ET-AL: Entropy-targeted active learning for bias mitigation in materials data

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Integrated DEsign Automation Laboratory



Materials Science with Data



Growing materials data + data-driven methods \rightarrow

- Accurate predictive modeling
- Efficient, on-demand materials design

Data Sources

Where materials informatics / data-driven design researchers get data



These data sources are often biased



Bias in Materials Databases



Why is bias a problem?

From a materials science perspective

- Microstructure information helps modeling materials properties
- Microstructure relies on ΔE of phases
- Bias in $\Delta E \rightarrow$ problematic property models

From a data science perspective

Lower bias → better coverage of the design space →
 better generalizability of models



Problem Formulation

- Data bias in properties of interest
 - Deviates from known nature
 - Lack of representativeness
- Bias is ubiquitous in materials data, but its level can be reduced





Goals:

- Detect (quantify) bias
- Reduce bias by adding new data

Information Entropy as a Bias Metric

Define bias among groups



Here, use crystal system (a natural, trivial grouping)

Information entropy

$$h(Y) = -\int p(y) \ln p(y) \, \mathrm{d}y$$

 \rightarrow Diversity of a set of Y values.

Here we consider $h(\Delta E)$ in each system

- Diversity of ΔE in a crystal system
- If low, the system is underrepresented

Fairness metric

• Difference of h among groups \rightarrow bias

Demonstration of the Bias Metric





ET-AL: Entropy-Targeted Active Learning

To mitigate bias: add data in underrepresented crystal system to increase h.



Uncertainty Estimation for h



For every x in the unlabeled sample pool, we can calculate expected improvement (EI) in h.

Experiments for Demonstration



- Mitigate artificial structure-stability bias
- ML: bulk & shear moduli
 (B & G), important
 mechanical properties

Testbed: Jarvis dataset (~11K)

- remove H, VIIA, VIII, and radioactive elements
- $N_{\rm L} = 1000, N_{\rm U} \sim 5000, N_{\rm T} = 5000$

Experimental Results

ET-AL successfully fixed the artificially created bias.



ET-AL samples in underrepresented regions.





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H. Zhang et al. ET-AL: Entropy targeted active learning for bias mitigation in materials data. *Applied Physics Reviews*, 2023.

Experimental Results



Tried multiple different ML models: NN, trees, SVM, ...

- Hyperparameters are tuned
- Tree-based ensemble models perform better
- ETAL dataset shows systematic advantage



Conclusions

- We developed and presented
 - A metric for measuring bias in (materials) data
 - ET-AL framework to mitigate bias by guiding data acquisition

• ET-AL can mitigate data bias, thus benefiting data-driven informatics



Help improve dataset quality



Guide database construction



Applicable to other scientific domains

/ Searching for: bias in materials science databases

/ Generating answers for you...

Yes, there can be bias in materials science databases. Researchers have different focuses and preferences of what materials to study; some experiments and simulations are easier to conduct than others which can contribute to bias¹.

However, there are methods to mitigate that bias such as developing an entropy-targeted active learning method ¹.

The bias can cause problems such as limiting the scope of research and development ².

Are there ways to solve this problem?

- Searching for: methods to mitigate bias in materials science databases
- Generating answers for you...

3 P & ...

Yes, there are methods to mitigate bias in materials science databases such as developing an entropytargeted active learning method ¹. The team settled on information entropy as a metric to measure bias ¹. Using this metric, they organized existing data into regions in a materials space and constructed their algorithm to more heavily prioritize regions that received less attention ¹. They also identified regions that would most benefit from future research efforts to reduce data bias ¹.

Other methods include pre-processing techniques such as sampling, massaging, reweighing to more complex methods like optimized data transformation which reduces bias and the predictability of the protected or sensitive attribute².

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Thanks for your attention!