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Cara(o) candidata(o),

O texto *Researchers buil an 'AI Scientist' - what can it do*, escrito por Davide Castelvecchi, foi publicado na versão *on-line* do periódico científico *Nature*, em 30 de agosto de 2024. Leia-o com atenção para resolver as questões.

Researchers built an 'AI Scientist' — what can it do?

The large language model does everything from reading the literature to writing and reviewing its own papers, but it has a limited range of applicability so far.
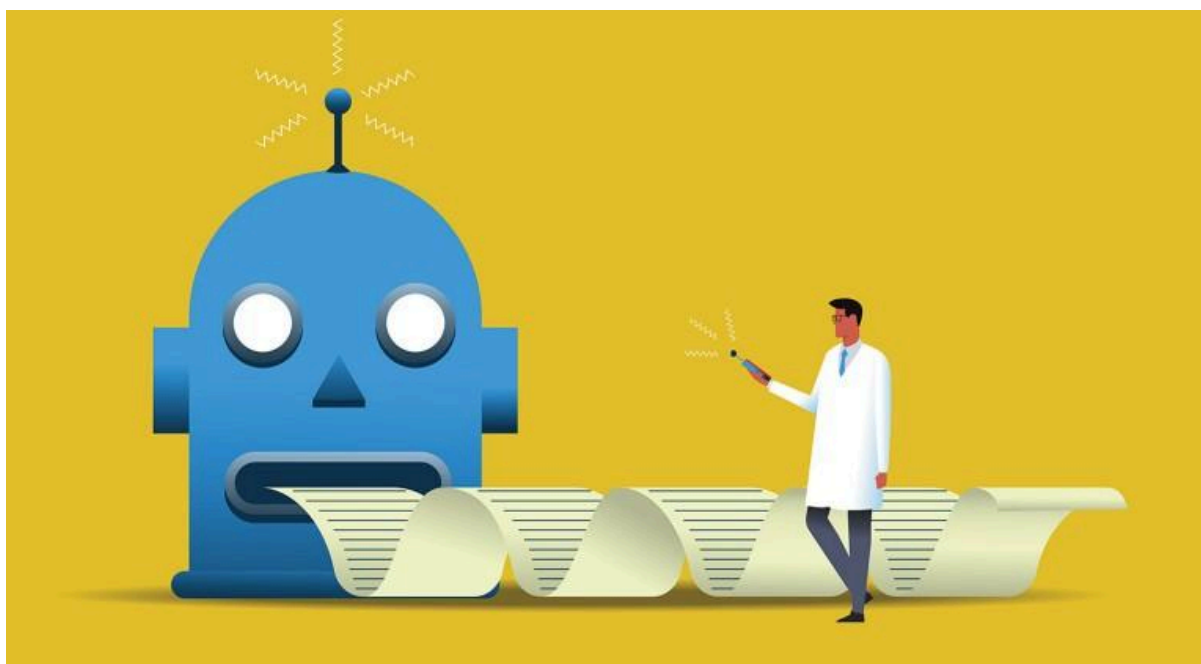
Credit: Moor Studio/Getty.

Could science be fully automated? A team of machine-learning researchers has now tried.

'AI Scientist', created by a team at Tokyo company Sakana AI and at academic labs in Canada and the United Kingdom, performs the full cycle of research from reading the existing literature on a problem and formulating hypotheses for new developments to trying

out solutions and writing a paper. AI Scientist even does some of the job of peer reviewers and evaluates its own results.

AI Scientist joins a slew of efforts to create AI agents that have automated at least parts of the scientific process. "To my knowledge, no one has yet done the total scientific community, all in one system," says AI Scientist co-creator Cong Lu, a machine-learning researcher at the University of British Columbia in Vancouver, Canada. The results[1] were posted on the arXiv preprint server this month.

"It's impressive that they've done this end-to-end," says Jevin West, a computational social scientist at the University of Washington in Seattle. "And I think we should be playing around with these ideas, because there could be potential for helping science."

The output is not earth-shattering so far, and the system can only do research in the field of machine learning itself. In particular, AI Scientist is lacking what most scientists would consider the crucial part of doing science — the ability to do laboratory work. "There's still a lot of work to go from AI that makes a hypothesis to implementing that in a robot scientist," says Gerbrand Ceder, a materials scientist at Lawrence Berkeley National Laboratory and the University of California, Berkeley. Still, Ceder adds, "If you look into the future, I have zero doubt in mind that this is where much of science will go."

Automated experiments

AI Scientist is based on a large language model (LLM). Using a paper that describes a machine learning algorithm as template, it starts from searching the literature for similar work. The team then employed the technique called evolutionary computation, which is inspired by the mutations and natural selection of Darwinian evolution. It proceeds in steps, applying small, random changes to an algorithm and selecting the ones that provide an improvement in efficiency.

