Abstract

A recent paper by Davies et al (2021) describes how deep learning (DL) technology was used to find plausible hypotheses that have led to two original mathematical results: one in knot theory, one in representation theory. I argue here that the significance and novelty of this application of DL technology to mathematics is significantly overstated in the paper under review and has been wildly overstated in some of the accounts in the popular science press. In the knot theory result, the role of DL was small, and a conventional statistical analysis would probably have sufficed. In the representation theory result, the role of DL is much larger; however, it is not very different in kind from what has been done in experimental mathematics for decades. Moreover, it is not clear whether the distinctive features of DL that make it useful here will apply across a wide range of mathematical problems. Finally, I argue that the DL here “guides human intuition” is unhelpful and misleading; what the DL does primarily does is to mark many possible conjectures as false and a few others as possibly worthy of study.

Certainly the representation theory result represents an original and interesting application of DL to mathematical research, but its larger significance is uncertain.

1 Introduction

A recent paper by Davies et al. (2021), published in Nature, discusses two newly proved theorems — one in knot theory, one in representation theory — where the authors were to some extent guided by computational experiments carried out using deep learning.

The paper has gathered a great deal of attention in the popular scientific press, in uncritical articles with overheated headlines, such as “DeepMind AI collaborates with humans on two mathematical breakthroughs” in NewScientist (Sparkes, 2021); “Maths researchers hail breakthrough in applications of artificial intelligence” in phys.org, (U. Sydney, 2021); “Researchers create AI that can create brand new math theorems” in iflscience.com (Spalding, 2021). An article in ScienceAlert (Neild, 2021) claims “AI is discovering patterns in pure mathematics that have never been seen before . . . . We can add suggesting and proving mathematical theorems to the long list of what artificial intelligence can do.”

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1For AI readers: “representation theory” here is a subfield of abstract algebra. It has essentially no connection to either the knowledge representation used in symbolic AI, or the representations studied in machine learning.

2The proofs of the theorems are published separately, in (Davies, Lackenby, Juhasz, and Tomasev, 2021) and (Blundell et al., 2021), and are included in the supplemental material.
intelligence is capable of.” An article in LiveScience (Pappas, 2021) describes the results as “the first-ever important advances in pure mathematics generated by artificial intelligence.”

On careful examination, however, this excitement is excessive and the articles are misleading. The AI in these two mathematical research projects neither suggested nor proved any theorems. The use of AI in these projects is not very different in kind from what has been done in experimental mathematics (Borwein and Bailey, 2008) for decades. In the case of the knot theory result, though not the representation theory result, the insight provided by deep learning could have been achieved through more traditional statistical analysis. The claim that the AI was used to “guide human intuition” is misleading and unhelpful; a more accurate claim is that the experimentation indicated that some specific conjectures might be true and therefore deserve study while others almost certainly were not, and therefore should be abandoned.

Before going further, let me make two disclaimers. The first has to do with my own limitations. The work here draws on three different fields, and I am not an expert in any of them. I have some knowledge of machine learning generally and deep learning specifically, but I am not an expert. I know very little about knot theory and almost nothing at all about representation theory. So it is certainly possible that my account below has some misstatements or misjudgments. If you find a mistake, please do let me know.

Second, let me clearly set out the limits of what I am claiming here. I am not at all arguing against the value of computational experiments in mathematical research or against the development of AI tools for mathematics; there is a lot of excellent, exciting work going on in both directions. I am not arguing against the significance of these new mathematical results as mathematics; I am in no position to judge that. I am not arguing that the Nature paper misrepresents how the AI tools were used or how helpful the mathematicians involved found them; I am working from the assumption that that is all accurately set forth.

What I want to do in this review is to lay out clearly the role of AI in these projects and to discuss the implications of that role. Since many lay readers and even many people involved in machine learning technology have little idea of research in pure mathematics, and since many mathematicians do not follow machine learning closely, claims such as the ones I have quoted above can easily be accepted uncritically, leading to miscommunication and misunderstanding.

Ordinarily, when someone praises a tool that they have been using — a gardener praises a particular hedge trimmer, a mathematician says that they constantly use Brouwer’s fixed point theorem — there is no reason to be at all skeptical. In this case, however, there is a perverse incentive to focus the role of the DL in this research, not just for the ML specialists from Deep Mind, but even for the mathematicians. The remarkable fame that these works have achieved — the prestigious article in Nature, the excitement in all kinds of science venues across the internet — has nothing to do with their merits as pure mathematics, and everything to do with the fact that AI was involved. Everyone involved, therefore, has an interest in highlighting and even exaggerating the extent and impact of that involvement.

