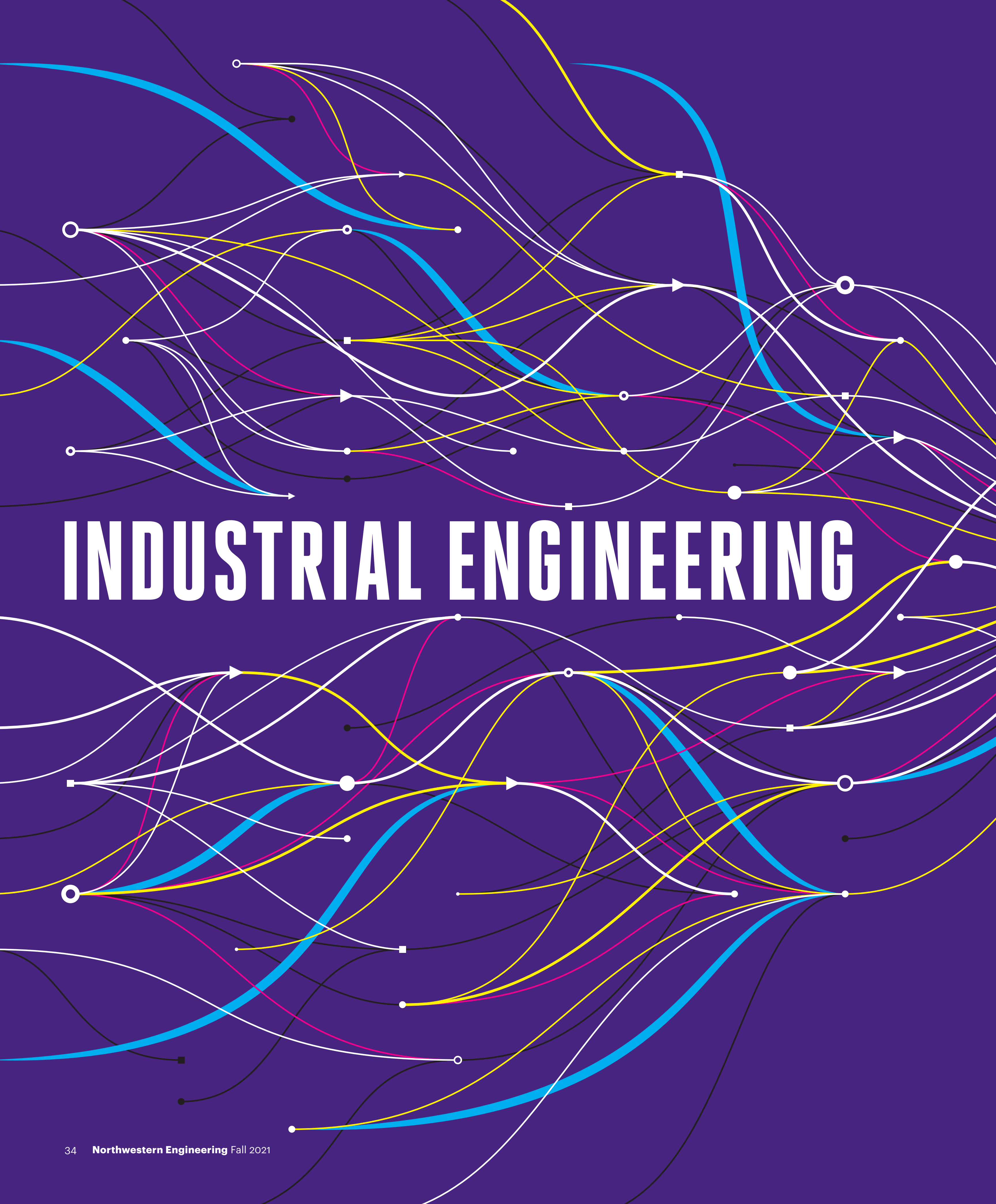

INDUSTRIAL ENGINEERING

The Department of Industrial Engineering and Management Sciences is a leader in the science of decision-making in complex environments through innovation in algorithms, computation, and mathematical modeling.

LEADING DECISION-MAKING IN THE AGE OF MACHINE LEARNING

As artificial intelligence and machine learning become more integrated into daily lives, IEMS faculty members are improving decision-making and addressing societal challenges across industries, businesses, and disciplines.

"WE'RE DEVELOPING ENABLING TECHNOLOGIES. NOT ONLY ARE OUR ALGORITHMS USED IN ALL THESE DIFFERENT INDUSTRIES, THEY ALSO MAKE IT POSSIBLE FOR SCIENTISTS AND ENGINEERS TO DO NEW RESEARCH."

ANDREAS WÄCHTER Professor of Industrial Engineering and Management Sciences

THE FAR REACH OF IEMS ALGORITHMS

Building a chemical plant. Developing an airline route. Modeling the shapes of proteins.

Each of these endeavors requires optimization algorithms: the combination of math and theory translated into code that ultimately finds the best way to design, plan, or perform an action. While engineers often develop algorithms for specific uses, two IEMS professors have earned the distinction of having developed optimization algorithms that are used broadly across industries and scientific disciplines.

L-BFGS and KNITRO, developed by Jorge Nocedal, and Ipopt, developed by Andreas Wächter, have been used in everything from designing computer chips to modeling pandemics to understanding the effects of climate change on arctic ice.

Optimization algorithms take a problem—the best airline route from Chicago to Atlanta, for example—and consider variables, like air traffic and wind, before presenting the optimal solution.

