Machine learning accelerates development of advanced manufacturing techniques

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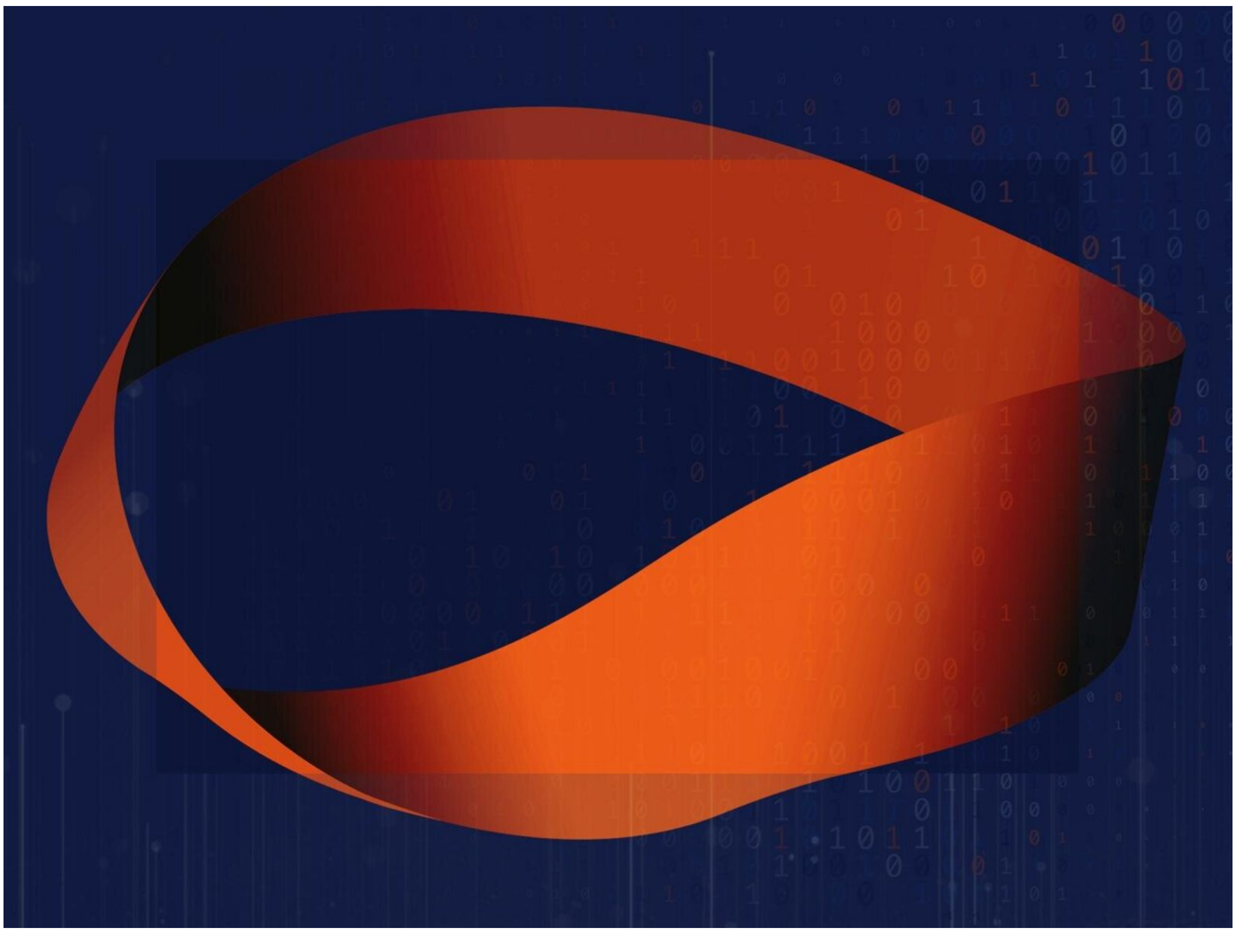

Scientists are pioneering approaches in machine learning to design and train computer software programs that guide the development of new manufacturing processes. Credit: Composite image by Jeff London | Pacific Northwest National Laboratory

Despite the remarkable technological advances that fill our lives today, the ways we work with the metals that underlie these developments haven't changed significantly in thousands of years. This is true of everything from the metal rods, tubes, and cubes that provide cars and trucks with their shape, strength, and fuel economy, to wires that move electrical energy in everything from motors to undersea cables.

But things are changing rapidly: The materials manufacturing industry is using new and innovative technologies, processes, and methods to improve existing products and create new ones. Pacific Northwest National Laboratory (PNNL) is a leader in this space, known as advanced manufacturing.