2 The knot theory result

My discussion of the mathematical aspects of the two results will be minimal; only as much as is necessary to explain the role of the AI in achieving them. For a little more detail, go to (Davies et al., 2021); for a lot more detail, look up the works cited there.

A knot in mathematical parlance is a closed loop in a three-dimensional space. There are many different numerical features of a knot that can be defined that describe different geometric characteristics. These features are categorized into a number of different categories, corresponding to
the kind of math used to define them. Two of the most important categories are *algebraic invariants* and *hyperbolic invariants*. The goal of the research here was to find a relation between one particular algebraic invariant, called the *signature* and a number of hyperbolic invariants; that would exciting because it would be a connection between two completely separate approaches to characterizing a knot.

The research project proceeded along a number of steps:

**Step 1:** The mathematicians selected about 12 hyperbolic invariants as promising candidates.

**Step 2:** They created a data set with 2.7 million examples of knots, labelled with the signature and these 12 hyperbolic invariants.

**Step 3:** Using the data set, they trained a neural network (3 hidden layers, 300 units in each, fully connected) with the task of predicting the signature from the hyperbolic invariants.

**Step 4:** They observed that the trained NN could predict the signature from the inputs with an accuracy of 78%. This indicated that, indeed, there is a relation.

**Step 5:** Using standard techniques for analyzing neural networks, they determined that they can reduce the input to three hyperbolic invariants — the real and imaginary parts of the meridional translation and the longitudinal translation — without losing much accuracy.

**Step 6:** Thinking about these particular quantities, the mathematicians decided that it would be reasonable to combine them into a new, geometrically meaningful, quantity, the ‘natural slope’. If \( \mu \) is the meridional translation (a complex number, thus a pair of real numbers) and \( \lambda \) is the longitudinal translation, then \( \text{slope} = \text{Re}(\lambda/\mu) \).

**Step 7:** They plotted the signature against the slope. It turned out that there was an approximate linear relation: the signature is approximately half the slope. Using the slope as the sole predictive feature for the signature gave an accuracy of 78%; i.e. the slope constituted all the predictive power in the twelve hyperbolic features combined.

**Step 8:** They formulated an initial hypothesis:

\[
|2\sigma(K) - \text{slope}(K)| < c_1\text{vol}(K) + c_2
\]

where \( K \) ranges over knots, \( \sigma \) is the signature, \( \text{vol}(K) \) is the volume (a fourth hyperbolic parameter), and \( c_1 \) and \( c_2 \) are constants.

**Step 9:** They realized that there might be counter-examples to the initial hypothesis over a particular category of knots. They generated a data set with about 36,000 knots in this category. They indeed found some counter-examples.

**Step 10:** They formulated a revised hypothesis

\[
|2\sigma(K) - \text{slope}(K)| < c\text{vol}(K)/\text{inj}(K)^3
\]

where \( \text{inj}(K) \) is the injectivity radius, a fifth hyperbolic parameter, which can be a small real number.

**Step 11:** They were able to prove the revised hypothesis.

Note, first, that machine learning was used only in steps 4 and 5, and its sole outcome is to determine that three particular hyperbolic parameters are largely predictive of the signature. Step 7 involved doing a linear regression. Steps 2 and 9, the creation of two data sets, involved highly specialized non-AI software, almost certainly more sophisticated computationally and mathematically than the neural network, quite possibly more demanding computationally (the computation of

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3The description in (Davies et al. 2021) is not entirely clear on this point. The list of invariants given in the section Methods/Topology/Data-Generation is slightly different from the list in figure 3.
some of these parameters can be very difficult.) The other steps were all carried out by the human mathematicians.

Second, at the end of the day, all that the deep learning component accomplished was to isolate a mathematically simple relationship between four real-valued numerical parameters. If we write the complex meridional translation $\mu$ in the form $\mu = a + bi$, then the formula for slope becomes

$$\text{slope} = \Re(\lambda/a + bi) = \lambda a/(a^2 + b^2).$$

The relation detected by the neural network therefore has the form $\sigma \approx \lambda a/(2(a^2 + b^2))$ — linear in $\lambda$ and a simple function of $a$ and $b$. Again, the DL did not even extract the form of the relation; all it did was to report that $\sigma$ could be predicted with 78% accuracy from $\lambda$, $a$, and $b$.

