MACHINE LEARNING GLASSES RESULTS LOG

KIRK SWANSON

1. 11/26/2017

(1) Merged recent updates to GitHub
(2) Downloaded images from a while ago. This first one is batch size 80, learning rate 0.001, beta 0.01, dropout 0.5, including the recent change that each batch is chosen from a newly randomly chuffled metadata:

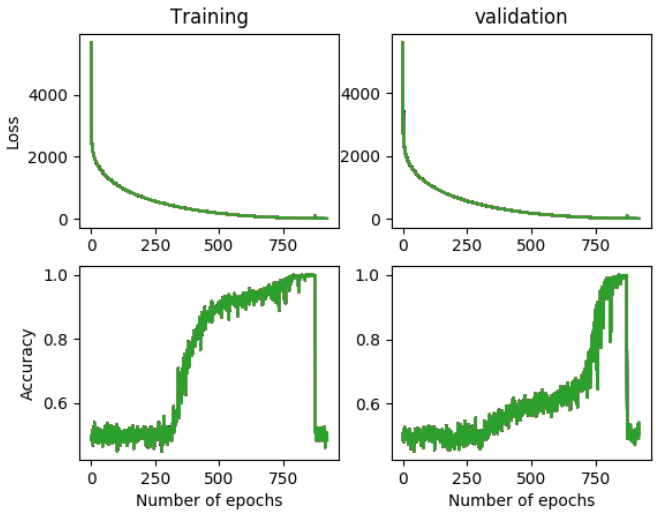


FIGURE 1. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(3) This run had an optimal validation accuracy of 99.7635 and an optimal test accuracy of 99.7297. I also tested this multiple times, running the SAME set of hyperparameters, to see what is going on with that weird spike. Does it keep showing up? What is going on? Here are more examples, all run at the same hyperparameters as above:

Date: June 26, 2018.

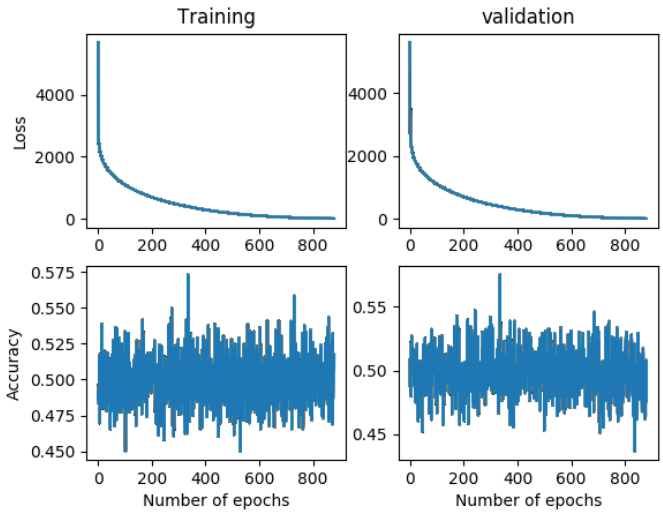


FIGURE 2. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(4) This run had an optimal validation accuracy of 47.0608, optimal test accuracy of 47.6689, and final validation accuracy of 49.223, test accuracy of 50.0338

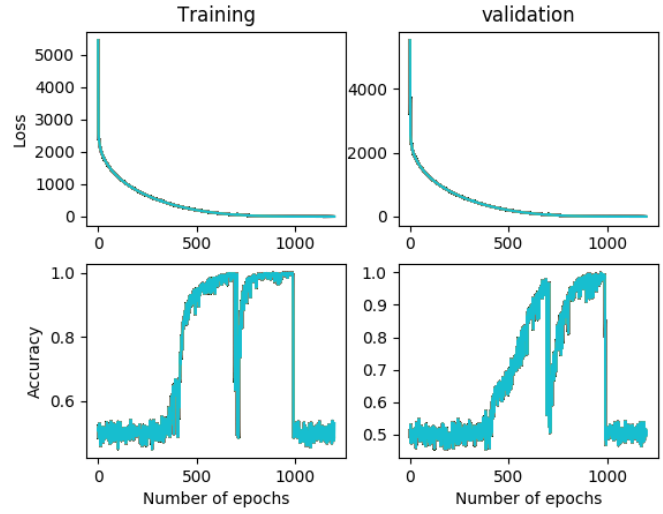


FIGURE 3. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(5) This run had an optimal validation accuracy of 99.4595, optimal test accuracy of 99.3243, and final validation accuracy of 50.777, test accuracy of 49.9662.

