

Model Training Analysis (Decorated Lattice)

1. Learning Curve

The learning curve shows a gradual decrease in training and validation loss.

However, the error remains quite high, indicating a challenging task for the model.

2. Test Set Evaluation

Results on the test set:

- Mean Absolute Error: 0.2865
- Median Absolute Error: 0.2248
- Mean Relative Error: 63.42%
- Median Relative Error: 52.62%

The errors are significantly higher compared to the 'simple' and 'molecule' cases, indicating that the model struggles with precise prediction for the 'decorated' lattice.

3. Prediction Errors

The error plots show a large spread in both absolute and relative errors.

Many samples have a high relative error (>50%), confirming the challenging nature of the task.

4. True vs Predicted Parameters

The 'True vs Predicted' plots show significant deviations from the ideal diagonal line.

This further highlights the model's difficulty in accurately capturing the parameter relationships for the decorated lattice.

5. Conclusion

At this stage, the result is unsatisfactory for practical applications.

Further work is needed to improve the model: enhancing architecture, increasing dataset size,

changing the loss function, or improving data preprocessing.