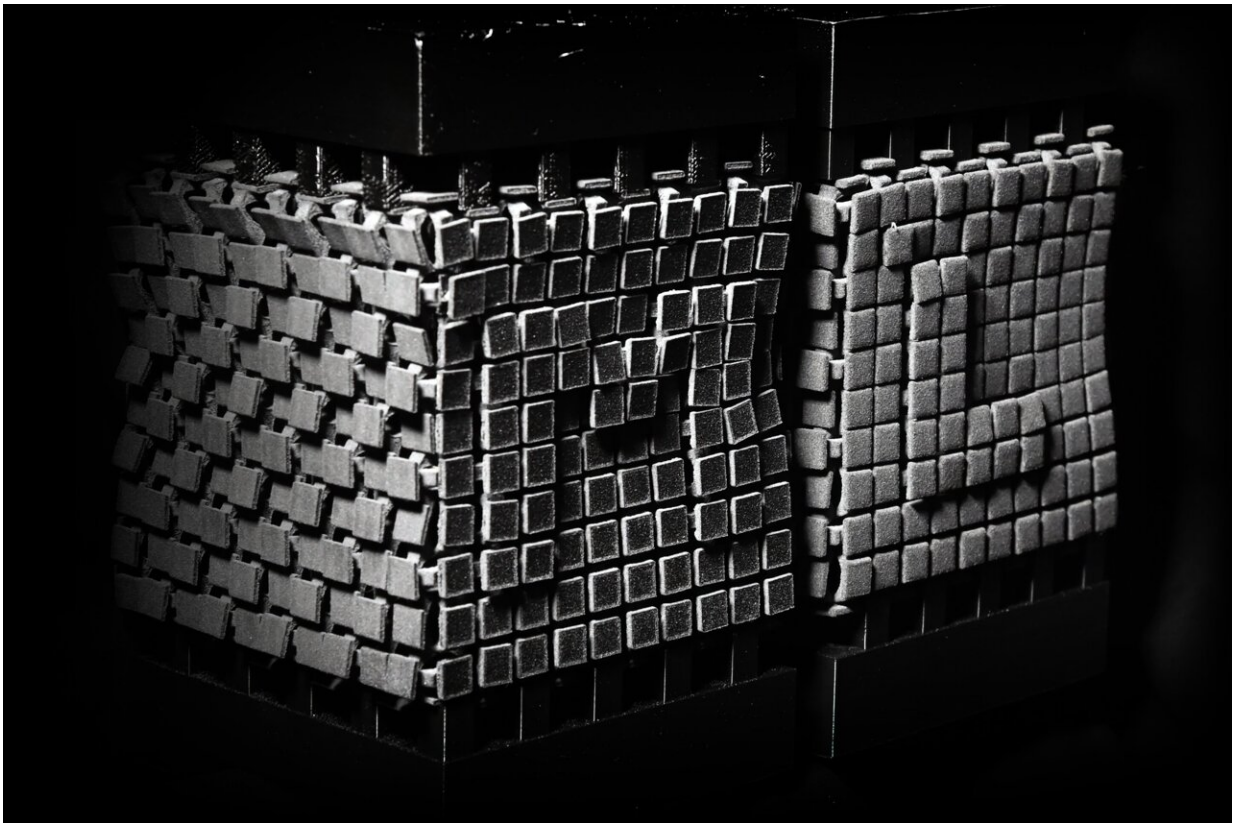
Using machine learning to infer rules for designing complex mechanical metamaterials

November 25 2022, by Ingrid Fadelli



Two combinatorial mechanical metamaterials designed in such a way that the letters M and L bulge out in the front when being squeezed between two plates (top and bottom). Designing novel metamaterials such as this is made easy by AI. Credit: Daan Haver and Yao Du, University of Amsterdam

Mechanical metamaterials are sophisticated artificial structures with

mechanical properties that are driven by their structure, rather than their composition. While these structures have proved to be very promising for the development of new technologies designing them can be both challenging and time-consuming.

Researchers at University of Amsterdam, AMOLF, and Utrecht University have recently demonstrated the potential of convolutional neural networks (CNNs), a class of machine learning algorithms, for designing complex mechanical metamaterials. Their paper, published in *Physical Review Letters*, specifically introduces two-different CNN-based methods that can derive and capture the subtle combinatorial rules underpinning the design of mechanical metamaterials.

"Our recent study can be considered a continuation of the combinatorial design approach introduced in a previous paper, which can be applied to more complicated building blocks," Ryan van Mastrigt, one of the researchers who carried out the study, told Phys.org. "Around the time when I started working on this study, Aleksi Bossart and David Dykstra were working on a combinatorial metamaterial that is able to host multiple functionalities, meaning a material that can deform in multiple distinct ways depending on how one actuates it."