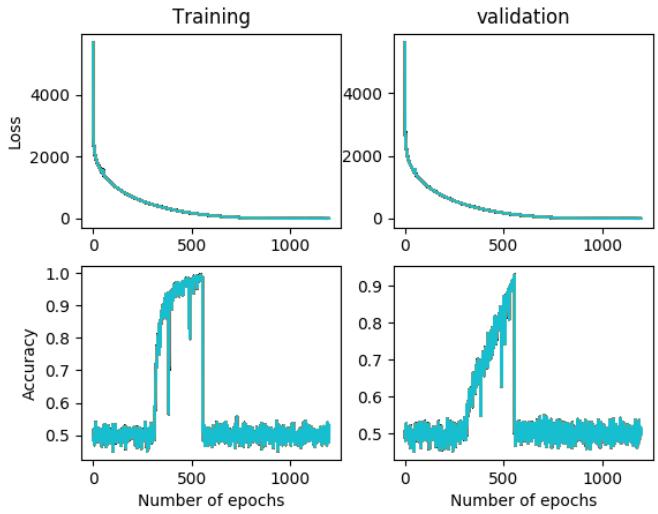


FIGURE 4. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(6) This run had an optimal validation accuracy of 992.5, optimal test accuracy of 91.7568, and final validation accuracy of 49.223, test accuracy of 50.0338.

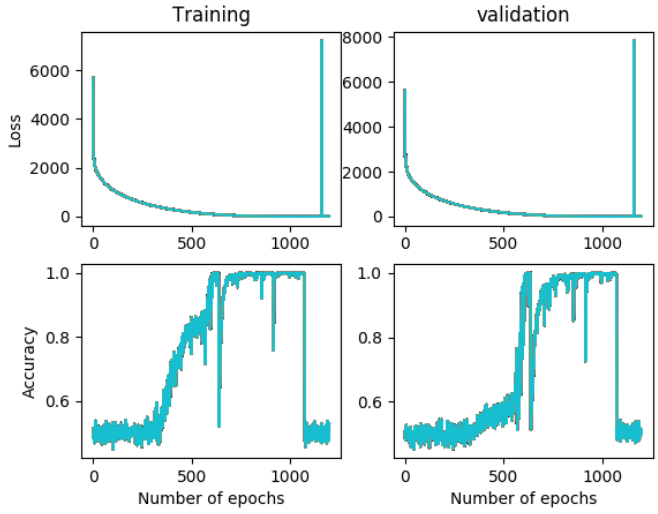


FIGURE 5. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(7) This run had an optimal validation accuracy of 99.8987, optimal test accuracy of 99.8649, and final validation accuracy of 50.777, test accuracy of 49.9662.

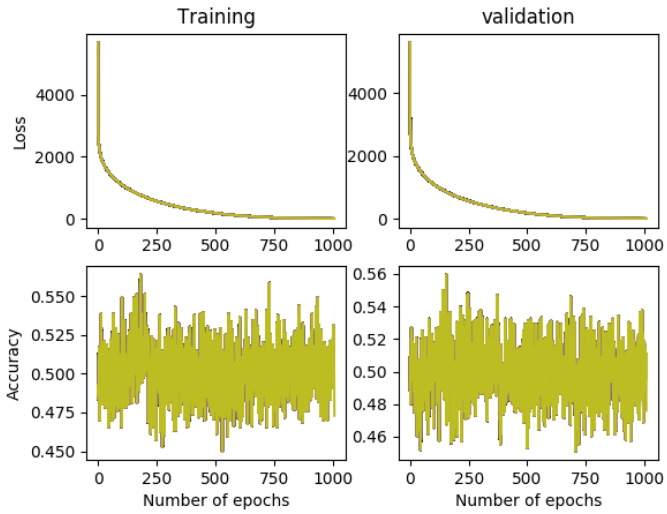


FIGURE 6. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(8) This run had an optimal validation accuracy of 55.4054, optimal test accuracy of 54.223, and final validation accuracy of 49,223, test accuracy of 50.0338.
(9) The following are images of runs on the dataset that consists of glasses and liquids that are each 12 time steps away from the assumed glass transition temperature of 0.21.

