CSC580 CTA5 Option 1 - Hyperparameter Tuning for Tox21 Dataset

Student Name: Arun Saxena

Date: June 2025

# Project Overview

In this assignment, I improved the performance of the Tox21 toxicity prediction model using hyperparameter tuning of a fully connected neural network architecture. The tuning process involved systematically varying multiple hyperparameters to search for the optimal model configuration. I also experimented with a Random Forest model for performance comparison.

# Random Forest Baseline Model

As a baseline, I trained a Random Forest classifier using 50 trees and balanced class weights. The weighted validation accuracy achieved by the Random Forest model was used as a reference point for deep learning model improvements.

# Hyperparameters Tuned

I tuned the following hyperparameters for the neural network:  
- Number of hidden units: [50, 100]  
- Number of layers: [1, 2]  
- Learning rate: [0.001, 0.0005]  
- Dropout probability: [0.3, 0.5]  
- Batch size: 100 (fixed)  
- Epochs: 20 (fixed for runtime stability)  
- Random seed sensitivity: Each setting repeated for 3 runs and averaged

# Tuning Rationale

The chosen hyperparameter values reflect a trade-off between model complexity, training time, and overfitting risk. Increasing hidden units and layers allows the model to capture more complex nonlinear relationships. Smaller learning rates prevent overshooting the loss surface. Dropout regularizes the model by preventing co-adaptation of neurons. Multiple repetitions smooth out randomness in neural network weight initialization.

# Results Summary

The hyperparameter grid search identified the following best configuration:  
- Hidden Units: 100  
- Layers: 2  
- Learning Rate: 0.0005  
- Dropout: 0.3  
  
This configuration achieved a weighted validation accuracy of approximately 84.2%, improving over both the baseline Random Forest and the default neural network settings.

# Screenshot

A screen shot of a computer program

AI-generated content may be incorrect.

A screenshot of a computer

AI-generated content may be incorrect.

# Conclusion

Hyperparameter tuning significantly improved the Tox21 model's performance. This exercise demonstrates the importance of systematic tuning in deep learning workflows, as even simple architecture changes combined with small learning rate adjustments can result in meaningful accuracy gains.