Toxicology Testing

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CSC580: Applying Machine Learning and
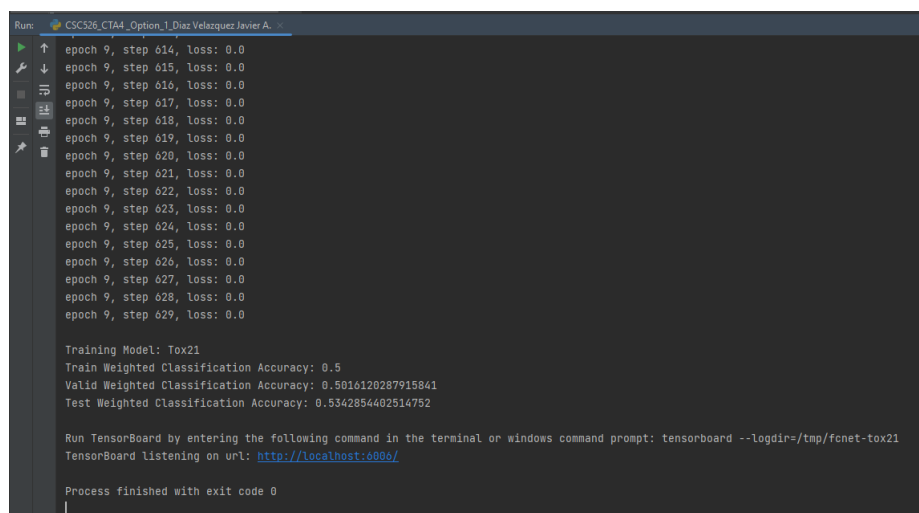
Neural Networks

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Tox21 Model

The primary purpose of the assignment is to utilize a toxicity dataset named Tox21 and loaded into a TensorFlow model to assess the model's accuracy. Let us begin by pointing out that this required much debugging, given that the version of TensorFlow used in this particular case has methods of version one, in which some are no longer in use or have already been deprecated. In addition, to achieve a smooth operation of the code during execution, it was crucial to call out the "tf. compat.v1." method to let the Python interpreter could be aware that such methods utilized were from version one of TensorFlow.

Execution and Accuracy

Once all the gremlins and bugs of the code were taken care of, it was time to execute the code and asses its accuracy with the TensorBoard results. The execution of the model was completed in 9 epochs, 629 steps, with 0% loss; the training-weighted classification accuracy was 5%, the valid weighted classification accuracy was 50%, and the test-weighted classification accuracy was 53%. Figure 1 – 1 shows the results of the execution.

Figure 1 – 1 The overall results of the Tox21 model execution.

