

Krátos Batteries

The Project:

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

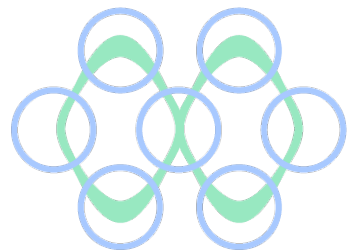
- Small Volume Change → Longer Battery Life
- Bigger Capacity → More Energy Stored

Predicting them is useful:

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

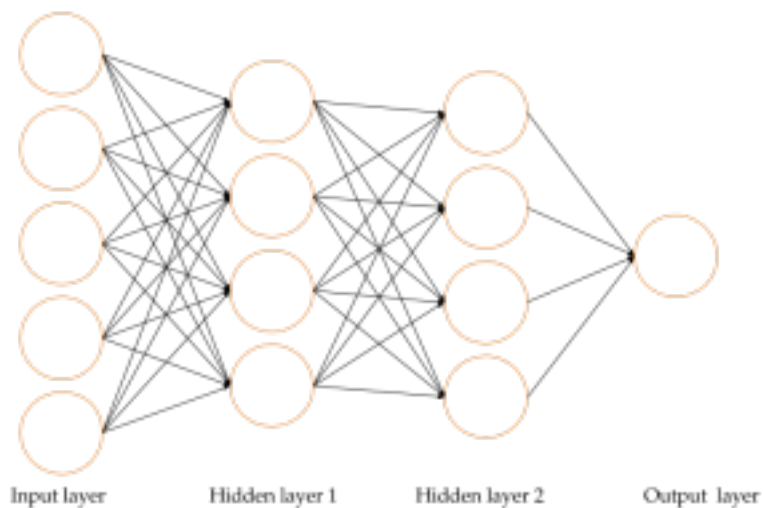


How It Works



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



| |  |  |
|-----------------------|---|--|
| Neural Network | Dynamic <ul style="list-style-type: none">Reverse-mode auto-differentiationImperative Programming<ul style="list-style-type: none">Define, change and execute nodes as you go through each line (similar to Python) | Static <ul style="list-style-type: none">'Data as code and code is data'Graph defined statically before a model can runChanging 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

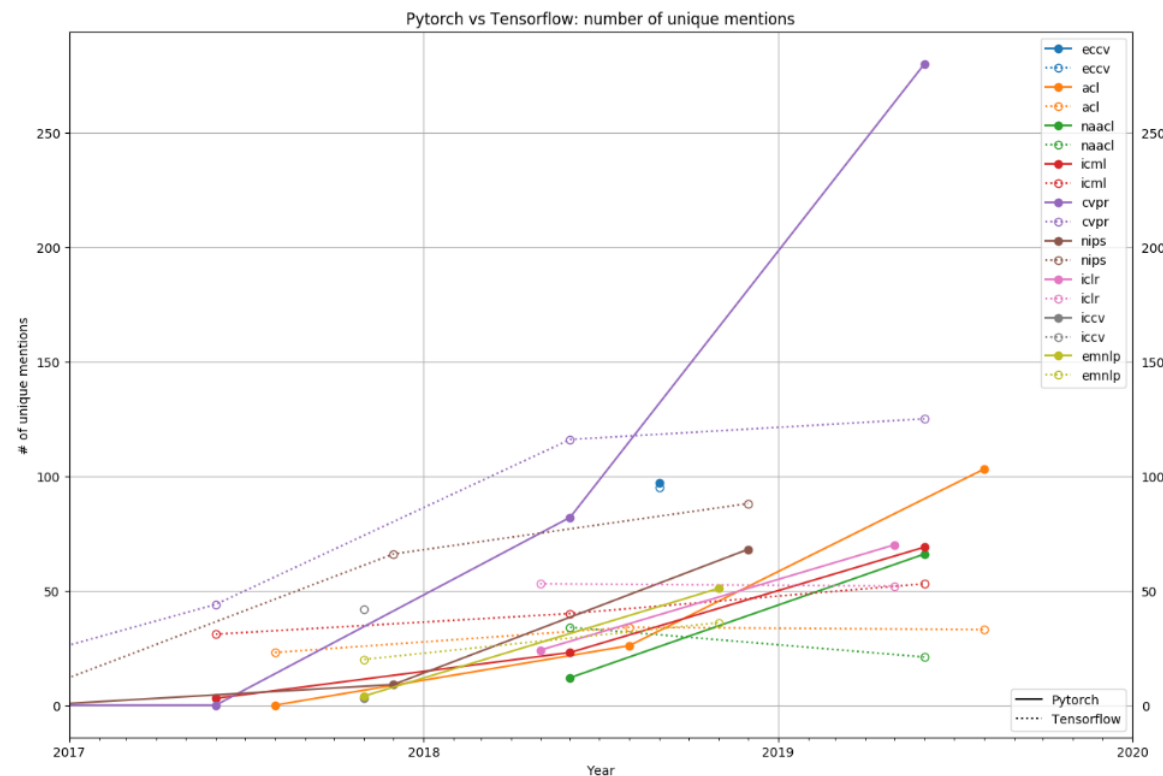


Image source: <https://thegradient.pub/>

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 | <div>build running</div> | <div>build running</div> | — |
| Linux GPU | <div>build running</div> | <div>build running</div> | — |
| Windows CPU / GPU | — | <div>build failing</div> | — |
| Linux (ppc64le) CPU | — | — | <div>build failing</div> |
| Linux (ppc64le) GPU | — | — | <div>build failing</div> |