Will AI help us in building better batteries?

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We have written a series of blogs on how artificial intelligence (AI) is advancing other megatrends:

- AI Continues to Build the Foundation for a Remarkable Future in Biology
- Can AI Replace People? The Truck-Driving Case Study
- The World Needs More Metals. Maybe AI can Find Them.

By exploring these connections between themes, we can view AI less as a black box of algorithmic complexity and more as something that is focused on solving concrete problems in the world.

A brief primer on electrochemical batteries1

What we know today as 'lithium-ion' batteries fall into the class of 'electrochemical batteries'. For the battery to generate power the chemical process has to generate electrons, and for the battery to be 're-charged' it has to store electrons.

The structure of the battery involves the anode (negative side), electrolyte and cathode (positive side). The current that the battery can generate relates to the number of electrons flowing across from negative to positive, and the voltage relates to the force with which the electrons are traveling.

Using the battery, that is, using your smartphone or driving your electric car, means that the electrons are flowing from the anode, through the electrolyte and to the cathode. Charging your devices means that you are forcing the process to occur in reverse, where the electrons are leaving the cathode, going back across the electrolyte and ending up in the anode.

Why do we have to know all of that?

Some of you might be like me and think—my last chemistry class was more than 20 years ago. The reason we set that foundation, however, is that it now allows us to think in terms of the following:

- The different parts of the battery can be fashioned out of different elements.
- Changing the mix of metals in the cathode, for example, may impact the energy density, speed of charging, heat dispersion or other battery characteristics.
- Researchers can experiment with all sorts of different anodes, cathodes and electrolytes as they seek to optimise the characteristics of a given battery to its use case.

Now we can better understand the ways in which an artificial intelligence process can be utilised to seek to improve different characteristics of the batteries that we use.

Who wants electric vehicles to charge faster?

One of the many obstacles to the wider usage of electric vehicles is the time it takes to charge a battery vs. filling a tank with petrol. Since filling the tank is much faster, they opt for the internal combustion engine over the battery electric vehicle.

There is huge marketability for automobile manufacturers and battery-makers for every unit of time they can shave off of charging times.

Researchers at Carnegie Mellon used a robotic system to run dozens of experiments designed to generate different electrolytes that could enable lithium-ion batteries to charge faster. The system is known as Clio, and it was able to both mix different solutions together as well as measure performance against critical battery benchmarks. These results were then fed into a machine-learning system, known as Dragonfly2.

Dragonfly is where the process starts to get exciting—the system is designed to propose possible combinations of chemicals to be used in the electrolytes that could potentially work even better. Using this process during this particular time period led to six different electrolyte solutions that outperformed a standard one when they were placed into typical battery test cells. The best option showed a 13% improvement relative to the top-performing battery baseline3.

In reality, electrolyte ingredients can be mixed and matched billions of different ways, but the benefit of using the system of Clio and Dragonfly working together is that one can get through a wider array of possibilities faster than humans alone. Dragonfly also isn't equipped with information about chemistry or batteries, so it doesn't bring the 'bias of previous knowledge or experience' to the process.

Using AI to help the progress of solid-state batteries

While the aforementioned path involves improving liquid electrolytes, it is not the only critical area of battery research today.

If the flammable, liquid electrolyte is replaced by a stable solid, it's possible that there would be improvements in battery safety, lifetime and energy density. However, finding the appropriate materials to facilitate building solid-state batteries that fit all specifications and that can be produced at scale is not a simple matter.

Researchers at Stanford have noted a particular process where they compile data on 40 materials with both good and bad measured room temperature lithium conductivity values. This particular characteristic is thought to be the most restrictive of all the different constraints on candidate materials. The 40 examples are 'shown' to a logistic regression classifier, which can 'learn' to predict whether the material performed well or not based on the atomistic structure. After the training phase, the model can then evaluate more than 12,000 lithium-containing solids and find around 1,000 of them that have a better than 50% chance of exhibiting fast lithium conduction4.

Progressing solid state batteries along the development path is therefore another clear use-case for artificial intelligence.

Conclusion: energy storage is one of the most important considerations for the coming decades

Having better energy storage solutions will help global society in myriad different ways. The classic case—there are intermittent power generation sources like solar and wind that can use batteries to equilibrate the flows of energy across time. However, I think we'd all love smartphones that don't need a charge for a week or electric vehicle batteries with long range that can charge in similar times to what it previously took at a gas station.

1 Source: https://www.volts.wtf/p/a-primer-on-lithium-ion-batteries#details

2 Source: Temple, James. "How robots and AI are helping develop better batteries." MIT Technology Review. 27 September 2022.

3 Source: Temple, 27 September 2022.

4 Source: https://reedgroup.stanford.edu/research/eletrolyte.html

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