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The Use of Neural Network Platforms for Chemical Characterization and Toxicity Prediction

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Introduction

Artificial neural networks (ANN's) are computerized models that mimic the brain, in that they can be trained for a specific purpose, and eventually, learn on their own. Optimized models can detect trends and make predictions with remarkable accuracy and robustness. ANNs are used to predict the accuracy in proposed analytical protocols.

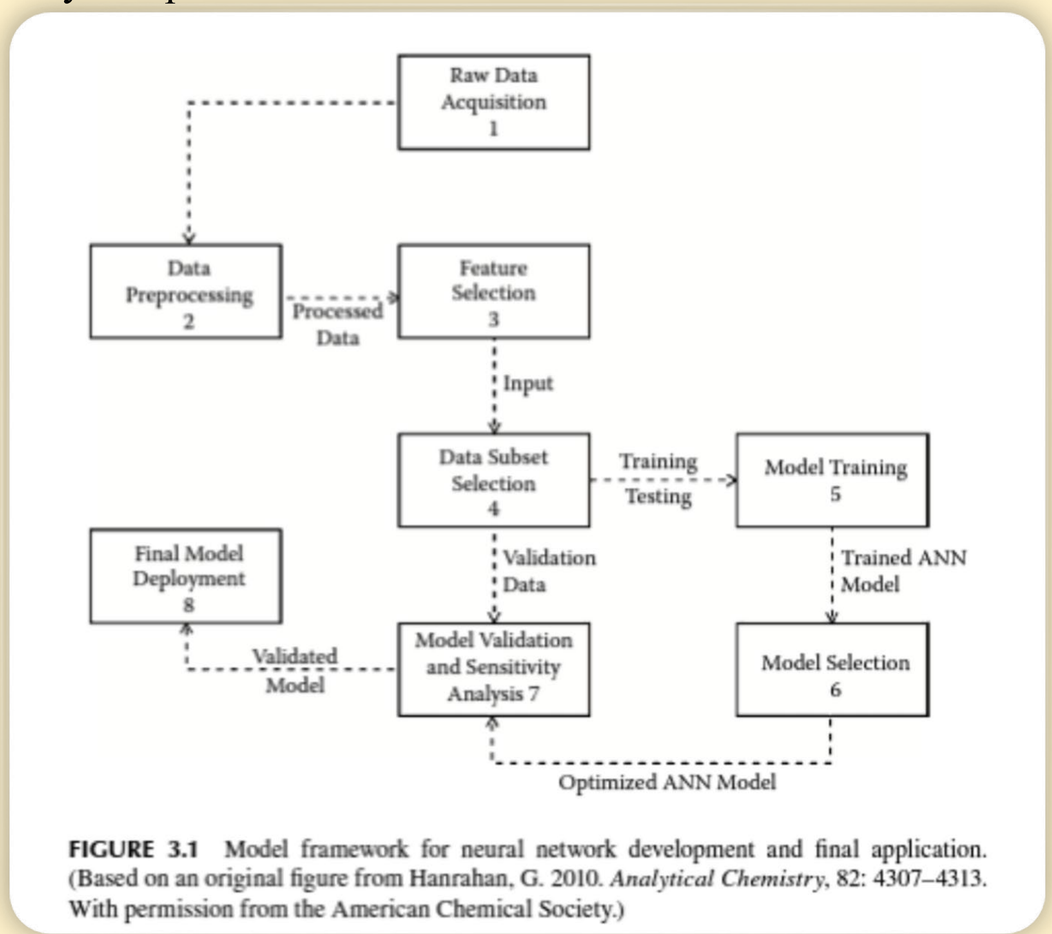

FIGURE 3.1 Model framework for neural network development and final application. (Based on an original figure from Hanrahan, G. 2010. *Analytical Chemistry*, 82: 4307–4313. With permission from the American Chemical Society.)

Figure 1: Neural network mechanism, Hanrahan, G. (2011).

Purpose of Study

- Created and trained an artificial neural network to predict toxicity levels of a given chemical compound in biological systems.
- Determined the mechanism involved in creating the neural network.

