Predictor of Acid Dissociation Constants

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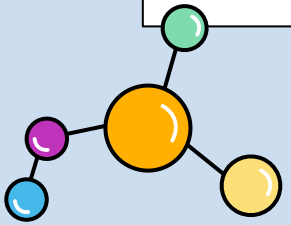
INTRODUCTION



INTRODUCTION

$$HA_{(aq)} + H_2O_{(l)} \rightleftharpoons H_3O^+_{(aq)} + A^-_{(aq)}$$

First, we need to:

- Define the problem
- Importance of the project
- Applications of the Acid Dissociation Constant

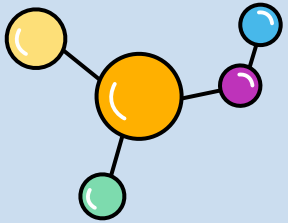
$$K_a = \frac{[H^+][A^-]}{[HA]}$$

$$pK_a = -\log K_a$$

$$pH = pK_a + \log_{10}\left(\frac{[A^-]}{[HA]}\right)$$

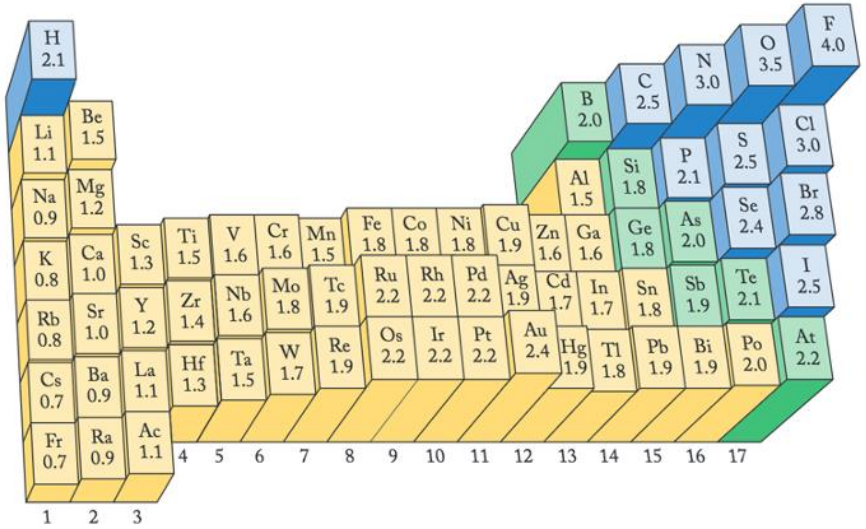
02

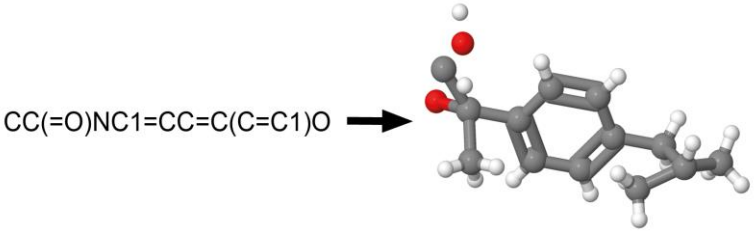
DATA COLLECTION



DATA COLLECTION

- Source: IUPAC Database
- Molecules: SMILES notation was used
- pKa Values: Collected at 20-25°C for consistency
- Molecules ➡ Graphs:
  - Atoms = Nodes (with attributes)
  - Bonds = Egdes (with attributes)