Nocedal developed L-BFGS after realizing that an existing optimization algorithm called BFGS could not be applied to problems with numerous variables. He tried to solve this throughout graduate school and succeeded only after becoming a faculty member and realizing the algorithm could not retain everything it learned, because that would exceed the capacity of every computer. Instead, it needed to retain only a limited amount of relevant information, called limited memory—the "L" in L-BFGS.

"My modification of the algorithm allowed it to solve problems with millions of variables," says Nocedal, Walter P. Murphy Professor of Industrial Engineering and Management Sciences. But this was before big data and its usefulness were widely understood. Nocedal kept refining it based on his increasingly deeper understanding of the problem. In the 1990s, the algorithm became popular with weather forecasters, and when machine-learning research took off 20 years later, the use of the algorithm accelerated.

Now, most everyone in the field of machine learning knows the term L-BFGS. Recently, the algorithm was used as part of the Google DeepMind project to help determine the 3D shapes of proteins—a breakthrough that could lead to major advances in biology and drug discovery. It was also used early in the pandemic by the federal government to model the COVID-19 pandemic's trajectory.

In the 1990s, Nocedal also began developing another nonlinear optimization algorithm called KNITRO. This algorithm took even longer to develop than L-BFGS and could solve more complicated problems with more restrictions. He and his graduate students ultimately commercialized the algorithm as software. Now, KNITRO is widely used in the energy, finance, economics, and robotics sectors.

Enabling new technologies with Ipopt

KNITRO has a companion in Ipopt, the nonlinear optimization algorithm developed by Wächter using a different algorithm than KNITRO. Wächter, professor of industrial engineering and management sciences, began developing the algorithm in the late 1990s when he was a chemical engineering graduate student. He continued working on Ipopt at IBM, where it became an open-source project.

For years, he used math, theory, and computer programming to test and refine Ipopt. When it was translated into the C++ programming language, it became known as the go-to open-source nonlinear optimization algorithm.

Wächter regularly hears about new applications of the algorithm—running trains, optimizing power grids, building chemical plants, developing airline routes, enhancing medical imaging, and even creating models of black holes.

"We're developing enabling technologies," he says. "Not only are our algorithms used in all these different industries, they also make it possible for scientists and engineers to do new research."

Both Nocedal and Wächter continue to develop new algorithms. The future, Nocedal says, lies in algorithms that can deal with uncertainty. One rich source of new problems is in machine learning where optimization must be performed in the presence of uncertainty in the data. Given the explosive growth of artificial intelligence, the demand for more capable optimization algorithms will only increase with time.

EMILY AYSHFORD

"Our work opens new pathways to the understanding and discovery of this class of materials."

JAMES RONDINELLI Morris E. Fine Professor in Materials and Manufacturing

AI-BASED TOOLS TO ACCELERATE ELECTRONIC MATERIALS DISCOVERY

One of the keys to designing new computer architectures, and to making current microelectronic devices faster and more energy efficient, has been the discovery of new materials with tunable electronic properties.

Materials that exhibit a metal-insulator transition (MIT) could pave the way for future information-processing devices, display, and energy harvesting applications. Although some materials that exhibit MITs have already been implemented in electronic devices, fewer than 70 are known, and even fewer exhibit the performance necessary for integration into new electronic devices.

An interdisciplinary team of scientists from IEMS and the Department of Materials Science and Engineering used artificial intelligence techniques to build new, free, and easy-to-use tools that allow scientists to accelerate the rate of discovery and subsequent study of materials that exhibit MIT. The team also identified new features that can describe this class of materials.

The project was led by James Rondinelli, Morris E. Fine Professor in Materials and Manufacturing, and Daniel Apley, professor of industrial engineering and management sciences.

Combining their knowledge of MIT materials with natural language processing, the researchers scoured existing literature to identify the known MIT compounds, as well as 300 materials that are similar in chemical composition but do not show an MIT. The team has provided the resulting materials—as well as features it's identified as relevant—to scientists as a freely available database for public use.

Using machine-learning tools, the scientists then identified important features to characterize these materials. They confirmed the importance of certain features, such as the distances between transition metal ions or the electrostatic repulsion between some of them, as well as the accuracy of the model.

The team used that information to develop a reliable machine-learning model for MIT materials, which has been packaged into an openly accessible format. "Our work opens new pathways to the understanding and discovery of this class of materials," Rondinelli says.

BRIAN SANDALOW

HELPING BUSINESSES CAPITALIZE ON THE INTERNET OF THINGS

The "things" that comprise the Internet of Things (IoT)—mostly physical devices embedded with sensors and software that enable them to connect over the internet with other systems to share data—are becoming ubiquitous.

Northwestern Engineering professors have crafted a new system that allows all businesses to capitalize on this burgeoning IoT ecosystem. REFIT, developed by Northwestern's Center for Deep Learning and built by the McCormick School of Engineering's computer science and industrial engineering and management sciences departments, combines the University's machine learning and data science research with state-of-the-art artificial intelligence to produce predictive results.

REFIT ingests device and real-time business data and employs modern machine-learning approaches to infer the status of various IoT system components. The system allows users to develop, experiment, and deploy a powerful IoT framework quickly that makes work done by IoT components more efficient and with the same resources. The design allows REFIT to evolve and continuously improve its predictive abilities, while not disrupting the deployment of the current machine-learning or deep-learning approaches.

REFIT is especially useful for data scientists and engineers in companies with limited in-house resources. For example, current applications include determining real-time street traffic flows and predicting demand of Divvy bikes at stations.

"Data engineering is one of the most despised tasks," says Diego Klabjan, professor of industrial engineering and management sciences and director of the Center for Deep Learning. "Northwestern's system facilitates it by automatically generating a variety of statically based features from streaming IoT data and by using a single point of logic for features throughout the system during training or real-time scoring."

BRIAN SANDALOW