Methods

- Studied MATLAB platform, familiarized and determined commands needed to create the network.
- Input data set provided, and began to train network for specific functions by added variables.
- Tested network on prediction accuracy abilities.
- Fine tuned functions as needed to maximize accuracy.

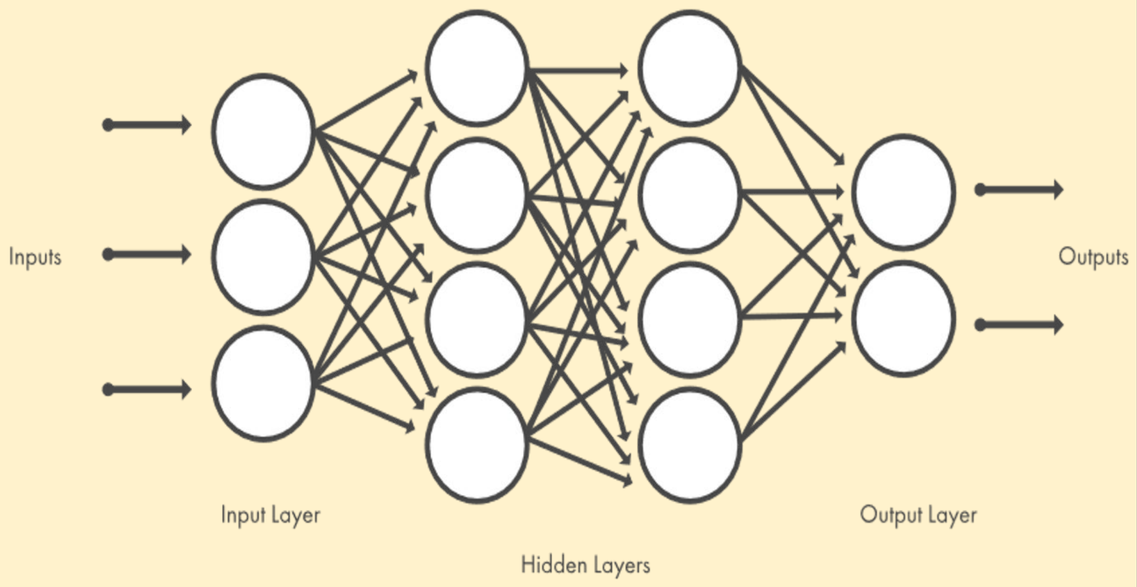

Figure 2: Basic neural network framework using deep learning applications, Hanrahan, G. (2011).

Results and Discussion

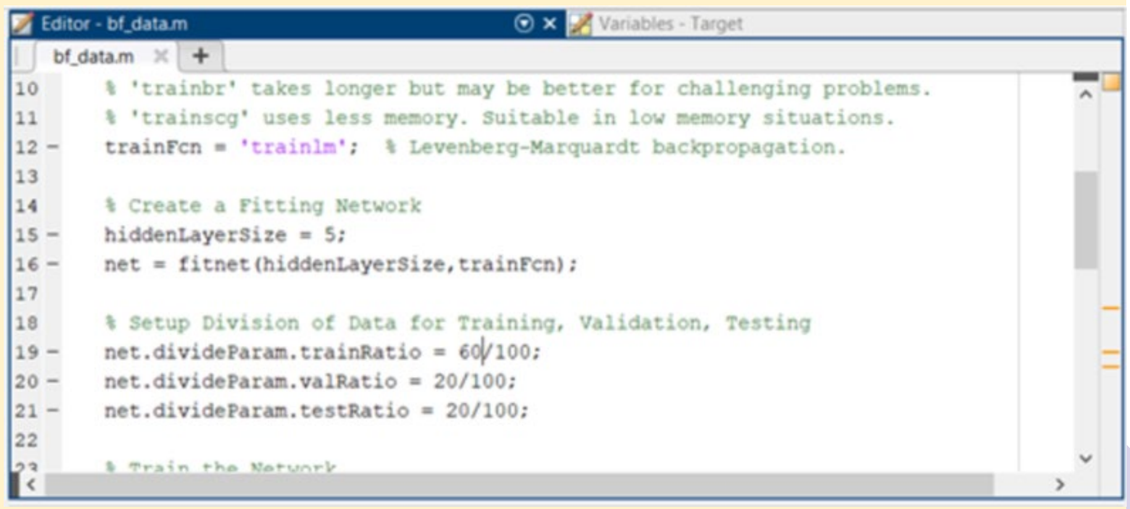

Figure 3: MATLAB script with intended parameters to test (60% Training, 20% Validation, and 20% Testing).