As part of their previous research, van Mastrigt and his colleagues tried to distill the rules underpinning the successful design of complex metamaterials. They soon realized that this was far from an easy task, as the "building blocks" that make up these structures can be deformed and arranged in countless different ways.

Previous studies showed that when metamaterials have small unit cell-sizes (i.e., a limited amount of "building blocks"), simulating all the ways in which these blocks can be deformed and arranged using conventional physics simulation tools is possible. As these unit cell-sizes become larger, however, the task becomes extremely challenging or impossible.

"Since we were unable to reason about any underlying design rules and conventional tools failed at allowing us to explore larger unit cell designs in an efficient way, we decided to consider machine learning as a serious option," van Mastrigt explained. "Thus, the main objective of our study became to identify a machine learning tool that would allow us to explore the design space much quicker than before. I think that we succeeded and even exceeded our own expectations with our findings."

To successfully train CNNs to tackle the design of complex metamaterials, van Mastrigt and his colleagues initially had to overcome a series of challenges. Firstly, they had to find a way to effectively represent their metamaterial designs.

"We tried a couple of approaches and finally settled on what we refer to as the pixel representation," van Mastrigt explained. "This representation encodes the orientation of each building block in a clear visual manner, such that the classification problem is cast to a visual pattern detection problem, which is exactly what CNNs are good at."

Subsequently, the researchers had to devise methods that considered the huge metamaterials class-imbalance. In other words, as there are currently many known metamaterials belonging to class I, but far fewer belonging to class C (the class that the researchers are interested in), training CNNs to infer combinatorial rules for these different classes might entail different steps.

To tackle this challenge, van Mastrigt and his colleagues devised two different CNN-based techniques. These two techniques are applicable to different metamaterial classes and classification problems.

"In the case of metamaterial M2, we tried to create a training set that is class-balanced," van Mastrigt said. "We did this using naïve undersampling (i.e., throwing a lot of class I examples away) and

combine this with symmetries which we know some designs have, such as translational and rotational symmetry, to create additional class C designs.

"This approach thus requires some domain knowledge. For metamaterial M1, on the other hand, we added a reweight term to the loss function such that the rare class C designs weigh more heavily during training, where the key idea is that this reweighting of class C cancels out with the much larger number of class I designs in the training set. This approach requires no domain knowledge."

In initial tests, both these CNN-based methods for deriving the combinatorial rules behind the design of mechanical metamaterials achieved highly promising results. The team found that they each performed better on different tasks, depending on the initial dataset used and known (or unknown) design symmetries.

"We showed just how extraordinarily good these networks are at solving complex combinatorial problems," van Mastrigt said. "This was really surprising for us, since all other conventional (statistical) tools we as physicists commonly use fail for these types of problems. We showed that neural networks really do more than just interpolate the design space based on the examples you give them, as they appear to be somehow biased to find a structure (which comes from rules) in this design space that generalizes extremely well."

The recent findings gathered by this team of researchers could have far reaching implications for the design of metamaterials. While the networks they trained were so far applied to a few metamaterial structures, they could eventually also be used to create far more complex designs, which would be incredibly difficult to tackle using conventional physics simulation tools.

The work by van Mastrigt and his colleagues also highlights the huge value of CNNs for tackling combinatorial problems, optimization tasks that entail composing an "optimal object" or deriving an "optimal solution" that satisfies all constraints in a set, in instances where there are numerous variables at play. As combinatorial problems are common in numerous scientific fields, this paper could promote the use of CNNs in other research and development settings.

The researchers showed that even if machine learning is typically a "black box" approach (i.e., it does not always allow researchers to view the processes behind a given prediction or outcome), it can still be very valuable for exploring the design space for metamaterials, and potentially other materials, objects, or chemical substances. This could in turn potentially help to reason about and better understand the complex rules underlying effective designs.

"In our next studies, we will turn our attention to inverse design," van Mastrigt added. "The current tool already helps us enormously to reduce the design space to find suitable (class C) designs, but it does not find us the best design for the task we have in mind. We are now considering machine learning methods that will help us find extremely rare designs that have the properties that we want, ideally even when no examples of such designs are shown to the machine learning method beforehand.

"This is a very hard problem, but after our recent study, we believe, that neural networks will allow us to successfully tackle it."

More information: Ryan van Mastrigt et al, Machine Learning of Implicit Combinatorial Rules in Mechanical Metamaterials, *Physical Review Letters* (2022). DOI: 10.1103/PhysRevLett.129.198003

Corentin Coulais et al, Combinatorial design of textured mechanical metamaterials, *Nature* (2016). DOI: 10.1038/nature18960

Anne S. Meeussen et al, Topological defects produce exotic mechanics in complex metamaterials, *Nature Physics* (2020). DOI: 10.1038/s41567-019-0763-6

Aleksi Bossart et al, Oligomodal metamaterials with multifunctional mechanics, *Proceedings of the National Academy of Sciences* (2021). DOI: 10.1073/pnas.2018610118