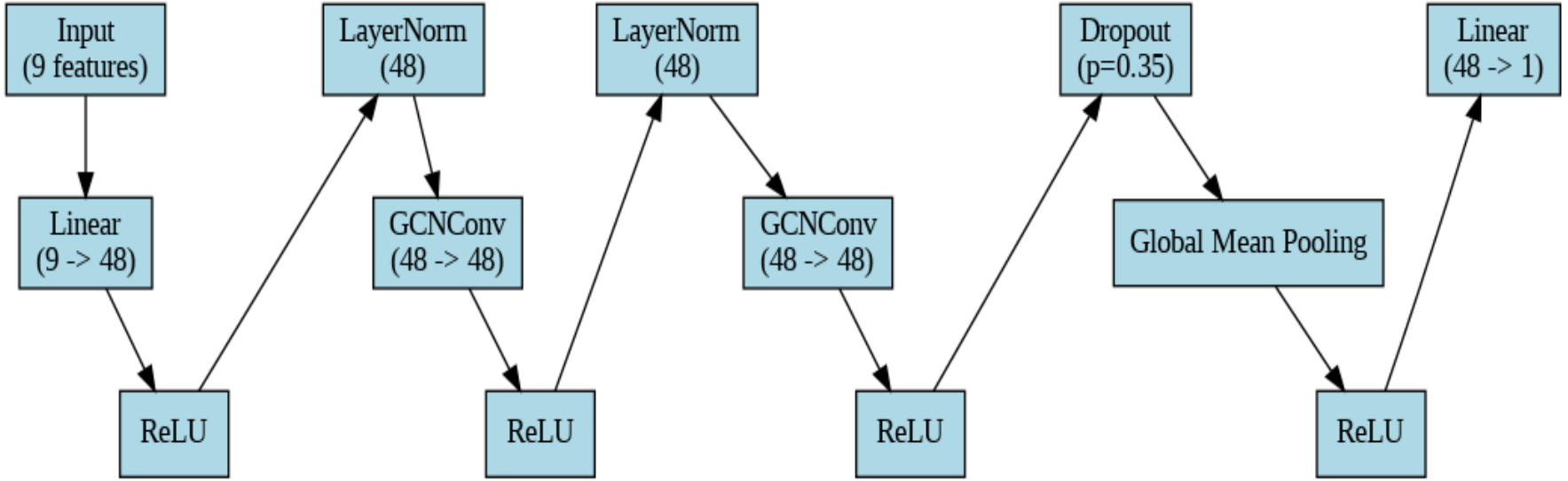
03

MODEL TRAINING

MODEL TRAINING

- Data Processing: Preparing molecular data for neural network use
- Data Splitting:
  - 70% for training
  - 15% for validation
  - 15% for testing
- The neural network contains:
  - Linear Layer
  - GCN Layer (Graph Convolutional Networks)
  - Layer Normalization
  - Dropout
  - Global Mean Pooling