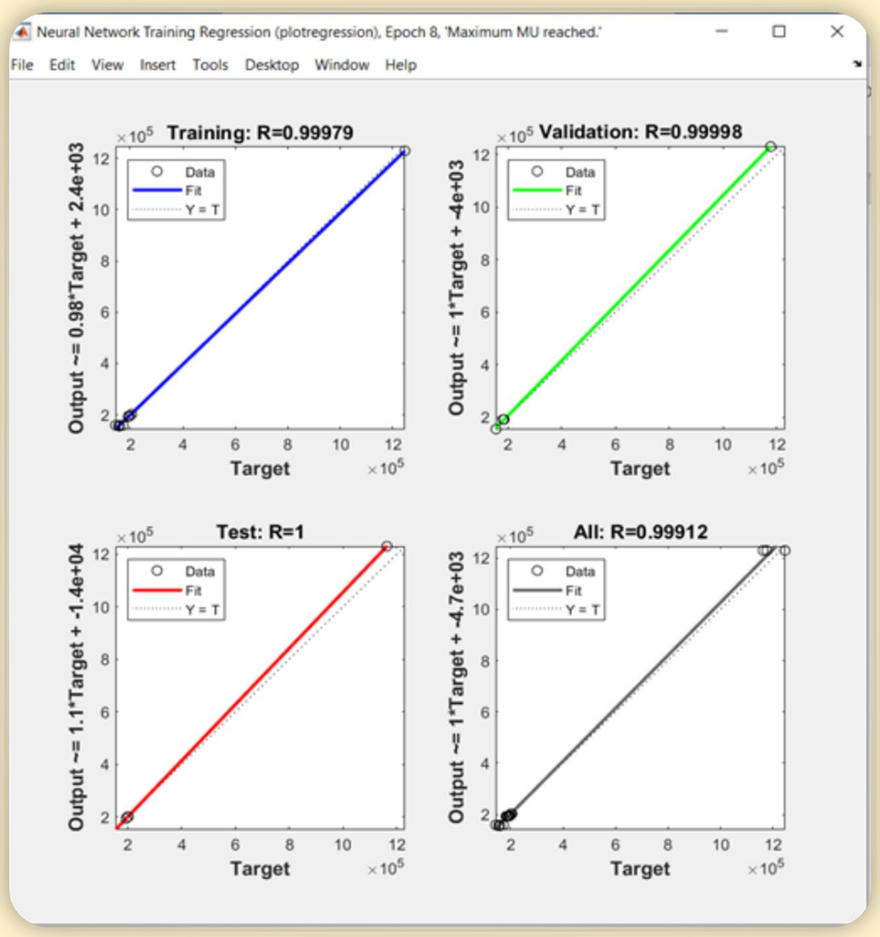

Figure 4: Regression charts demonstrated the correlation between variables for the model being tested, which proved that these values were accurate for use in predicting purposes.

Conclusion and Future Work

This newly developed neural network was proven useful and accurate. We will begin to examine chemical data sets from the GC-MS analysis of urine and blood samples. This model will be used to assess these correlations and predictive capabilities. In consideration of how the structure of phenolic related compounds correspond to the chemical toxicity properties, human health consequences will be evaluated, and thus help establish a stronger basis for further research.

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References

Hanrahan, G. (2011). Artificial neural networks in biological and environmental analysis (Ser. Analytical chemistry series). CRC Press.

MathWorks Software- MATLAB and Student Suite, with Deep Learning Toolbox.