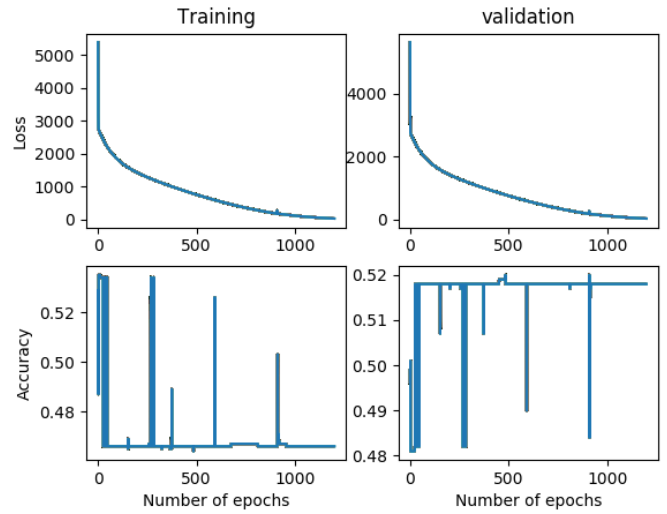


FIGURE 7. Batch Size = 100, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

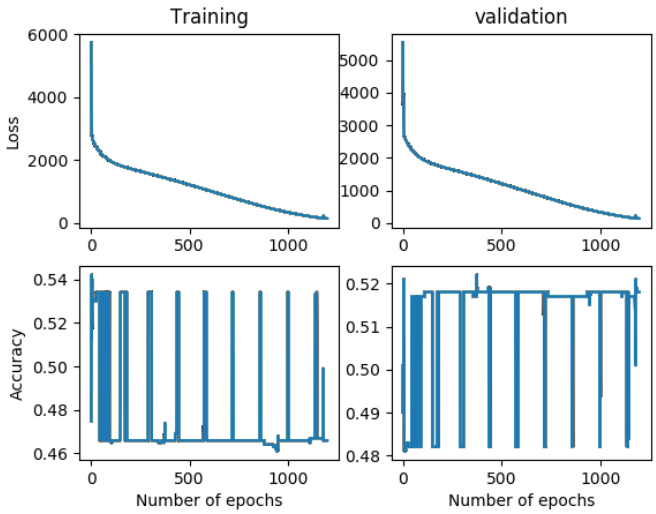


FIGURE 8. Batch Size = 10, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

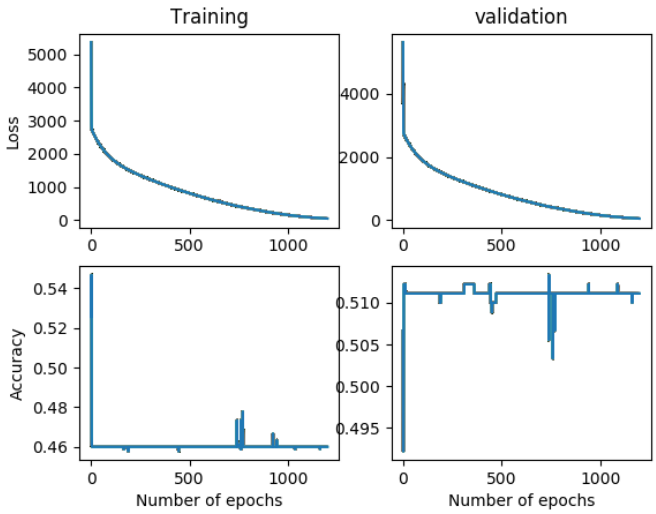


FIGURE 9. Batch Size = 150, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

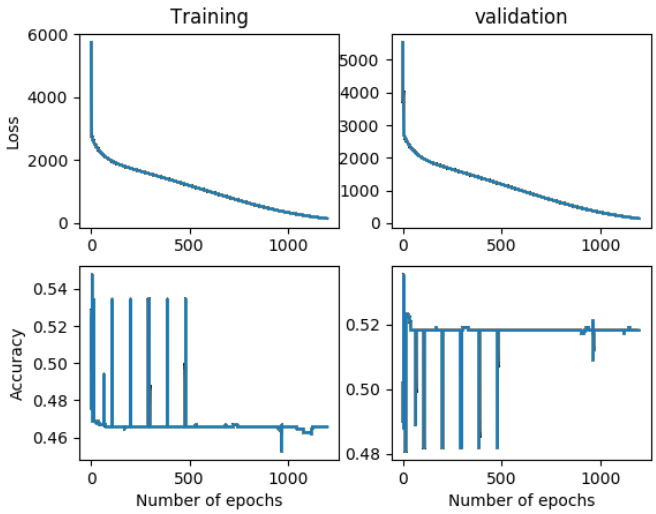


FIGURE 10. Batch Size = 15, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

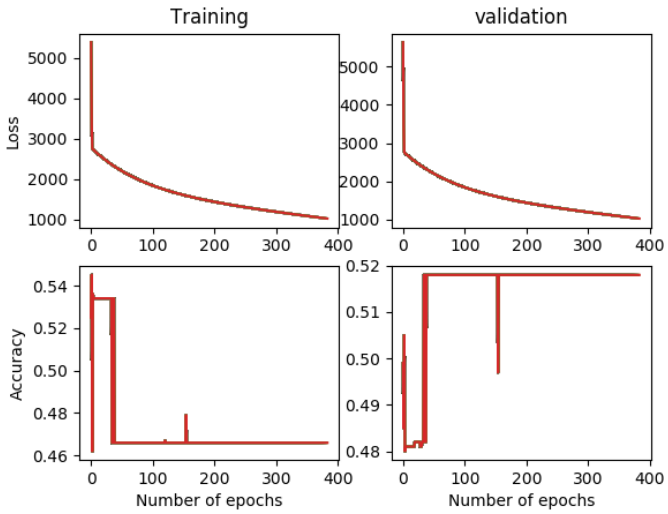


FIGURE 11. Batch Size = 200, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

