An evidential framework to measure similarities between materials with considering uncertainty for materials discovery

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Materials with multiple principal elements and under different names such as high-entropy alloys and complex concentrated alloys, are becoming increasingly popular for their exceptional properties and wide range of applications [1]. Scientists utilize various data-driven techniques to uncover new HEAs and gain insight into their underlying mechanisms. However, due to the limited and inconsistent data available on these alloys, the efficacy of these methods in discovering innovative HEAs with more elements is challenging. Consequently, evaluating the prediction's uncertainty is crucial, yet it has not been seriously considered in prior studies. Addressing this limitation, our study introduces a novel framework [2-3] based on evidence theory [4] to measure the similarity between alloys while considering uncertainty to predict their properties and elucidate associated physical mechanisms. The proposed framework converts alloy data into evidence regarding similarities between alloys based on their properties. This evidence is then modeled and combined using the evidence theory to infer the similarities between alloys. Finally, the obtained similarity information is employed to predict the properties of candidate alloys, facilitating the exploration of new high-entropy alloys and the understanding of underlying physical mechanisms. To demonstrate the versatility of our framework, we utilized two datasets of quaternary alloys with target properties, specifically Curie temperature, and magnetization. By leveraging the extracted similarity information, we applied unsupervised learning techniques to extract cluster structures that enhance the interpretation of underlying mechanisms. Our experimental results indicate that the obtained similarities, as our framework measures, effectively detect anomalies and identify groups of materials with diverse correlations between composition and properties. Moreover, by incorporating the extracted similarities, we significantly improved the accuracy of predictions for Curie temperature and magnetization in the quaternary alloys, reducing mean absolute errors (MAE) by approximately 40%. In conclusion, our proposed framework, known as the evidence-based similarity measurement (eRSM) approach, offers a robust solution to measure similarities between materials, considering uncertainty. Furthermore, by addressing the challenges associated with data-driven methods in discovering novel alloys, our framework is promising to contribute to the advancement of materials research and enable more informed decision-making in alloy design and development.

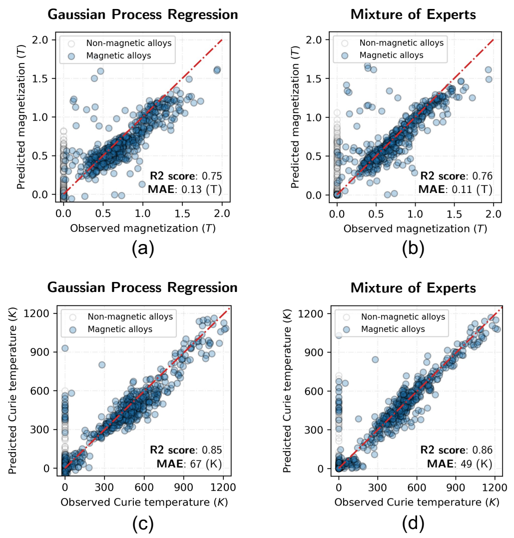

Figure 1:Prediction accuracies for magnetization (a) and (b) and Curie temperature (c) and (d) of the alloys with tenfold cross-validations. Sub-figures (b) and (d) show the results as introducing similarity measured by our proposed framework.

References:

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