Broadly speaking, this knot theory problem is not actually the kind of problem where DL typically outshines other machine-learning or statistical methods. DL’s strength is in cases like vision or text where each instance (image or text) has a large numbers of low-level input features, it is hard to reliably identify high-level features, and the function relating the input features to the answer is, as far as anyone can tell, immensely complex, with no small subset of the input features being at all determinative. With only twelve input features, of which only three are relevant, with a simple mathematical approximate relation involved, and with three million data points, it is hard to see why a neural network with 200,000 parameters would be the method of choice; simple, conventional statistical methods or a support vector machine would be more suitable.

3 The representation theory result

Like the knot theory result, the representation theory result involves connecting two different views of a mathematical object. The objects involved in representation theory are much more abstract than those in knot theory, and I will not make the slightest attempt to explain them; I will merely quote them. (The account of the math in (Davies et al. 2021) is likewise noticeably sketchier for the representation theory than the knot theory, for the same reason.)

Symmetric groups are a very important category of mathematical structure; generally speaking, they describe the ways that a set of some kind can be mapped into itself. If you have two elements of a symmetry groups, then the relation between those can be characterized in two different ways: the unlabelled Bruhat interval graph and the Kazhdan-Lusztig (KL) polynomial. The Bruhat interval graph rapidly becomes quite complex, even for fairly simple elements; the KL polynomial is much simpler. For instance, in the examples they used, some of the graphs had $9! = 362,880$ nodes, whereas the polynomials were at most of degree four.

A long-standing conjecture, known as the “combinatorial invariance” conjecture states that the KL polynomial can be computed from the Bruhat interval graph. One of the obstacles to proving this is that the graphs are so large that it is hard for researchers to get an intuitive feeling for their structure.

What the project here accomplished was to prove a result that is a major step toward the full conjecture: There is a way to pre-process the interval graph, called “a hypercube decomposition along its extremal reflection”, and once you have done that, then the KL-polynomial can be computed using a simple formula. The only problem is, there can be many different hypercube decompositions along extremal reflections, and all that Blundell et al. have proved is that one of these will work; they haven’t given a method of finding the right one. They have now formulated the further conjecture that, in fact, any hypercube decomposition along extremal reflections will work, and their experiments bear that out, but they have not proved it. If they can prove that, then that will settle the combinatorial invariance conjecture.

The project involved the following steps:
**Step 1:** They designed a specialized, comparatively shallow (4 propagation steps), deep learning system that takes as input an encoding of the interval graph and produces as output the coefficients of the KL polynomial. The architecture of the network was designed to be “algorithmically aligned” with existing knowledge about techniques for computing KL-polynomials from “labelled Bruhat intervals” i.e. Bruhat intervals with some extra information.

**Step 2:** They created a training set of 24,000 examples, labelled by the Bruhat interval graph and the KL polynomial.

**Step 3:** They trained the network on the training set, attaining accuracies for the four coefficients ranging from 63% to 98%. This success gave some encouragement that the Bruhat interval graph does indeed determine the polynomials.

**Step 4:** “By experimenting on the way in which we input the Bruhat interval to the network, it became apparent that some choices of graphs and features were particularly conducive to accurate predictions. In particular, we found that a subgraph inspired by prior work may be sufficient to calculate the KL polynomial, and this was supported by a much more accurate estimated function.” Accuracies on this subgraph ranged between 95.6% and 99% for the different coefficients.

**Step 5:** By analyzing the states of the DL network generated in the experiments of step 4, they determined that edges in the Bruhat graph corresponding to “extremal reflections” tended to be particularly important in the successful experiments. The authors state that they did not at all anticipate this.

**Step 6:** They used the information gathered in steps 4 and 5 to formulate a conjecture that they were able to prove.

Clearly the role of deep learning is much greater here than in the knot theory work. In particular my comment about the knot theory work, that other kinds of statistical analysis would have worked as well, does not at all apply here. The number of input features is enormous, and the relation between the input feature and the output is complex.

However, a number of points should be observed.

