DEEPMIND'S AI HELPS UNTANGLE THE MATHEMATICS OF KNOTS

The machine-learning techniques could benefit other areas of maths that involve large data sets.

By Davide Castelvecchi

For the first time, machine learning has spotted mathematical connections that humans had missed. Researchers at artificial-intelligence (AI) powerhouse DeepMind, based in London, teamed up with mathematicians to tackle two separate problems — one in the theory of knots and the other in the study of symmetries. In both cases, AI techniques helped the researchers discover new patterns that could then be investigated using conventional methods.

"I was very struck by just how useful the machine-learning tools could be as a guide for intuition," says Marc Lackenby at the University of Oxford, UK, one of the mathematicians who took part in the study. "I was not expecting to have some of my preconceptions turned on their head."

Computer simulations and visualizations of knots and other objects have long helped mathematicians to look for patterns and develop their intuition, says Jeffrey Weeks, a mathematician based in Canton, New York, who pioneered some of those techniques. But, he adds, "Getting the computer to seek out patterns takes the research process to a qualitatively different level."

The authors say the approach, described in a paper in the 2 December issue of *Nature* (A. Davies *et al*. *Nature* **600**, 70–74; 2021), could benefit other areas of maths that involve large data sets.

Maths versus machine

DeepMind, a sister company of Google, has made headlines with breakthroughs such as cracking the game Go, but its long-term focus has been scientific applications such as predicting how proteins fold.

The idea for a maths collaboration was sparked by a casual conversation in 2019 between mathematician Geordie Williamson at the University of Sydney in Australia and DeepMind's chief executive, neuroscientist Demis Hassabis. Lackenby and a colleague at Oxford, András Juhász, both knot theorists, soon joined the project.

Initially, the work focused on identifying mathematical problems that could be attacked using DeepMind's technology. Machine learning enables computers to feed on large data sets and make guesses, such as matching a surveillance-camera image to a known face from a database of photographs. But its answers are inherently probabilistic, and mathematical proofs require certainty.

The team reasoned that machine learning could help to detect patterns, such as the relationship between two types of object. Mathematicians could then try to work out the precise relationship by formulating what they call a conjecture, and then attempting to write a rigorous proof that turns that statement into a certainty.

Because machine learning requires lots of data to train on, one requirement was to be able to calculate properties for large numbers of objects: in the case of knots, the team calculated several properties, called invariants, for millions of different knots.

The researchers then moved on to working out which AI technique would be most helpful for finding a pattern that linked two properties. One technique in particular, called saliency maps, turned out to be especially helpful. It is often used in computer vision to identify which parts of an image carry the most-relevant information. Saliency maps pointed to knot properties that were likely to be linked to each other, and generated a formula that seemed to be correct in all cases that could be tested. Lackenby and Juhász then provided a rigorous proof that the formula applied to a very large class of knots (A. Davies *et al*. Preprint at https://arxiv.org/abs/2111.15323; 2021).

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"The fact that the authors have proven that these invariants are related, and in a remarkably direct way, shows us that there is something very fundamental that we in the field have yet to fully understand," says Mark Brittenham, a knot theorist at the University of Nebraska–Lincoln who frequently uses computational techniques. Brittenham adds that although machine learning has been used in knot theory before, the authors' technique is novel in its ability to discover surprising connections.

Solving symmetries

Williamson focused on a separate problem, regarding symmetries. Symmetries that switch around finite sets of objects have an important role in several branches of maths, and mathematicians have long studied them using various tools, including graphs — large abstract networks linking thousands of nodes — and algebraic expressions called polynomials. For decades, researchers have suspected that it would be possible to calculate the polynomials from the networks, but guessing how to do it seemed like a hopeless task, Williamson says. "Very quickly, the graph becomes beyond human comprehension."

With the computer's help, he and the rest of the team noticed that it should be possible to break down the graph into smaller, more manageable parts, one of which has the structure of a higher-dimensional cube. This gave him a solid conjecture to work on for the first time.

"I was just blown away by how powerful this stuff is," says Williamson. Once the algorithm zeroed in on a pattern, it was able to guess very precisely which graphs and polynomials came from the same symmetries. "How quickly the models were getting accuracy — that for me was just shocking," he says. "I think I spent basically a year in the darkness just feeling the computers knew something that I didn't."

Whether Williamson's conjecture will prove true is still an open question. Conjectures sometimes take a long time for the mathematical community to crack, but they can help to shape entire fields.

Wider applications

Throughout the project, the researchers had to tailor the AI techniques to the two different mathematical problems, says Alex Davies, a computer scientist at DeepMind. "We did not originally expect these to be the most useful techniques," he says.

"Any area of mathematics where sufficiently large data sets can be generated could benefit from this approach," says Juhász, adding that the techniques they demonstrated could also find applications in fields such as biology or economics.

Adam Zsolt Wagner, a mathematician at Tel Aviv University, Israel, who has used machine learning, says that the authors' methods could prove valuable for certain kinds of problems. "Without this tool, the mathematician might waste weeks or months trying to prove a formula or theorem that would ultimately turn out to be false." But he adds that it is unclear how broad its impact will be.

"My personal guess is that computer-generated conjectures will become ever more useful in 'filling in the details', but will never replace human intuition and creativity," says Weeks.