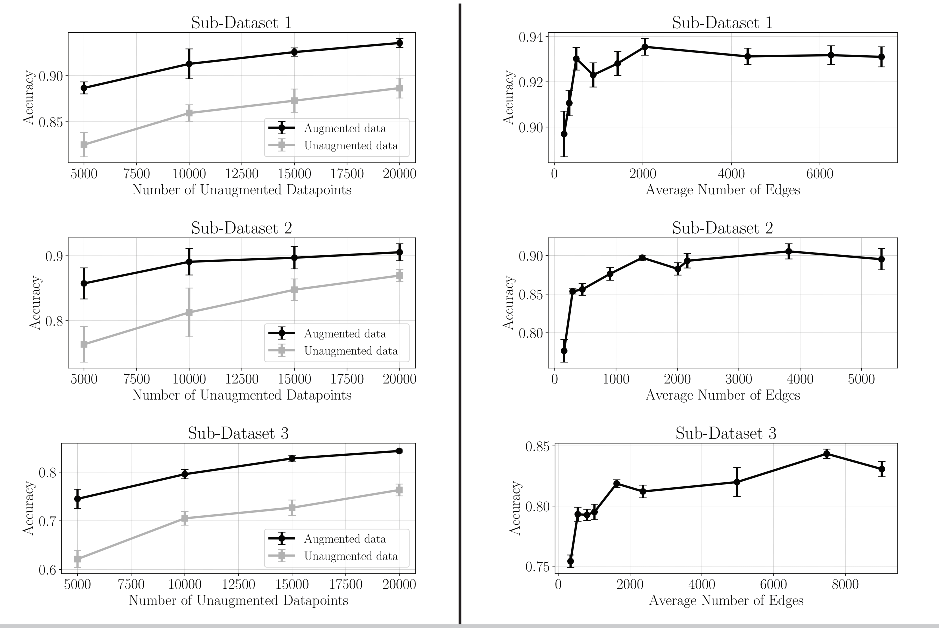
Dataset (Fig.1)



Preliminary Results (Fig. 3)



Metamodeling Pipeline (Fig. 2)