In step 3, the DL provided little more than general encouragement that the project on the whole was on the right track and that the deep learning system might be able to detect the relation of the KL polynomial to the. In step 4, it distinguished successful from unsuccessful experiments with different forms of input. Presumably all these experiments were carefully selected by the mathematicians as possibly promising avenues of research. It would be interesting to know how many such experiments were run and how many were successful; i.e. how much useful pruning did the DL provide here? In step 5, analysis of the DL identified certain edges as particularly important; here the DL did, indeed, provide information that the mathematicians had not anticipated.

Unlike the knot theory project, which used a generic DL architecture, the neural network was carefully designed to fit deep mathematical knowledge about the problem. Moreover, the DL worked much better, with something like 1/40th the error rate, on pre-processed data than on the original data. This cuts both ways. On the one hand, in the past, critics of DL, including myself, have often objected that it is difficult to incorporate domain knowledge; this cuts against that criticism. On the other hand, enthusiasts for DL have often praised DL as a “plug-and-play” learning methodology that can be thrown at raw data for whatever problem comes to hand; this cuts against that praise.

Deep mathematical knowledge of the problem was required here at practically every stage: In designing the DL architecture in step 1, in creating the data set in step 2, in choosing the experiments in step 4, in interpreting them in step 5. and of course in proving the theorem in step 6.

In both projects, the DL was entirely in the dark about the larger mathematical setting of the problem it was solving. In the knot theory project, it was not given the actual geometric structure
of the knots, just the invariants as a collection of uninterpreted numbers. In the representation theory project, it was not given the group or the group elements, just the Bruhat graph and the KL polynomials.

In applications of deep learning of this kind, success may depend critically on the way in which the training data is generated and the way that the mathematical structures are encoded, in ways that are quite specific to a particular task (Charton, 2021). Finding the best way to generate and encode data involves a mixture of theory, experience, art, and experimentation. The burden of all this lies on the human expert. Deep learning can be a powerful tool, but it is not always a robust one.

In view of all this, it seems to me that DL as used here is best viewed as another analytic tool in the toolbox of experimental mathematics rather than as a fundamentally new approach to mathematics. How powerful a tool it is and how broadly applicable remains to be seen. Experimental mathematics in general can only be applied to certain kinds of mathematical questions, and this technique is further limited. Davies et al. (2001) themselves express hesitation on that:

There are limitations to where this framework will be useful — it requires the ability to generate large datasets of the representations of objects and for the patterns to be detectable in examples that are calculable. Further, in some domains the functions of interest may be difficult to learn in this paradigm.

Additionally, there are examples where other analysis tools are more effective.

So far, we have one quite impressive example of the use of DL in mathematical research and one that is much less impressive. The history of AI has had its share of one-offs: remarkable successes that were achieved on one particular task that seemed promising but could never be matched on a second task.

4 “Guiding Intuition”

Finally, “guiding intuition” seems to me an seriously inaccurate description of the assistance that mathematicians have gained, or can hope to gain, from this use of DL systems. The word “intuitive” is a useful, though informal, one in mathematical writing. Because it is a useful word, it is important not to misuse it. In the mathematical setting, the word “intuitive” means that a concept or a proof can be grounded in a person’s deep-seated sense of familiar domains such as numerosity, space, time, or motion, or in some other way “makes sense” or “seems right” in a way that does not involve explicit calculation or step-by-step reasoning. Math teachers work hard to try to give their students an intuitive understanding of concepts and proofs by tying them to the familiar; this can involve diagrams, videos, examples from everyday life, and similar tools. Mathematicians and math students work hard to achieve an intuitive understanding by similar means. Contrary to the dictionary definition, “consisting in immediate apprehension, without the intervention of any reasoning process”, an intuitive grasp of a mathematical concept often requires hard mental work to attain. Often, gaining an intuitive grasp requires working through multiple specific examples. But no teacher ever tries to guide their students’ intuitions by telling them, “I have looked at millions of examples, and I can report that there is a pattern that works X% of the time, mostly on the basis of features A,B,C” which is what the DL tells the mathematician, and all that the DL tells the mathematician. The mathematicians in these projects may well have attained an intuitive understanding of the concepts they have defined, the theorems they have prove, and the conjectures

4Of course, the phrase “intuitively obvious” is often abused, either to bully students into quiet acceptance or as a euphemism for “I haven’t thought it through but I’m pretty sure it’s right.”
they have put forward, but they did not get that from the DL. What the DL did was to give them some advice as to which features of the problem seemed to be important and which seemed unimportant. That is not to be sneezed at, but it should not be exaggerated.

Acknowledgements

Thanks to François Charton for helpful suggestions.

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