Prediction of the Hamiltonian using equivariant neural networks(ENN)

Current Research Overview

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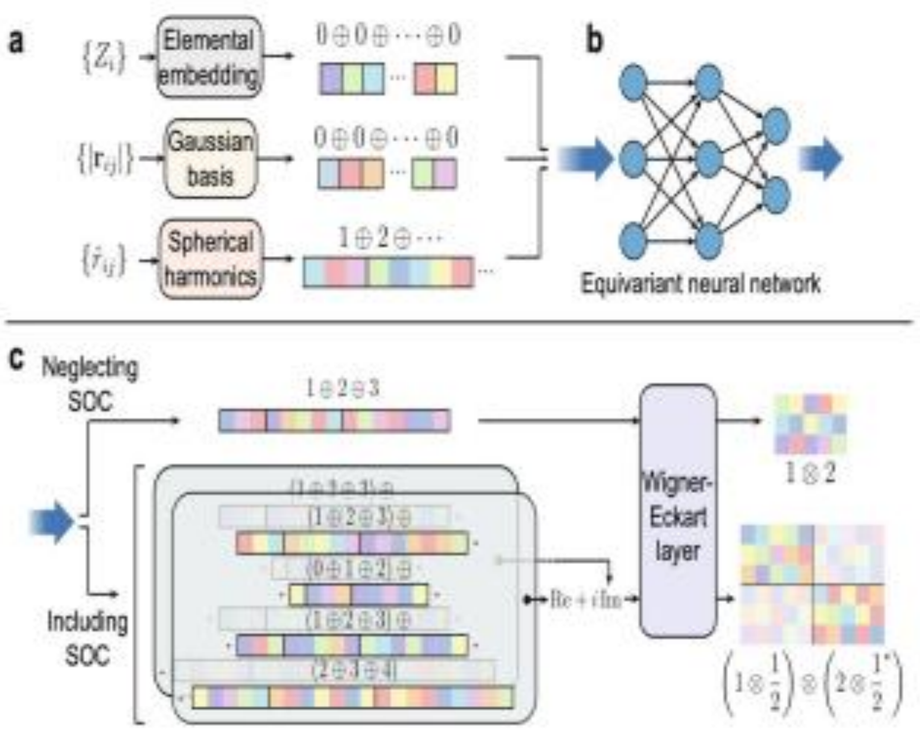
Background

- 1. The Hamiltonian in density functional theory (DFT) encompasses all electronic structure properties of the material, allowing predictions about the material.
- 2. Equivariant neural networks are used to address symmetry design issues related to the O3 group.

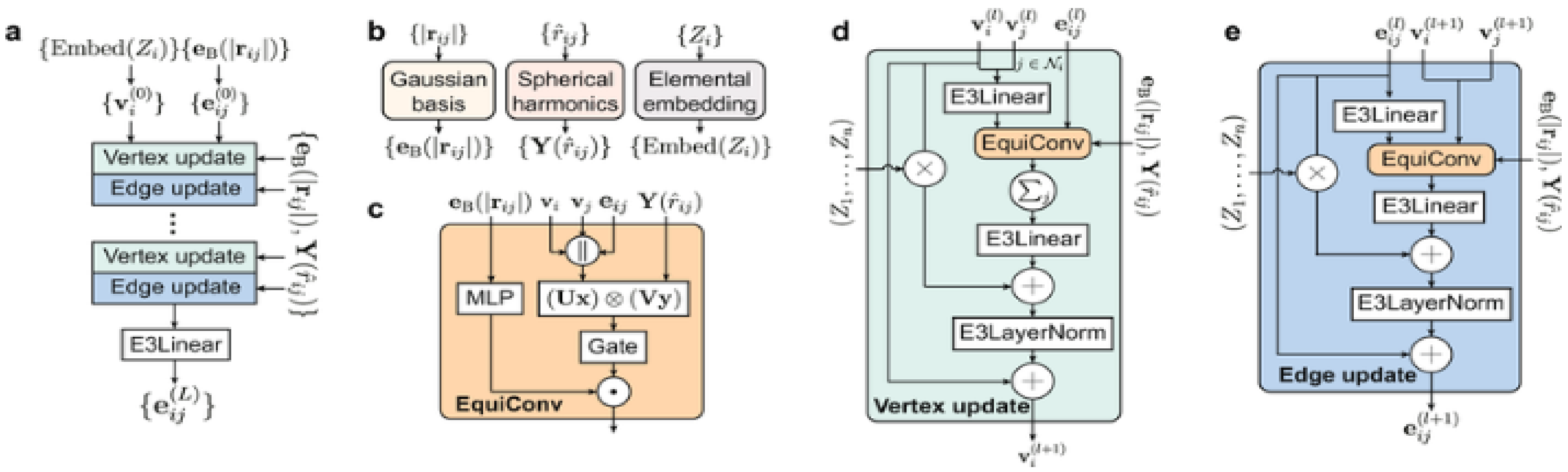
Benefit

- Geometric symmetry is inherent to equivariant neural networks, eliminating the need for additional processing constraints (e.g., data augmentation) on the input data.



Logic and Current Work

- Logic:
- Mapping geometric graph structures to higher-order vectors.
- Here, the geometric graph structure refers to converting information about the crystal cell structure of different
- materials into input, such as element embedding, angular, and radial features.
- The higher-order vector we seek is the Hamiltonian, which is a second-order tensor.
- The mapping process is done by the model: DeepHe3.



MEERL-H Model Structure

- We have developed a new model based on Deephe3, we currently call it: Meerl-H model. In our model there exists two parts, main model and auxiliary model.
- **Main model**:

  Based on the DeepHe3 architecture, responsible for predicting the Hamiltonian matrix.
- **Auxiliary Model**:

  Also based on DeepHe3, focused on estimating uncertainty of the main model's predictions.

  Uses Evidential Learning to quantify Epistemic and Aleatoric Uncertainty, providing feedback to enhance the reliability of predictions.
- **Dynamic Weight Adjustment**:

  Adjusts task weights during training based on uncertainty feedback. Prioritizes optimization of critical matrix elements.

MEERL-H Model Principles

- **1. Input Material Data**:
  Geometric structure and basis set information are encoded as high-dimensional geometric features.
- **2. Hamiltonian Matrix Prediction**:
  The main model predicts values for all matrix elements, forming a complete Hamiltonian matrix.
- **3. Reliability Assessment**:
  The auxiliary model evaluates the uncertainty of predictions, generating quantitative reliability scores.
- **4. Dynamic Optimization**:
  Adjusts main model's optimization direction based on uncertainty feedback.
  Allocates more resources to uncertain regions and reduces focus on reliable areas.
- **5. Final Output**:
  Outputs an optimized Hamiltonian matrix and quantified uncertainty for reliable results.

Current Work and Future Work

- **My current work**:

  Reproduce DeepHe3 on the SACADA dataset.

- **Future Work**:

  Verify the potential of equivariant neural networks in robotic optimization problems.

- **Milestone**:

  Plan to submit findings to Nature Machine Intelligence.