Artificial intelligence expands the materials universe

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Video Abstract

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Abstract

Artificial intelligence is transforming our way of life. Able to spot patterns invisible to the human eye, algorithms are learning how to make our lives easier, safer, and more fun. That power is not lost on materials researchers. During the next decade, artificial intelligence or AI-driven research could fundamentally transform how new and better materials are developed. What's more, it might even revamp how materials research itself is carried out, enabling promising new materials and processes to be developed more quickly. Machine learning methods come in a variety of flavors, with some requiring more guidance, or "supervision," from researchers. But, generally, a machine-learning algorithm designed to discover and understand the behavior of materials looks for patterns connecting the composition, structure, and properties of known materials. Once trained on a sufficiently large data set, and incorporating the latest understanding of materials behavior, the algorithm then makes educated guesses at what unique combinations are most likely to yield better thermoelectric or battery cathode materials, for example. As easy as that process might sound, researchers still face hefty challenges in probing the vast materials universe. For one, machine-learning methods are only as smart as their training data allow. Despite their unrivaled computational muscle, machine-learning algorithms work best with massive amounts of data to make reliable inferences. Unfortunately for materials researchers, data are hard to come by in bulk, given the numerous ways materials can be combined and processed from the elements. Consider that the entirety of materials research history has produced somewhere between 200,000 and 500,000 inorganic compounds to date. Dazzling, no doubt. But that number represents only a small patch of the full space of possible material combinations. Then, of course, there's the problem of translating the predictions of these algorithms to the lab. A material that takes minutes to arrive at by computer could take years to synthesize in any useful form. For this second challenge, machine learning could be co-opted to do more than just search for new materials. Algorithms trained on experimental synthesis data could teach researchers how best to go about producing stable materials in the lab—literally generating recipes for success. Other algorithms might help design and conduct new experiments, perhaps in automated loops that barely require human intervention. Continued research will make machine-learning algorithms more powerful for materials scientists and engineers. Data sets will expand, and computational methods will become savvier. But machine reasoning will take a long time, if ever, to substitute for human reasoning. For now at least, materials researchers may look forward to the future of AI as a collaboration between human and machine in the pursuit of new and improved materials.