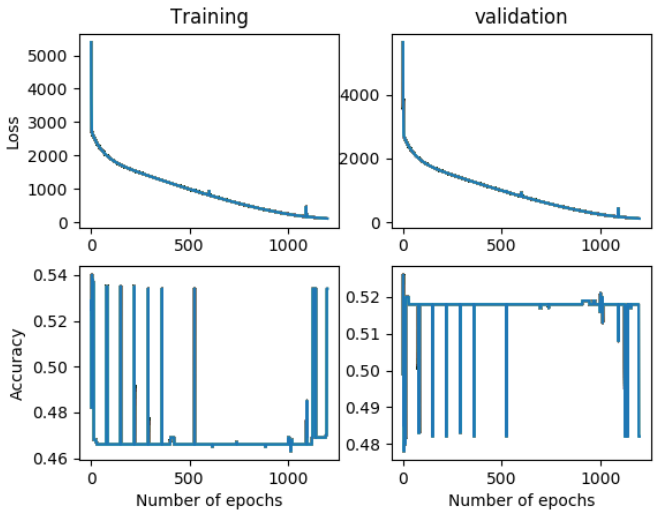


FIGURE 12. Batch Size = 20, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

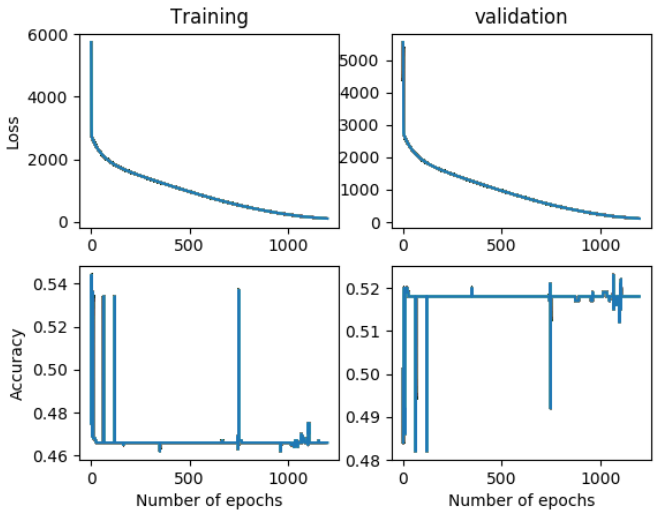


FIGURE 13. Batch Size = 25, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

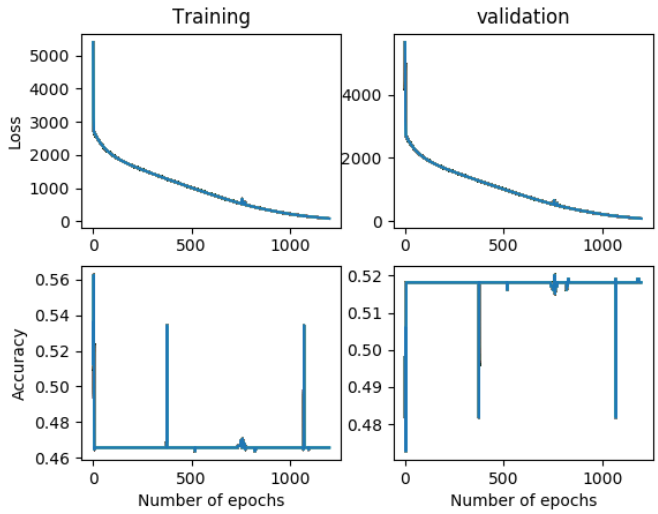


FIGURE 14. Batch Size = 30, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