To do so, AI Scientist conducts its own 'experiments' by running the algorithms and measuring how they perform. At the end, it produces a paper, and evaluates it in a sort of automated peer review. After 'augmenting the literature' this way, the algorithm can then start the cycle again, building on its own results.

The authors admit that the papers AI Scientists produced contained only incremental developments. Some other researchers were scathing in their comments on social media. "As an editor of a journal, I would likely desk-reject them. As a reviewer, I would reject them," said one commenter on the website Hacker News.

West also says that the authors took a reductive view of how researchers learn about the current state of their field. A lot of what they know comes from other forms of communication, such as going to conferences or chatting to colleagues at the water cooler. "Science is more than a pile of papers," says West. "You can have a 5-minute conversation that will be better than a 5-hour study of the literature."

West's colleague Shahan Memon agrees — but both West and Memon praise the authors for having made their code and results fully open. This has enabled them to analyze the AI Scientist's results. They've found, for example, that it has a "popularity bias" in the choice of earlier papers it lists as references, skirting towards those with high citation counts. Memon and West say they are also looking into measuring whether AI Scientist's choices were the most relevant ones.

Repetitive tasks

AI Scientist is, of course, not the first attempt at automating at least various parts of the job of a researcher: the dream of automating scientific discovery is as old as artificial intelligence itself — dating back to the 1950s, says Tom Hope, a computer scientist at the Allen Institute for AI based in Jerusalem. Already a decade ago, for example, the Automatic Statistician was able to analyse sets of data and write up its own papers. And Ceder and his colleagues have even automated some bench work: the 'robot chemist' they unveiled last year can synthesize new materials and experiment with them.

Hope says that current LLMs "are not able to formulate novel and useful scientific directions beyond basic superficial combinations of buzzwords". Still, Ceder says that even if AI won't able to do the more creative part of the work any time soon, it could still automate a lot of the more repetitive aspects of research. "At the low level, you're trying to analyse what something is, how something responds. That's not the creative part of science, but it's 90% of what we do." Lu says he got a similar feedback from a lot of other researchers, too. "People will say, I have 100 ideas that I don't have time for. Get the AI Scientist to do those."

Lu says that to broaden AI Scientist's capabilities — even to abstract fields beyond machine learning, such as pure mathematics — it might need to include other techniques beyond language models. Recent results on solving maths problems by Google Deep Mind, for example, have shown the power of combining LLMs with techniques of 'symbolic' AI, which build logical rules into a system rather than merely relying on it learning from statistical patterns in data. But the current iteration is but a start, he says. "We really believe this is the GPT-1 of AI science," he says, referring to an early large language model by OpenAI in San Francisco, California.

The results feed into a debate that is at the top of many researchers' concerns these days, says West. "All my colleagues in different sciences are trying to figure out, where does AI fit in in what we do? It does force us to think what is science in the twenty-first century — what it could be, what it is, what it is not," he says.

References:
Lu, C., Lu, C., Lange, R. T., Foerster, J., Clune, J. & Ha, D. Preprint at arXiv https://arxiv.org/abs/2408.06292 (2024).
Ghahramani, Z. Nature 521, 452–459 (2015).
Szymanski, N. J. et al. Nature 624, 86–91 (2023).

QUESTIONS:

1. AI Scientist is a new development in the field of machine learning, designed to perform the full cycle of scientific research. However, it has some limitations. Which of the following is a significant limitation of AI Scientist as described in the text?
- ☐ A) It cannot write research papers.
- ☐ B) It can only perform research in the field of machine learning.
- ☐ C) It is unable to generate any hypotheses.
- ☐ D) It cannot conduct literature reviews.
- ☐ E) It performs better than human scientists in all aspects.

2. The AI Scientist is praised for its innovative approach to scientific research, but it has not yet revolutionized the field. What is one reason that AI Scientist has not had a groundbreaking impact according to the text?
- ☐ A) It has produced results that are only incremental developments.
- ☐ B) It relies too heavily on outdated research papers.
- ☐ C) It requires constant human supervision to function correctly.
- ☐ D) It is too expensive to be widely adopted.
- ☐ E) It was designed primarily for educational purposes.

3. Researchers have differing opinions about the potential of AI Scientist. Some believe it will eventually perform all aspects of scientific work, while others are skeptical. What aspect of scientific work is AI Scientist currently unable to perform?
- ☐ A) Writing and reviewing research papers.
- ☐ B) Conducting experiments in a laboratory setting.
- ☐ C) Analyzing data from completed experiments.
- ☐ D) Reviewing the scientific literature.
- ☐ E) Formulating hypotheses for new developments.

