
THE ENERGY CRISIS

There is a significant—and rising—gap between sources of energy and energy consumption, which has led in recent years to the largest energy crisis since the 1980s. Because it is hard to change household energy consumption, I targeted industrial use. This allows sustainable energy sources to catch up to demand and create a smoother transition away from fossil fuels.

RESULTS

Currently, many catalysts used in production are outdated and costly. I demonstrate a method which aids in the design of optimal catalysts. In addition, I illustrate high-speed analysis of catalysts for efficiency in design.

METHODOLOGY

I designed a machine learning algorithm which satisfies two capabilities: to design new, optimized catalysts based on preselected characteristics; and, to perform real-time analysis of X-ray absorption spectroscopy that is hundreds of times faster than traditional methods. The Multi-task Algorithm for Variational auto-ENcoding (MAVEN) uses a novel mathematical framework that incorporates both physics-informed and statistics-informed constraints.

CONCLUSIONS

1. Explainability MAVEN demonstrates interpretability because scientists can understand the relationships between spectra and properties using the latent space as a proxy (as seen in fig. 6). It is well established that a major problem with deep learning is explainability, or it is not possible to manage.

2. Interpolation for Materials Discovery Interpolations along known nanocatalyst descriptors give insight when inverting the effects of properties on spectra and materials. While previous methodologies were able to decode structure from spectra and simulations were able to construct spectra from structural parameters, my algorithm is the first to be able to reverse-engineer materials in a self-consistent manner (as demonstrated in fig. 4). I can pinpoint the material at previously unknown points in the latent space with pre-selected catalyst properties so that I can find optimized solutions for manufacturing.

3. Real-time identification of nanocatalyst properties I demonstrate that MAVEN provides faster and more accurate identification of crucial properties for designing optimal nanocatalysts than state-of-the-art techniques for materials analysis. In previous methodologies, there was an unsatisfactory degree of accuracy in experimental data due to a lack of denoising capability, which would inhibit this from being used in real-world industrial situations. MAVEN allows for the understanding of physicochemical properties in complex, fast reactions through incomplete, noisy, time-modulated data, demonstrated in fig. 5 and fig. 6.

REFERENCES