For example, scientists working in PNNL's Mathematics for Artificial Reasoning in Science initiative are pioneering approaches in the branch of artificial intelligence known as machine learning to design and train computer software programs that guide the development of new manufacturing processes.

These software programs are trained to recognize patterns in manufacturing data and use this pattern recognition capability to recommend, or predict, settings in manufacturing processes that will yield materials with improved properties—lighter, stronger, or more conductive, for example—than materials produced using traditional methods.

"The components we make using advanced manufacturing processes are so attractive to industry that they want to see these technologies launched as quickly as possible," said Keerti Kappagantula, a materials scientist at PNNL.

A challenge is that industry partners are reluctant to invest in new technologies before the underlying physics and other complexities of advanced manufacturing techniques are fully fleshed out and validated.

To bridge the gap, Kappagantula teamed up with PNNL data scientists Henry Kvinge and Tegan Emerson to build machine learning tools that predict how various settings in the manufacturing process affect material properties. The tools also present the predictions in a visual way that offers immediate clarity and understanding to industry partners and others.

Using these machine learning tools, the team believes it can shorten to months, instead of years, the timeline from lab to factory floor. With the guidance of the tools' predictions, the materials scientists only need to perform a handful of experiments, instead of dozens, to determine, for example, what settings lead to desired properties in an aluminum tube.

"The goal for us was to use machine learning as a tool to help guide the person who is running the advanced manufacturing process as they try out different settings on their device—different process parameters—to find one that lets them achieve what they actually want to achieve," Kvinge said.

Solving the right problem

In traditional manufacturing, computer models built on the well-understood physics of a manufacturing process show scientists how different settings impact material properties.

In advanced manufacturing, the physics are less understood, Kappagantula said. "Without that understanding, there's a delay in deployment."

Kappagantula, Kvinge, and Emerson's Artificial Intelligence Tools for Advanced Manufacturing project aims to identify ways that machine learning can be leveraged to extract patterns between process parameters and the resulting material properties, which provides insight to the underlying physics of advanced manufacturing techniques and can accelerate their deployment.

"The approach that we've taken, the unifying theme, is understanding how material scientists view their field—What are the mental models they have?—and then using that as a scaffold on which to build our models," Kvinge said.

Too often, he explained, data scientists develop solutions to the problems that the data scientists think need to be solved rather than the problem that other scientists want solved.

In this project, Kvinge said he thought the team would want a machine learning model that predicted the properties of a material produced when given specific parameters. In consultation with the materials scientists, he soon learned that they really wanted to be able to specify a property and have a model suggest all the process parameters that could be used to achieve it.

An interpretable solution

What Kappagantula and her colleagues required was a machine learning framework that could provide results that help her team make decisions about what experiment to try next. In the absence of such guidance, the process of tuning parameters to develop a material with desired properties is trial and error.

In this project, Kvinge and his colleagues first developed a machine learning model called differential property classification that leverages machine learning's pattern matching capability to distinguish between two sets of process parameters to determine which, if either, will more likely result in a material with the desired properties.

The model allows materials scientists to home in on optimal parameters before setting up an experiment, which can cost be costly and require a lot of prep work.

Before moving forward with an experiment recommended by a machine learning model, Kappagantula said she needs to trust the model's recommendation.

"I want to be able to see how it's doing its analysis," she said.

This concept, known as interpretability, or explainability, in the field of machine learning, has different meanings for experts in different domains. For data scientists, the explanation of how a machine learning model arrived at its prediction may be entirely different than an explanation that makes sense to materials scientists, noted Kvinge.

As Kvinge, Emerson, and their colleagues tackled this problem, they tried to understand it from the mental framework of materials scientists.

"It turned out that they very much understand it through these pictures of material microstructures," Kvinge said. "If you ask them what went wrong, why the experiment didn't go well or why it went well, they will look at the pictures and point things out to you and say these grain sizes are too big, or too small, or what have you."

To make the results of their machine learning model interpretable, Kvinge, Emerson, and colleagues used images and related data of microstructures from previous experiments to train a model that generates images of the microstructures that would result from manufacturing process tuned with a given set of parameters.

The team is currently validating this model and aims to make it a part of a software framework that materials scientists can use to determine which experiments to perform while developing advanced manufacturing techniques that promise to transform materials production and properties.

"It's not just doing things more energy efficiently," Kappagantula said of advanced manufacturing, "it's unlocking properties and performance that we've never seen before."

Provided by Pacific Northwest National Laboratory

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