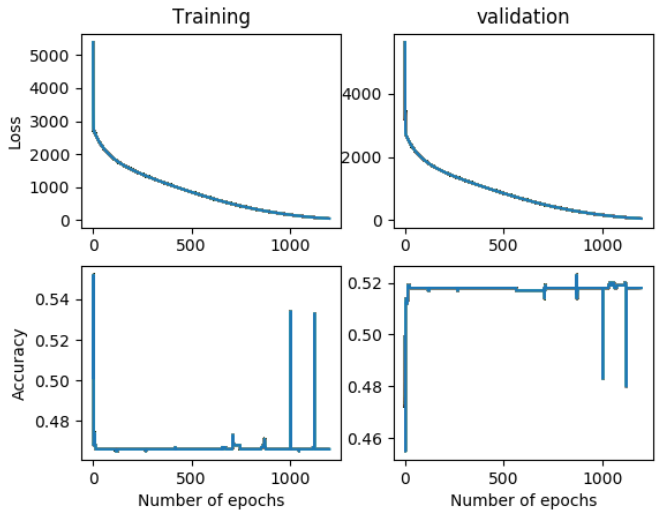


FIGURE 15. Batch Size = 50, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

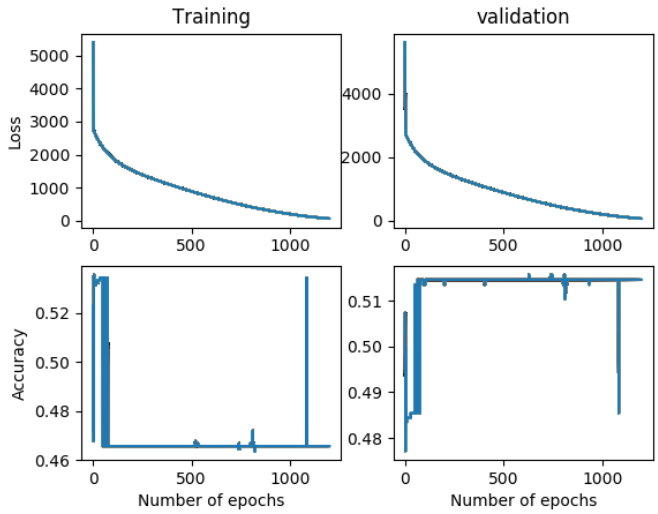


FIGURE 16. Batch Size = 80, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

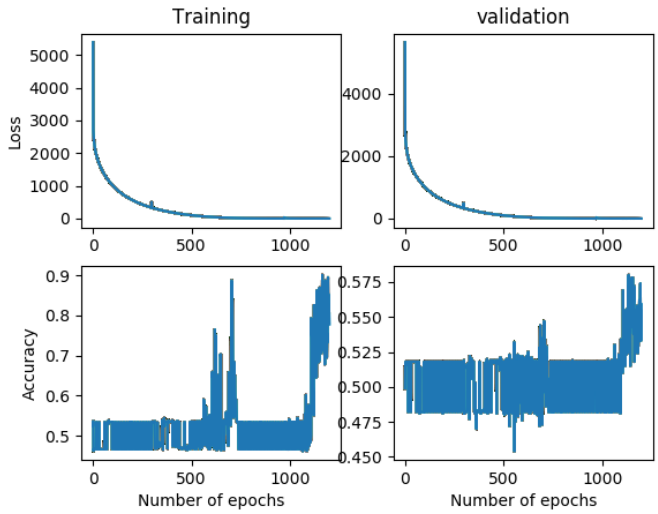


FIGURE 17. Batch Size = 100, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

