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Are you sure? – Uncertainty in MLIPs

Uncertainty – *"that which is not known precisely"*[1]

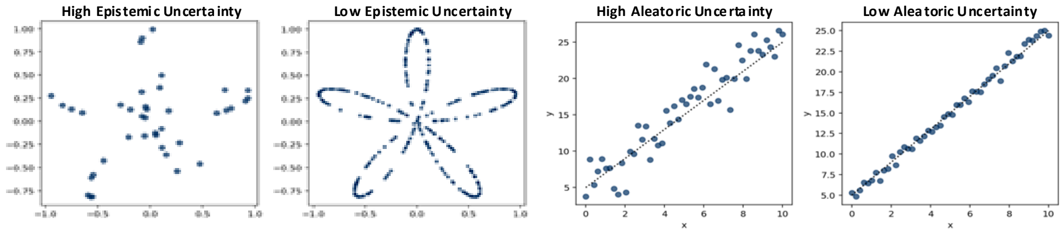
Types of Uncertainty

Epistemic uncertainty:[2]

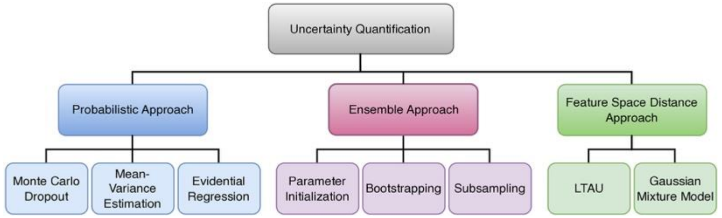
- Uncertainty that arises from a lack of knowledge.
- Can be systemically reduced (e.g., by adding data, improving the model)

Aleatoric uncertainty:[3]

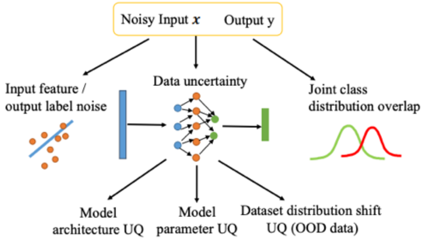
- Uncertainty that arises from the stochastic nature of the data collection or model training process
- Generally irreducible



Uncertainty Quantification: "*The systematic assessment and documentation of uncertainty in computational results.*"[4]



Examples of uncertainty quantification methods in machine learning.



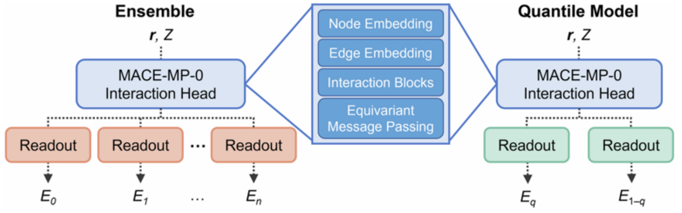
Possible sources of uncertainty in machine learning.

Why understand uncertainty?

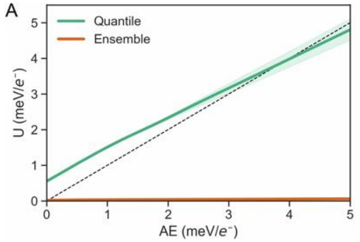
Understanding uncertainty helps us determine how confident we should be in a model's predictions. This insight can help guide how we should make improvements to the model, leading to more **accurate** and **reliable predictions**.

Examples of Uncertainty Quantification in MLIPs

Bilbery *et al.* [7] used readout ensembling (estimates *epistemic* uncertainty) and quantile regression (estimates *aleatoric* uncertainty) to quantify the uncertainty of MACE-MP-0.



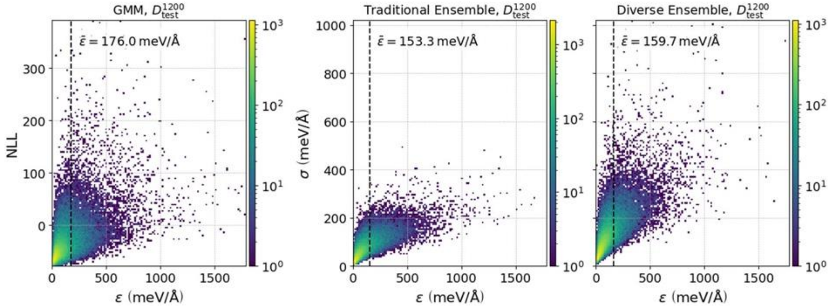
Schematic of the readout ensemble and Quantile model used by Bilbery *et al.*



Uncertainty in the MACE-MP-0, fine-tuning on 90,000 structures selected from the MPtrj dataset. Showing the regression uncertainty (U) vs absolute error (AE).

Zhu *et al.* [8] proposed a method aimed at bypassing more expensive ensemble approaches by using a Gaussian mixture model (GMM) to estimate predictive uncertainty of an NequIP model.

Comparison of GMM uncertainty estimates to uncertainty estimates obtained from traditional ensemble methods.



References

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[2] Hüllermeier *et al. Machine Learning* **2021**, *110,* 457.
[3] Kläs *et al.* In *SAFECOMP Workshops* **2018**.
[4] Frömbgen *et al. ChemRxiv* **2025.**
[5] Dai *et al. Reviews in Chemical Engineering* **2025**, *41,* 333.
[6] He *et al. arXiv* **2023**, abs/2302.13425.
[7] Bilbrey *et al. NPJ Computational Materials* **2025**, *11,* 109.
[8] Zhu *et al. J. Chem. Phys.* **2023**, *158,* 164111.
[9] Grasselli et al. *Digital Discovery* **2025**, *4,* 2654.