Exploring Flow Matching for Bifurcation: A Preliminary Framework for Buckling in Mechanical Metamaterials

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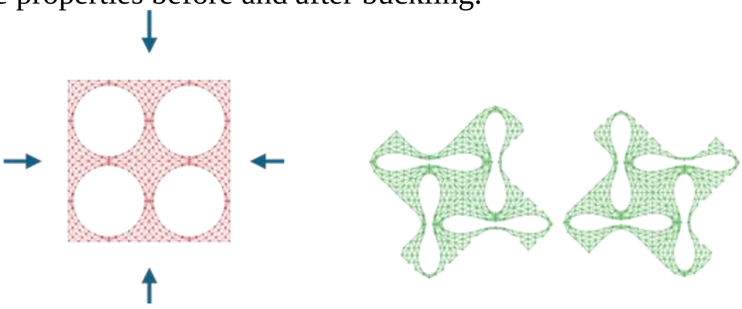
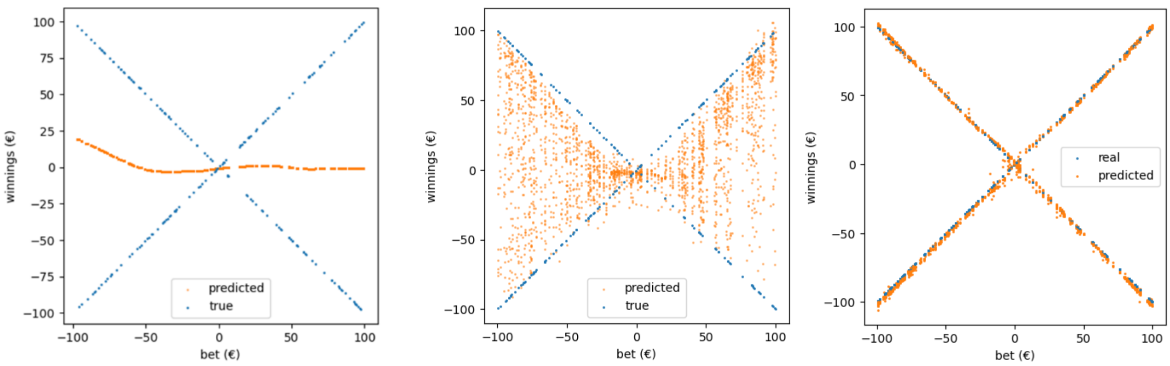
Introduction

Mechanical metamaterials are materials with a specially engineering microstructure, such that they exhibit specific mechanical behavior [1], which is usually triggered by buckling, a form of bifurcation. Specifically, bifurcation refers to a sudden qualitative change in a system's behavior due to small parameter variations, often leading to multiple possible outcomes. Sharp transitions are characteristic of bifurcations. In the case of mechanical metamaterials, buckling involves breaking of a symmetry, leading to multiple equivalent solutions, as shown in Figure 1. It also leads to a sudden change in the material behavior. We aim to predict this deformation and the effective properties before and after buckling.



(a) (b)

Figure 1: (a) Undeformed geometry of a mechanical metamaterial, with arrows indicating the applied deformation. (b) Two equally valid output configurations that result because of symmetry breaking, in this case some of the mirror symmetries and translation symmetry. Their effective properties will be the same, however.



(a) (b) (c)

Figure 2: The results of predicting outcomes of a coin flip using three different methods: (a) a regular neural network, (b) a conditional VAE, and (c) flow matching. Each method makes 10 predictions per test data point.

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Machine learning

Traditional machine learning models struggle to predict the buckling modes accurately due to their tendency to average out the possible outcomes, as shown in Figure 2a. In the case of the buckling modes in Figure 1b, the average of them would be a completely wrong prediction. Generative machine learning techniques such as VAEs do have the ability to predict multiple modes, however they tend to give 'blurry' results, as shown in Figure 2b.

Flow matching

We show that a newer technique within generative AI, flow matching, can accurately capture sharp transitions between different outcomes, which means it has the potential to be able to predict buckling modes such as the ones shown in Figure 1b. Flow matching efficiently maps an initial (noise) distribution to a target distribution [2]. This method is particularly useful for capturing complex distributions and sharp transitions, making it ideal for applications like bifurcation analysis. We use flow matching to assign probabilities to different outcomes without averaging them, thus preserving the distinct pathways a system might take, see for example Figure 2c.

Results

We show for multiple small test systems that flow matching outperforms conventional neural networks and a conditional VAE approach. These include predicting the results of a coin flip (Heads or Tails), a test system where two entities need to coordinate because they cannot collide (Three Roads) and a problem on a small graph, where permutation symmetry is broken (Four Node Graph). We present our results both qualitatively in the form of plots showing the predicted distributions (see Figure 2), as well as quantitatively in the form of the Wasserstein distance (see Table 1). We also discuss the role of symmetries and the breaking of them during bifurcation.

Table 1: Wasserstein distance of a set of 100 predictions to the actual distribution of allowed outcomes, for three different test systems.

Test System	Non-probabilistic	VAE	Flow Matching
Heads or Tails	56.2	33.0	**8.30**
Three Roads	21.4	17.3	**3.88**
Four Node Graph	10.0	9.89	**2.02**

Conclusion

Flow matching holds significant potential for the simulation of mechanical metamaterials with buckling, which will allow for more efficient investigation of their effective properties and ultimately exploration of the available design space and functionalities.

References

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