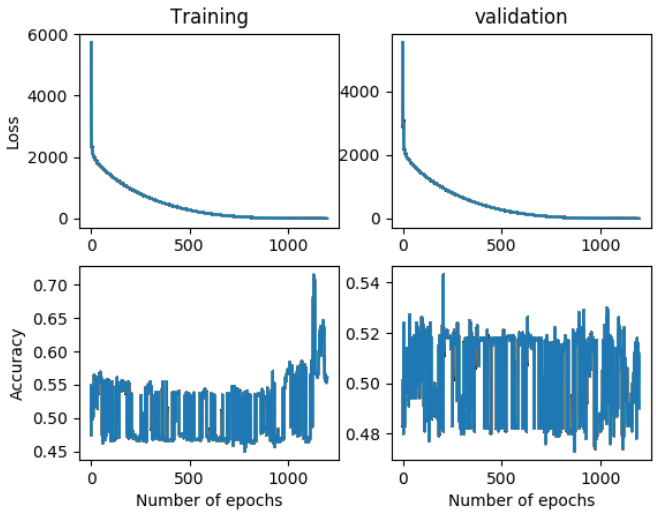


FIGURE 18. Batch Size = 10, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

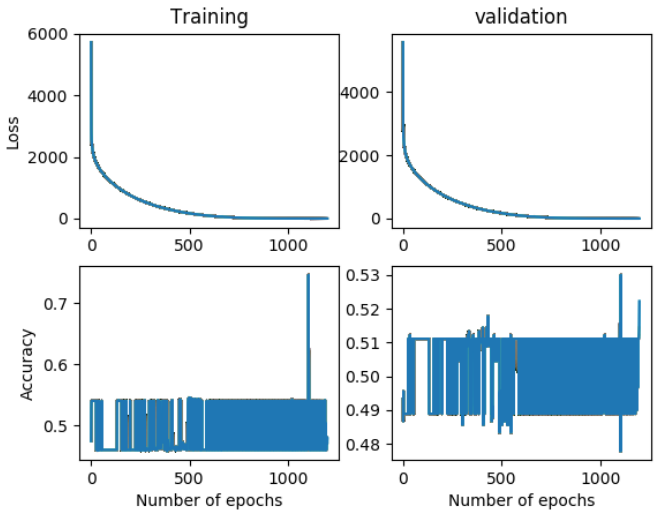


FIGURE 19. Batch Size = 150, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