4. Despite the current limitations of AI Scientist, researchers are optimistic about its future. Which of the following statements best reflects the long-term potential of AI Scientist as suggested in the text?
- ☐ A) AI Scientist will soon replace human researchers entirely.
- ☐ B) AI Scientist will never be able to contribute to scientific discovery.
- ☐ C) AI Scientist might eventually automate much of the scientific process, but creative work will remain human-driven.
- ☐ D) AI Scientist's usefulness is limited to specific research fields and will not expand.
- ☐ E) AI Scientist is expected to fail due to its inherent limitations.

5. The development of AI Scientist has sparked a debate about the role of artificial intelligence in scientific research. What concern do some researchers have about the reliance on AI in this context?

☐ A) AI Scientist may produce biased results based on popular papers.
☐ B) AI Scientist could completely take over the field of scientific research.
☐ C) AI Scientist is too complex for most scientists to use effectively.
☐ D) AI Scientist's findings are often too advanced for peer review.
☐ E) AI Scientist has no practical applications in modern science.

6. According to the text, one of the major strengths of AI Scientist is its ability to automate repetitive tasks in research. Which of the following tasks is AI Scientist particularly good at automating?

☐ A) Developing entirely new scientific theories.
☐ B) Performing creative and innovative experiments.
☐ C) Synthesizing new materials without human intervention.
☐ D) Running algorithms and measuring their performance.
☐ E) Engaging in scientific discussions at conferences.

7. The article discusses the potential improvements needed for AI Scientist to expand its capabilities. What is one method mentioned that could help AI Scientist handle more abstract fields beyond machine learning?

☐ A) Increasing its access to scientific literature.
☐ B) Incorporating symbolic AI techniques into its system.
☐ C) Improving its ability to write and review papers.
☐ D) Expanding its database of scientific conferences.
☐ E) Enhancing its ability to perform laboratory experiments.

8. The creators of AI Scientist have made their code and results fully open to the public. What is one reason given in the text for making these resources available?

☐ A) To encourage competition among researchers.
☐ B) To allow others to analyze and improve the AI Scientist's performance.
☐ C) To limit the use of AI Scientist in commercial projects.
☐ D) To ensure that AI Scientist remains free for educational purposes.
☐ E) To prevent the misuse of AI technology in scientific research.

9. AI Scientist's ability to formulate hypotheses is a key feature, but it is not without limitations. What is one challenge that AI Scientist faces when generating new scientific hypotheses?

☐ A) It cannot access the most recent scientific literature.
☐ B) It generates hypotheses that are too complex for peer review.
☐ C) It lacks the computational power to analyze complex data sets.
☐ D) It often fails to complete the scientific process.

□ E) It tends to rely on superficial combinations of existing ideas.

10. The text highlights both the achievements and the shortcomings of AI Scientist. What is one of the main reasons why some researchers are cautious about fully embracing AI Scientist for their work?

□ A) AI Scientist is not capable of fully autonomous scientific discovery.
□ B) AI Scientist is only available to researchers in specific countries.
□ C) AI Scientist has a tendency to produce inconsistent results.
□ D) AI Scientist requires a large amount of data storage.
□ E) AI Scientist is designed to replace human researchers entirely.

Gabarito:

1. B) It can only perform research in the field of machine learning.
The text states that AI Scientist is currently limited to conducting research specifically in the field of machine learning, which is one of its main limitations.

2. A) It has produced results that are only incremental developments.
The passage explains that the AI Scientist's results are not groundbreaking because they represent only incremental developments.

3. B) Conducting experiments in a laboratory setting.
The text mentions that AI Scientist lacks the ability to perform laboratory work, which is a critical component of scientific research.

4. C) AI Scientist might eventually automate much of the scientific process, but creative work will remain human-driven.
The text suggests that while AI Scientist could automate many aspects of research, creative and innovative work will likely continue to be driven by humans.

5. A) AI Scientist may produce biased results based on popular papers.
The text mentions that AI Scientist has a "popularity bias" towards papers with high citation counts, which is a concern for some researchers.

6. D) Running algorithms and measuring their performance.
The text describes how AI Scientist conducts its own experiments by running algorithms and measuring their performance, which is part of its strength in automating repetitive tasks.

7. B) Incorporating symbolic AI techniques into its system.
The text suggests that to broaden AI Scientist's capabilities, especially in more abstract fields, it might need to include symbolic AI techniques.

8. B To allow others to analyze and improve the AI Scientist's performance.
The text mentions that making the code and results open enables others to analyze the AI Scientist's results and potentially improve its performance.

9. E) It tends to rely on superficial combinations of existing ideas.
The text indicates that AI Scientist may struggle to formulate novel and useful scientific directions beyond basic superficial combinations of buzzwords.

10. A) AI Scientist is not capable of fully autonomous scientific discovery.
The text emphasizes that, while AI Scientist can automate parts of the research process, it is not yet capable of fully autonomous scientific discovery, which is a reason for researchers' caution.