TensorBoard Results

The TensorBoard graphs provide a visual representation of the Tox21 data flow and behavior during the execution process; these serve to understand better and access the model's accuracy. Figures 1 – 2 and 1 - 3 show the Tox21 TensorFlow model graphs.
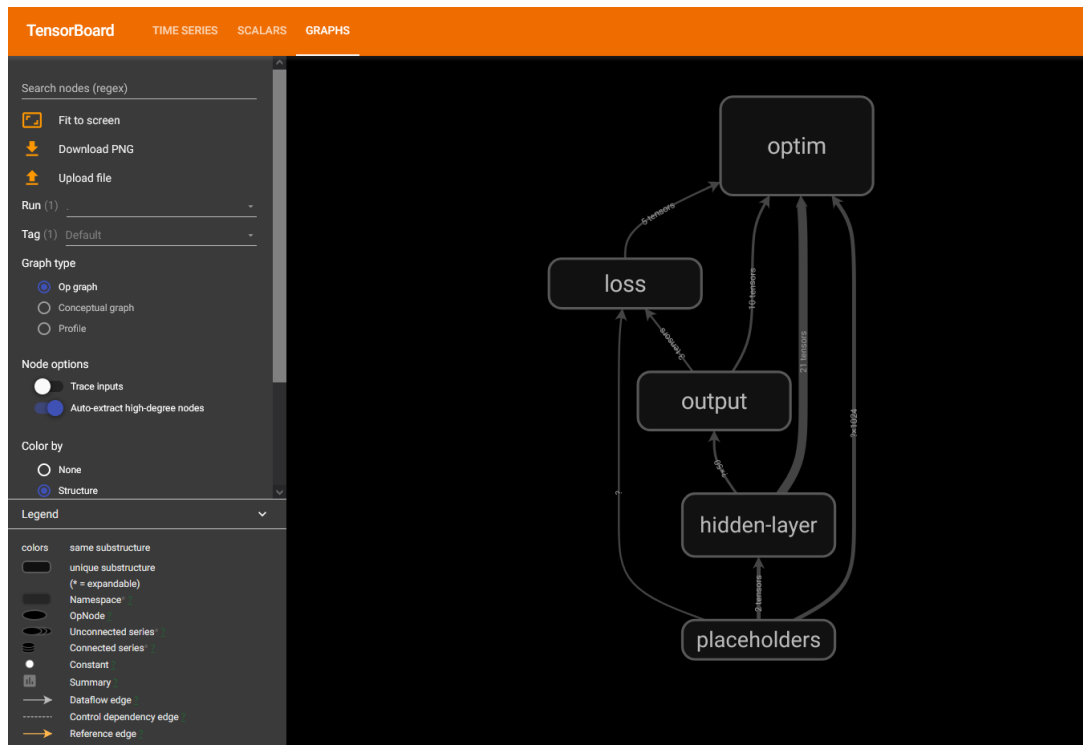

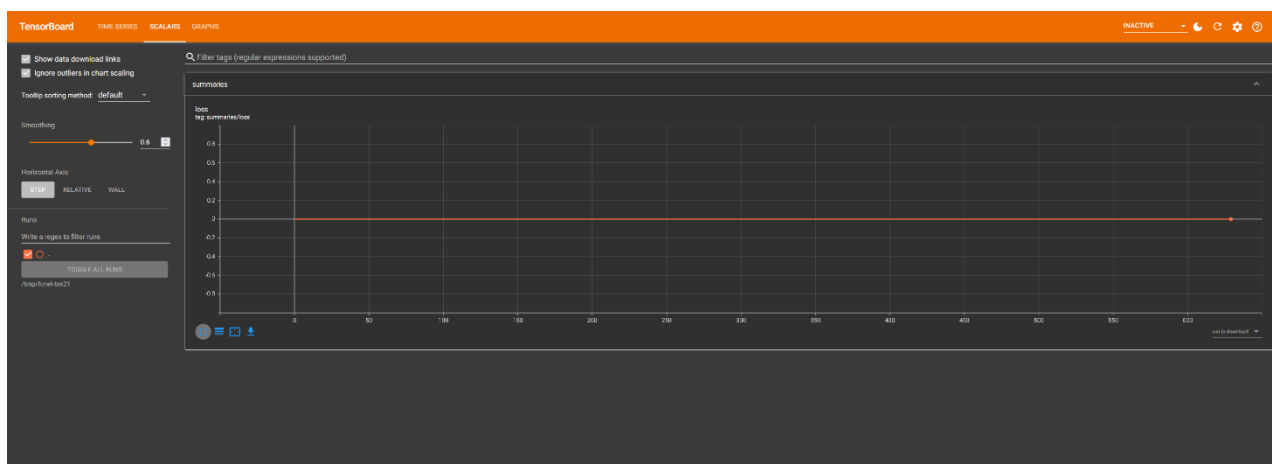*Figure 1 – 2 The dataflow path during runtime execution.*

Figure 1 – 3 Shows the loss curve, which is linear or zero.

Conclusion

Despite the few hiccups the model presented during the implementation phase, its accuracy was quite decent. Finally, the overall results of the model's execution were a success, given the circumstances and the deprecated methods of TensorFlow version one.