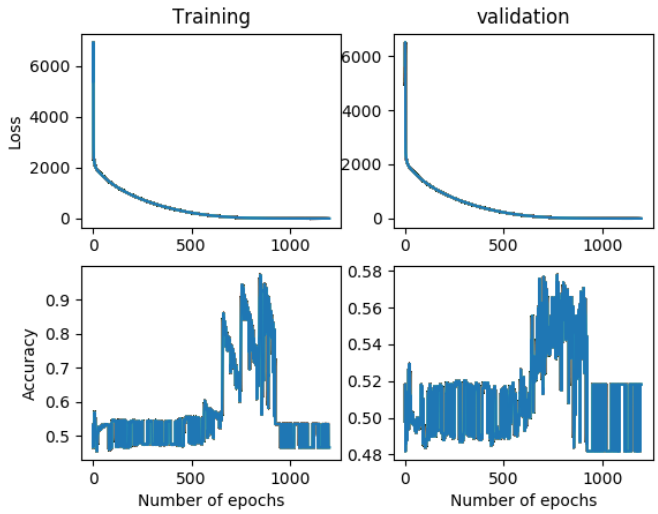


FIGURE 20. Batch Size = 15, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

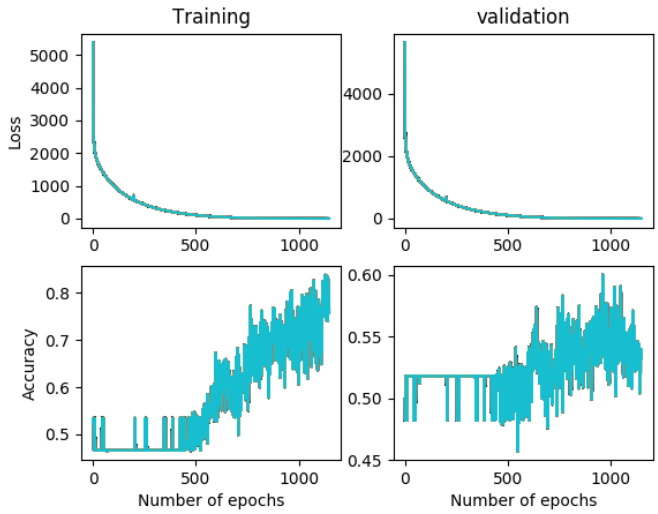


FIGURE 21. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.1

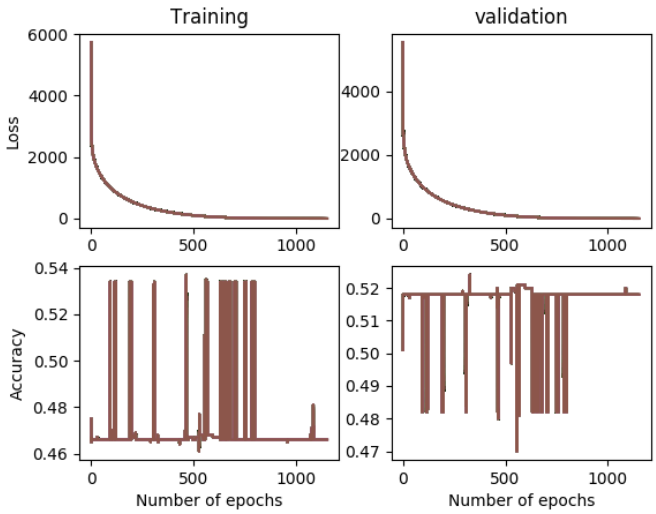


FIGURE 22. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.2

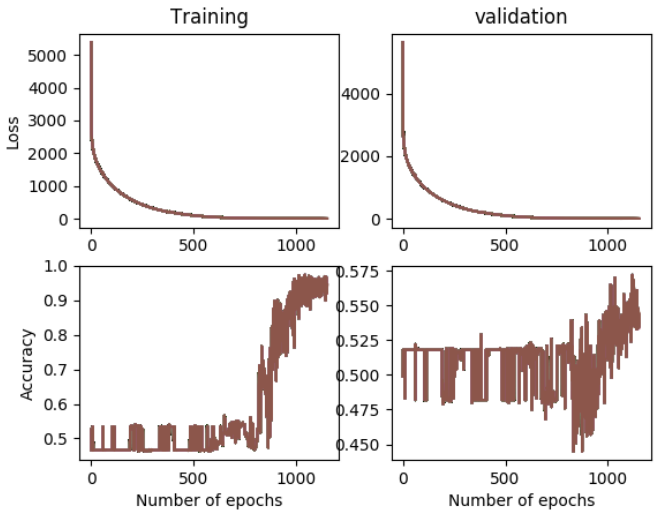


FIGURE 23. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.3

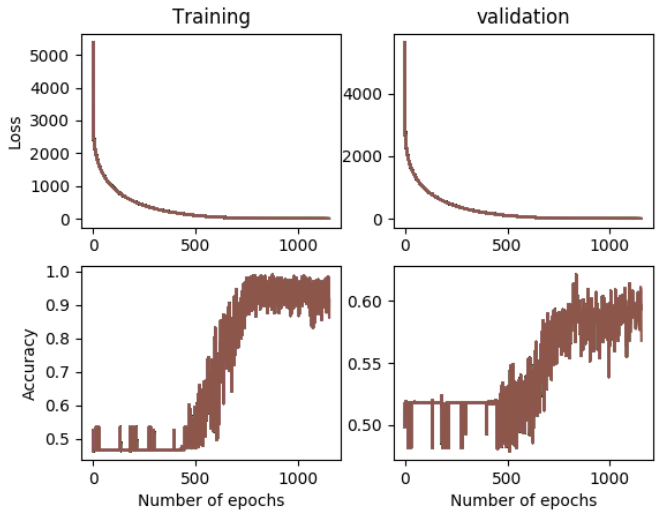


