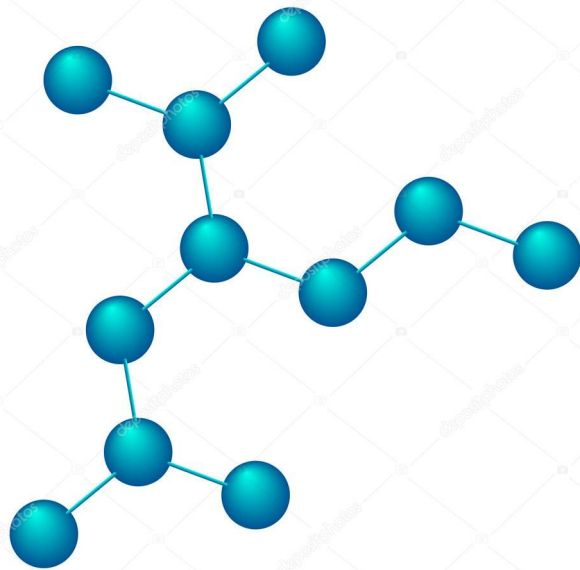
A decorative graphic in the top-left corner showing a network of interconnected nodes and edges. Some nodes are highlighted with blue circles, and the overall structure is rendered in light gray.

# Molecular Property Prediction

Hyunwook Paul Shin



# Business Problem

- ◎ Nuclear Magnetic Resonance (NMR)
  - Protein Target Drug design
- ◎ Coupling Constant
  - Limitation in Calculation

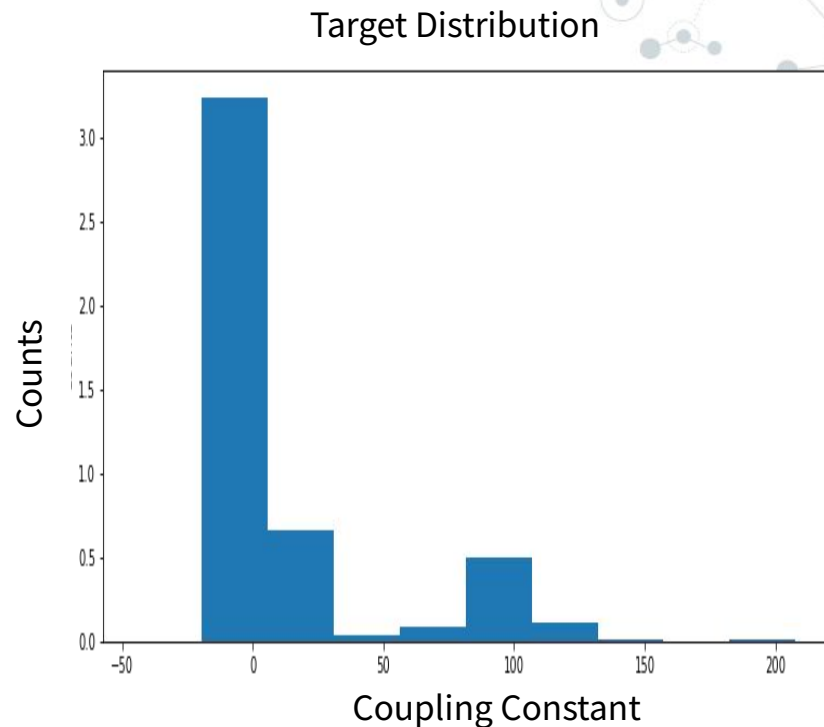


“

*Create a model that accurately  
predicts coupling constant in a  
small amount of time.*

# Data

- ⊙ Kaggle Competition
- ⊙ 85k Unique Molecules
- ⊙ 3D Structure Information
- ⊙ Imbalanced Target Variable
- ⊙ 8 Different Coupling Types



# Results

- ◎ Neural Network
- ◎ 94.6% variance explained
- ◎ Average error = 1.799
- ◎ Over 931k predictions

○ 90 seconds

# Conclusion

This model can be used to:

- ⦿ Predict Coupling Constant
- ⦿ Save time in interpreting NMR results

# Next Steps

- ① Additional Features
- ① More Molecule Samples
- ① Divide into Subset



# Thank You!

## Any questions?

Project Github:

[https://github.com/hps1795/Molecular\\_Properties\\_Prediction](https://github.com/hps1795/Molecular_Properties_Prediction)

Email:

paulshin17@gmail.com