MODEL TRAINING



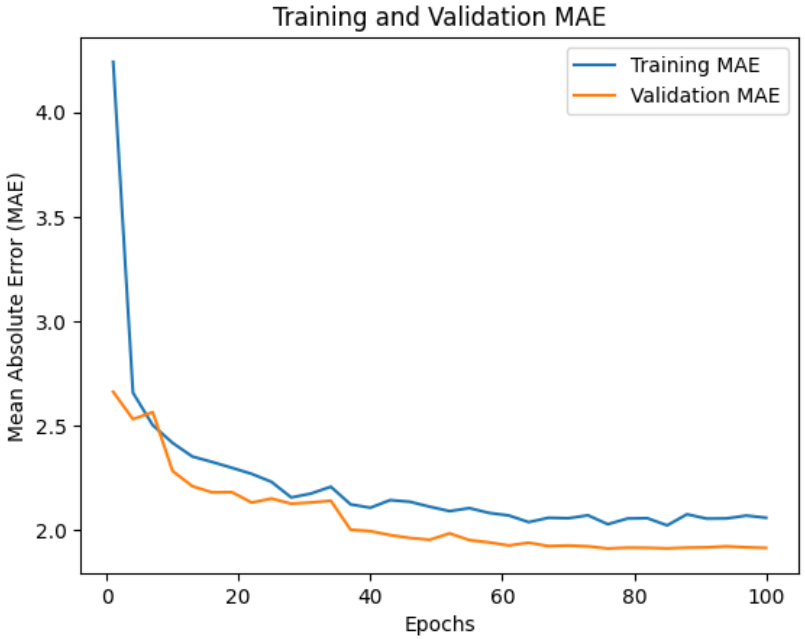
04

RESULTS

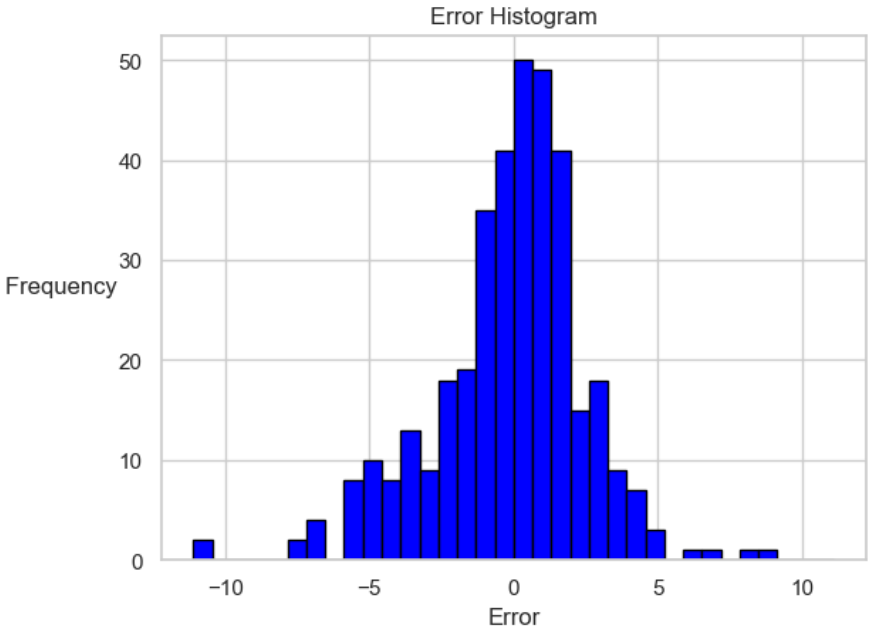
RESULTS

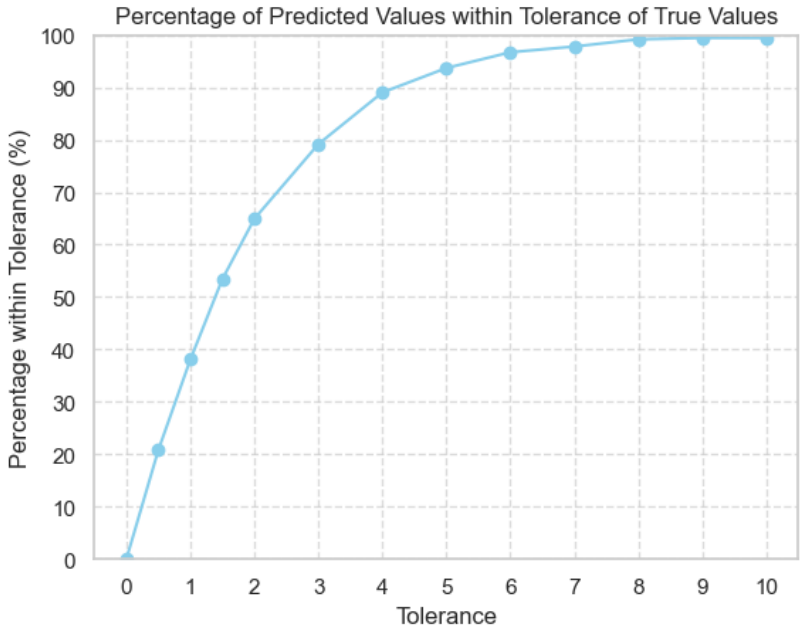
The evaluation metrics used were:

- Mean Squared Error (MSE = 6.45)
- Mean Absolute Error (MAE = 1.88)
- R^2 Score = 0.3727
- Percentage of predicted values within 1-unit tolerance of the true value: 37.3%



RESULTS AND PERSPECTIVES





Predictor of First Acid Dissociation Constants

References:

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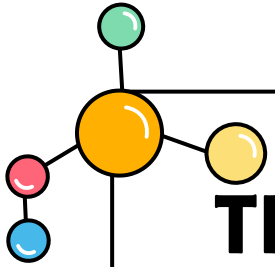
- Kristin S. Alongi, George C. Shields, Chapter 8 - Theoretical Calculations of Acid Dissociation Constants: A Review Article, Annual Reports in Computational Chemistry, Elsevier, Volume 6, 2010, Pages 113-138
- github.com/IUPAC/Dissociation-Constants



THANK YOU FOR YOUR ATTENTION!