CLUE: uncertainty-aware artificial intelligence in materials science

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1. Introduction

The rapid growth of data and AI technologies has significantly improved predictive accuracy across fields [1]. However, methods for quantifying prediction reliability –known as uncertainty quantification (UQ)– have not advanced at the same pace. This gap is particularly critical in materials science [2, 3, 4, 5], where small inaccuracies in predictions, such as ionic conductivity or material stability, can lead to costly experimental errors and misdirected resources.

The emergence of generative AI [6] has further highlighted the need for robust UQ methods. Without reliable UQ, distinguishing promising materials from flawed predictions remains a challenge, and recent failures in validating AI-generated candidates emphasize that accuracy alone is insufficient, while actionable insights require confidence measures.

Existing UQ methods offer partial solutions but often fall short of the computational efficiency and direct interpretability required in materials science. They are also limited in detecting and quantifying out-of-distribution (OOD) predictions, leaving a gap for more practical and scalable approaches.

We propose CLUE (Comparative Latent Uncertainty Estimator), a novel UQ method tailored for materials science. CLUE leverages latent space representations from deep learning models, directly assessing prediction similarity to training data [7, 8]. By identifying extrapolated cases outside the convex hull of known data, CLUE also flags high-risk predictions. Its computational efficiency enables retrospective application to existing models without retraining, making it a scalable and intuitive solution for uncertainty-aware AI in materials discovery.

2. Related work

State-of-the-art UQ methods primarily estimate epistemic uncertainty in predictions [3].These methods can be broadly categorized into two approaches: addressing model architecture limitations and evaluating target similarity to training data.

Bayesian methods [9, 10], a cornerstone of UQ, estimate posterior uncertainties by incorporating parameter distributions. Similarly, ensemble models [11, 12] and stochastic techniques, such as dropout-based uncertainty estimation, aggregate predictions from multiple models or randomized training variations. While effective in some cases, these approaches often suffer from limited accuracy and high computational overhead, making them resource-intensive and less practical for large-scale applications.

Emerging approaches leverage latent space representations to estimate uncertainty. These methods measure the similarity between latent embeddings of training and target data, offering an efficient way to gauge prediction confidence. Graph neural networks (GNNs), with their ability to encode complex material structures, are particularly suited for this task. However, existing latent-based methods typically rely on uncertainty calibration techniques that are manual, case-dependent, and lack generalizability.

CLUE addresses these challenges by refining latent-based uncertainty estimation. It eliminates the need for calibration or external parameters while incorporating the model's understanding of its own reliability. By assessing the relationship between known cases and target predictions, CLUE provides intuitive uncertainty estimates: predictions further from known cases in the latent space are considered less reliable.

Another important feature of CLUE relies on its ability to discern whether a prediction is an interpolation or an extrapolation. This is achieved by determining whether a target resides inside or outside the convex hull of latent representations, crucial for assessing the fidelity of predictions.

Our approach begins by collecting uncertainties from all observed cases, typically from a validation set that can also include training data. To estimate uncertainties for a new target set, CLUE performs a multilinear interpolation of these known uncertainties, using the latent representations of each material as coordinates (which often belong to high-dimensional latent spaces).

These latent representations, extracted from the final layer of the model, capture essential structural and compositional features of the materials. Although GNNs are used in this study, CLUE is versatile and can work with any model architecture capable of producing meaningful latent embeddings, taking or not as input graph representations of material as input [13]. Moreover, its adaptability extends beyond materials science, making it suitable for tasks in other scientific and technical domains.

3. Experiments

To validate the performance of CLUE, we conducted a benchmark study using a subset from the Materials Project database [14], encompassing 45,000 inorganic crystal structures. The task focused on predicting ground-state energies (Fig. Figure 1), a

Fig. 1: a) Training accuracy curve of the underfited GNN model, trained for ground-state energy prediction over 100 epochs, b) model predictions versus true values for the test set, with uncertainty bounds given by CLUE, c) deviations between CLUE-predicted uncertainties and ground-truth errors from reference data.

critical property in materials discovery.

Figure 1 illustrates the model's training process. We deliberately underfit the model to generate high inaccuracies, enabling robust testing of CLUE's capabilities. CLUE estimates the uncertainty of each sample independently of train-test splitting, eliminating the need for and surpassing the problems related to additional calibrations. Furthermore, by means of a convex-hull approach, CLUE distinguishes whether predictions fall within interpolation or extrapolation regimes, providing valuable insights into model performance, with special relevance on the assessment of material generation related tasks.

4. Data and models

The dataset was split into 40500 samples for training, 2250 for validation, and 2250 for testing. To test CLUE, we used training set uncertainties to configure the method and inferred uncertainties for the test set. In real-world applications, however, all available data –coming from training, test and any validation data– should be utilized to maximize the accuracy of uncertainty estimation for new cases.

Our GNN architecture consists of two graph convolutional layers with 32 neurons each, followed by three fully connected layers with 32, 16, and 1 neuron, respectively. Global mean pooling was applied for feature aggregation. The model was trained for 100 epochs with a batch size of 128, a dropout rate of 0.1, a learing rate of 0.001, and standard optimization techniques.

5. Conclusion

We present CLUE, a novel approach to uncertainty estimation based on parameter-free latent embeddings of materials. Using the Materials Project database as a benchmark, we demonstrated that CLUE provides rapid and confident uncertainty estimates for predictions. This method avoids the need for external model training or predefined parameters, instead intelligently utilizing validated cases. By delivering meaningful uncertainty estimates, CLUE represents a significant step toward reliable, uncertainty-aware AI in materials science.

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