Data-Driven Discovery and Design of Superionic Lithium Conductors for High Performance Lithium Ion Batteries

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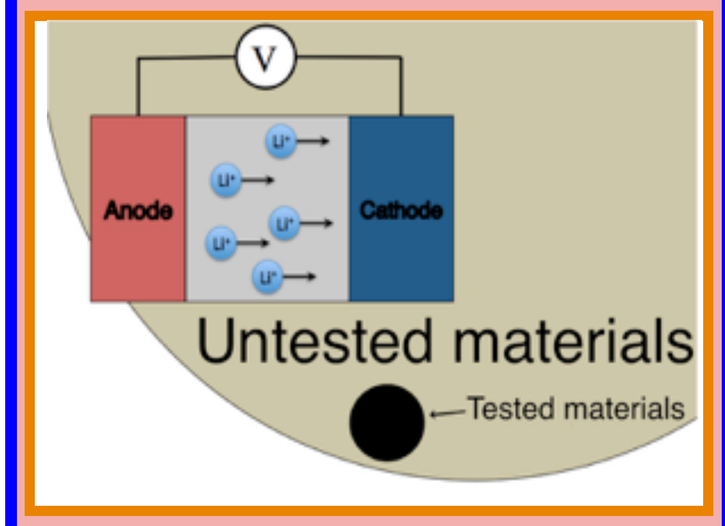
MOTIVATION

- Solid state lithium ion batteries show great promise as high performance energy storage devices; however, designing **high ionic conductivity solid electrolytes** remains a challenge.
- There has yet to be a model that **accurately** generalizes trends in ionic conductivity among crystal structures to rapidly identify promising electrolyte materials *in silico*.



KEY POINTS

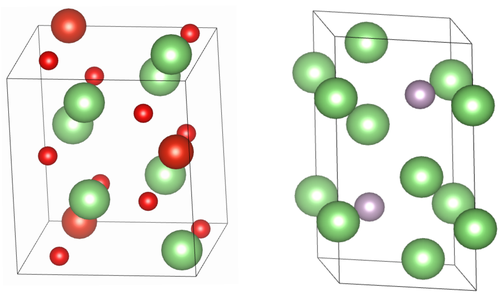
1) Implement multiple regression techniques to **predict ionic conductivity** in materials from structure alone.

2) Identify promising new candidate solid lithium conductors by screening over 1,000 lithium containing structures.

3) We find a number of promising candidate structures **which have not yet been studied in the literature**.

Data and Features

- Gather data on structure and ionic conductivity for **38 different materials** by searching the scientific literature
  - Structure files are down-loaded from the Inorganic Crystal Structure Database



- Extract **19 atomistic features** for each structure
  - These features do not require expensive electronic structure calculations
  - We avoid overfitting on our small training set by performing leave-one-out cross validation

Model Selection and Performance

We implement least squares linear regression with the following cost function:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

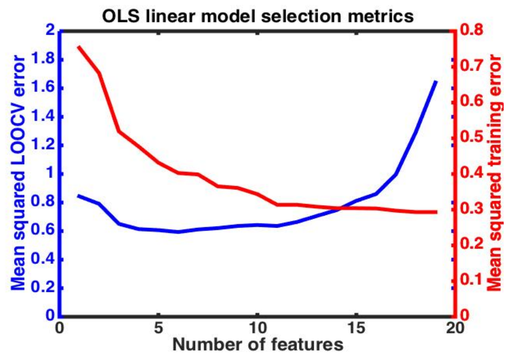
where $h_\theta(x) = \theta^T x$

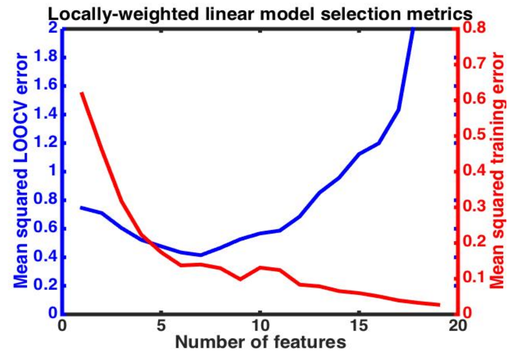
We also implement locally weighted least squares linear regression with the following cost function:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m} w^{(i)}(h_\theta(x^{(i)}) - y^{(i)})^2$$

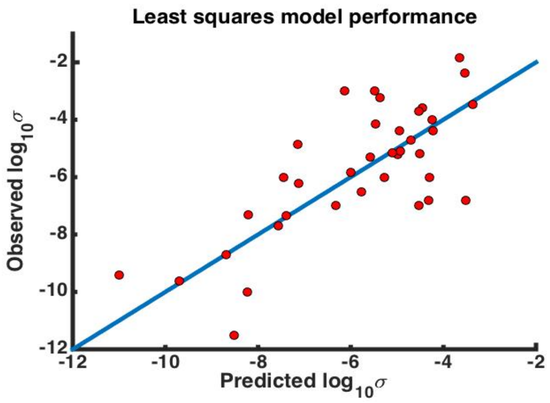
where $w^{(i)} = exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right)$

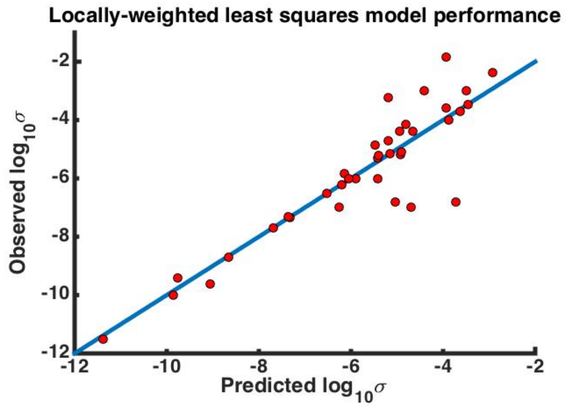
We search for the optimal model by performing leave-one-out cross validation over all models





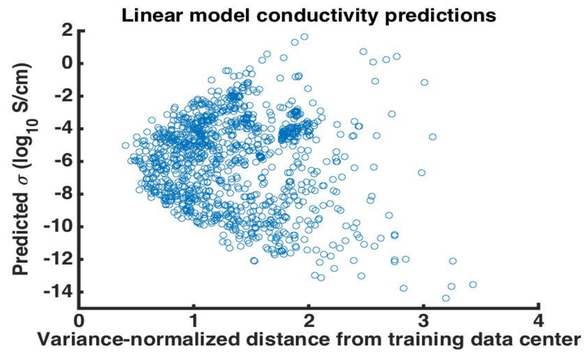
The optimal models show strong predictive capabilities with low training

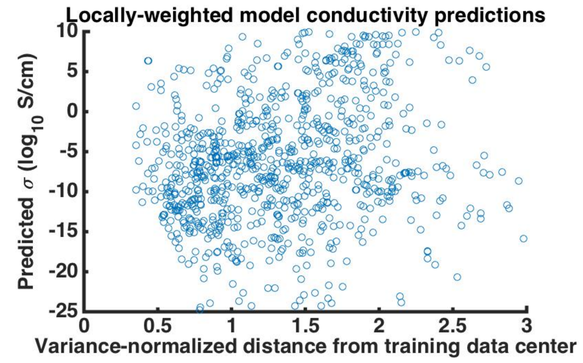




Screening

We apply our hypothesis functions to over 1,200 candidate materials and develop a PCA-based confidence metric for each prediction





Our models allow us to identify many promising candidate materials for further investigation

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