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Powerhouse UCSB team awarded big grant to investigate mathematical foundations of AI

When it comes to AI, two's company, but three — or more — can be a much harder problem.

Many current approaches to AI in science model interactions in pairs, according to UC Santa Barbara's Nina Miolane, whether between two atoms in a chemical reaction, two regions in the brain, or two stars in a galaxy.

But systems of all sizes often involve interactions between multiple components. Groups of molecules, planets and people can "create something that each pair independently couldn't have created," said Miolane, an assistant professor of electrical and computer engineering (ECE). "And AI often doesn't look at these higher-order interactions."

Now, Miolane and three fellow AI researchers in the Robert Mehrabian College of Engineering — ECE assistant professor Haewon Jeong, assistant professor of computer science Sanjukta Krishnagopal and ECE associate professor Yao Qin — are developing AI methods to uncover the scientific laws that govern such systems through a $1 million National Science Foundation award.

“Newton wrote the equations of mechanics, but there are other sciences that don’t have beautiful or known laws, Miolane said. “In neuroscience, for example, we don’t know much about the brain. And in other fields there are many scientific laws left to be discovered.”

The award is the first federal grant received by the Real AI initiative, launched earlier this year at UCSB and co-directed by Jeong, Miolane and Qin.

Rather than limiting AI models to pairwise relationships, the researchers want them to account for overlapping interactions among many components, across different scales and over time.

“This award matters to me because it directly addresses a major gap in today’s AI,” Jeong said. “LLMs are very good at answering a lot of our questions, yet if we ask them to predict the next state of a fluid flow, they still struggle. How can we build AI systems that understand not only human language, but also the physical world?”

The award also brings together four female early-career faculty members across multiple departments.

“This collaboration is unusual in engineering, because any single department doesn’t have a lot of women to begin with,” said Krishnagopal. “That makes it a really exciting space to be in.”

The team reflects one of UCSB’s strengths: researchers working across traditional boundaries in engineering and the physical sciences. In this case, the researchers’ combined expertise allows the group to approach the same problem from multiple directions, from developing new mathematical foundations to determining whether the resulting models are reliable and testing them across a range of scientific data.

In fact, the collaboration may be a prime example of the project’s underlying concept: a group has the potential for multiple interactions that can lead to novel, boundary-pushing results.

Meeting of the minds

Each of the co-PIs on the award, “Foundations for Discovering Higher-Order Scientific Laws with Deep Learning,” brings their own area of expertise.

Miolane has spent much of her career using novel mathematics to help AI extract information from data it would otherwise overlook, particularly through her work as director of UCSB's Geometric Intelligence Lab. She helped found topological deep learning, which lets AI capture group interactions in data, and has applied it to the complex interactions within the brain, including as AI core co-director at the Ann S. Bowers Women's Brain Health Initiative.

"The mathematics of topology gives AI a language to think about, and compute with, group interactions," Miolane said. "Once a model can see how many parts act together, it can start revealing the scientific rules that govern the whole system."

Jeong's research group specializes in machine learning for complex scientific systems. On this project, she is helping explore how new AI architectures might reveal information that conventional models leave hidden.

"We want to develop AI models that can accurately predict complex physical systems, but also go beyond prediction to interpret what they have learned," she said. "Ultimately, we hope to use techniques such as Kolmogorov-Arnold networks and topological neural networks to help uncover the governing equations and principles underlying the physical world."

Some of these promising architectures for science come without any underlying guarantees of their reliability, said Qin. That's where she comes in: her research has centered on the robustness and trustworthiness of machine learning, an area which is becoming increasingly important with the expansion of AI in scientific discovery.

Robustness and reliability have particular significance in molecular biology and drug discovery "where even small prediction errors can have serious downstream consequences," said Qin, who is leading the project's certified robustness work. "That gap is exactly the kind of problem I find compelling: these models are being adopted rapidly and enthusiastically, but without a theoretical foundation to tell scientists when their predictions can be trusted under the noise inherent in real experimental data. The chance to build that foundation — to bring provable robustness to an entirely new class of models at the frontier of AI for science — is what drew me into this project."

Krishnagopal, who received a Ph.D. in physics from the University of Maryland before shifting toward computer science, studies interconnected social and biological systems. Her background adds the behavior of systems over time to a project that

already spans different types and scales of interactions.

“I don’t just want something that explains what happens at a snapshot in time; I want something that explains what the entire system is doing over time,” Krishnagopal said.

The team ultimately wants the mathematical framework to work across different scales, systems and disciplines rather than for only one type of data.

“It’s important for the results to be robust, for them to be mathematically consistent, and for it to really be this foundational piece of work that is not dependent on a specific scale or a specific data set,” Krishnagopal said. “That opens up this new language for this analysis of these types of complex systems.”

Step by step

The team will start by establishing the mathematical foundations necessary to discover higher-order scientific laws, then test the framework using both synthetic and real-world data, including datasets drawn from Miolane’s neuroscience work, along with data from molecular biology and cosmology. Using such different scientific settings will allow the researchers to test whether the approach can extend beyond a single discipline or type or system.

Ultimately, the team plans to make its tools open source so scientists in other fields can use the methods without needing to become experts in robustness. Qin said that broader usefulness would be one measure of the project’s success.

“I’d consider it a real achievement if this work helps shift AI for science toward models that are not just accurate but demonstrably trustworthy,” Qin said.

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