Deep Learning for Batteries

2021-04-28



A Unique Research Institute in Deep Learning

Mission: To be a global pole for scientific advances that inspires innovation and the development of AI for the benefit of all



Founded in 1993 by Turing Award Laureate, Prof. Yoshua Bengio

In 2019, Mila moved to its unique location in O Mile-Ex creating a **distinctive Al ecosystem**, in which **Al researchers from academia and companies (large, medium and small) collaborate**





Distinctive Features of our Applied AI Team

Privileged access to Mila's 500+ faculty and student researchers Collaborative approach to transfer knowledge to industry researchers Significant part of the applied research team's costs covered by Mila funding

Mutually beneficial agreements regarding intellectual property

Meet some of our Experts



Scientific Direction

• 20+ years in ML/DL

Bengio

PhD in ML under the supervision of Y.



Project Management

Jean-Philippe Nantel

- 10+ years of data science project management
- Eng. and M.Sc. in Applied Math. & Computer Science



Project Lead

Gaétan Marceau Caron

- 9+ years in computer science and ML/DL
- Postdoc in ML





Polymer Properties Prediction

Searching in large parameter space

LambdaZero: ongoing project for targeted drug discovery

Surrogate Models of varying complexity for properties estimation

Combining Bayesian Deep Learning and Reinforcement Learning to search for drug candidates

Could be used for lithium-conducting polymers

Need data



Figure 1. Scheme for predicting properties of the solid polymer electrolytes by AI. Conductivity was predicted in this study.

From; *AI-Assisted Exploration of Superionic Glass-Type Li+ Conductors with Aromatic Structures.* K. Hatakeyama-Sato, T. Tezuka, M. Umeki, K. Oyaizu. JACS **142**, 3301-3305 (2020)

