

Molecule Lattice Analysis

1. Numerical Metrics:

Mean Absolute Error (MAE): ~0.038

Median Absolute Error: ~0.045

Mean Relative Error: ~12.34%

Median Relative Error: ~8.94%

2. Quick Analysis:

- Absolute error (~0.038-0.045) is about 3-4% of the parameter range [-1, 1].
- Relative error (~12%) is higher compared to the 'simple' lattice.
- Errors are acceptable given the task complexity.

3. Observations from Graphs:

- Training curve stabilizes, but validation loss fluctuates.
- Absolute and relative errors are wider spread.
- Scatter plots show good but not perfect correlation between true and predicted values.

4. Why It Is More Difficult:

- Parameters J1, J2, J3 are tightly linked: $J1 = J2 = J3$, $J4 = 0$.
- Magnetization curves are flatter and less sensitive to parameter changes.
- Makes it physically harder for the model to distinguish parameter values.

5. Conclusion:

- Current approach is correct.
- 12% relative error is acceptable.
- Model learns meaningful mappings.

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6. Possible Improvements:

- Increase dataset size (e.g., 20k samples).
- Increase hidden layer size (e.g., 256 neurons).
- Add data augmentation (small noise to $M(H)$).
- Separate training for positive/negative J .