Krátos Batteries

The Project:

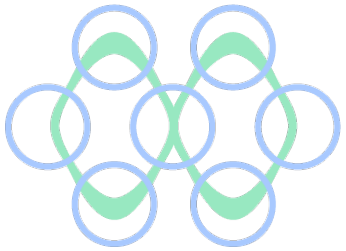
Using existing data to predict volume change and capacity of new electrode materials

- Small Volume Change → Longer Battery Life
- Bigger Capacity → More Energy Stored

Predicting them is useful:

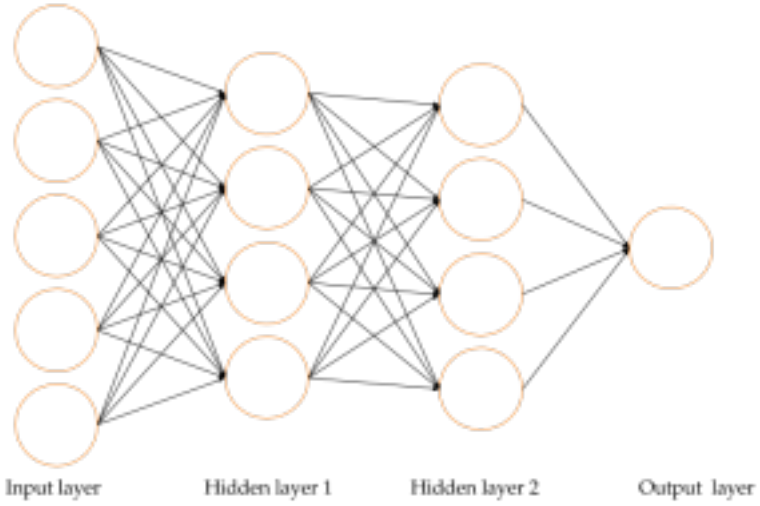
1. Guide experiments seeking to develop novel materials for battery applications
2. Perform a quick screening before starting synthesis procedures

How It Works



The Materials Project

Deep Neural Network



- Get dataset of electrodes for training from Materials Project Database and reference papers
- Figure out what parameters should be used by calculating correlations
- Use DNN, SVR, KRR machine learning methods to predict
- Test and optimise our model and algorithm
- Encapsulate our model as an API sharing on GitHub

PyTorch vs. TensorFlow

Krátos

Neural Network	**Dynamic** • Reverse-mode auto-differentiation • Imperative Programming • Define, change and execute nodes as you go through each line (similar to Python)	**Static** • ‘Data as code and code is data’ • Graph defined statically before a model can run • Changing network behavior = full restart
Commits	**24,138** commits Last Commit: “1 Hour ago”	**79,212** commits Last Commit: “15minutes ago”
Issues	3,863 Open ✓ **8,778 Closed** Last Resolve: “2 Hours ago”	3,141 Open ✓ **20,000 Closed** Last Resolve: “12 Hours ago”

PyTorch - Appeal

- More popular in the research community
- Made to be fast and lean
- Pretrained models
- Contains implementations of popular optimization algorithms
- Built to be deeply integrated into Python
- Easier debugging experience using built in debugging tools
- Official tutorials with examples

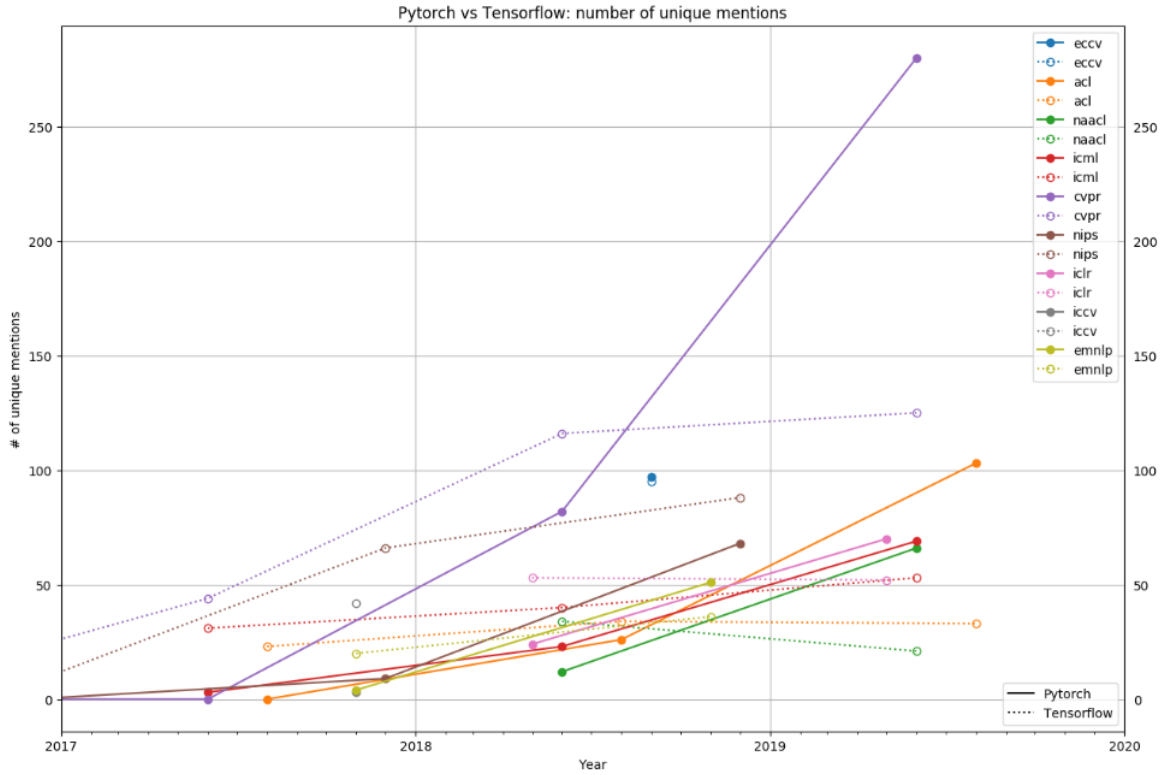


Image source: https://thegradient.pub/

PyTorch - Drawbacks

- PyTorch is a newer system
  - Less documentation
  - Lower amount of tutorials online (compared to packages like TensorFlow)
- PyTorch is not available for Windows (only Linux and MacOS)
  - However, there are unofficial builds
- Generally Considered Low-Level
- No commercial support

System	2.7	3.5	3.6
Linux CPU	build running	build running	—
Linux GPU	build running	build running	—
Windows CPU / GPU	—	build failing	—
Linux (ppc64le) CPU	—	—	build failing
Linux (ppc64le) GPU	—	—	build failing