FIGURE 24. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4

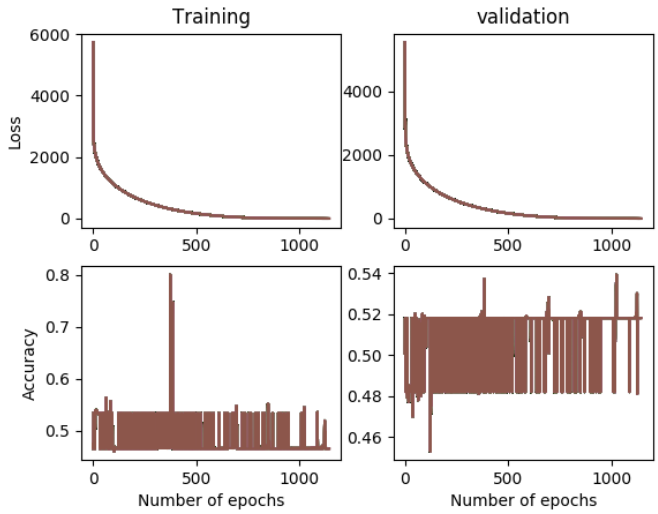


FIGURE 25. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

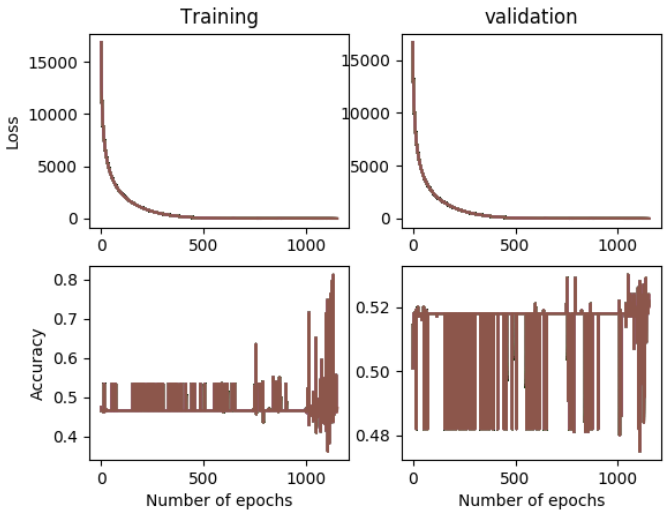


FIGURE 26. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.3

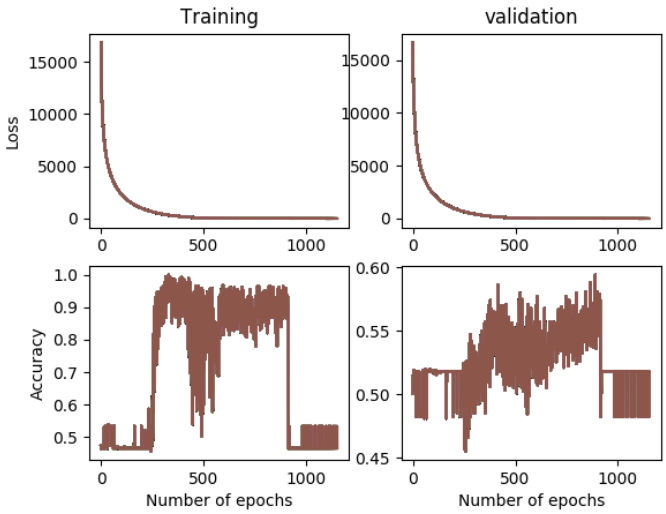


FIGURE 27. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4

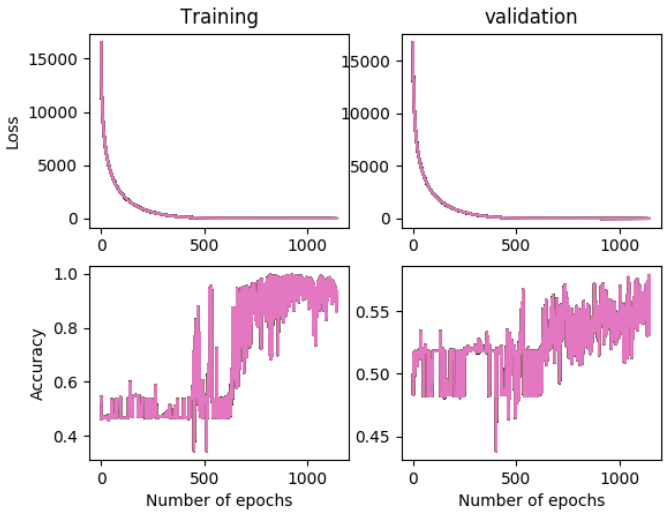


FIGURE 28. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4

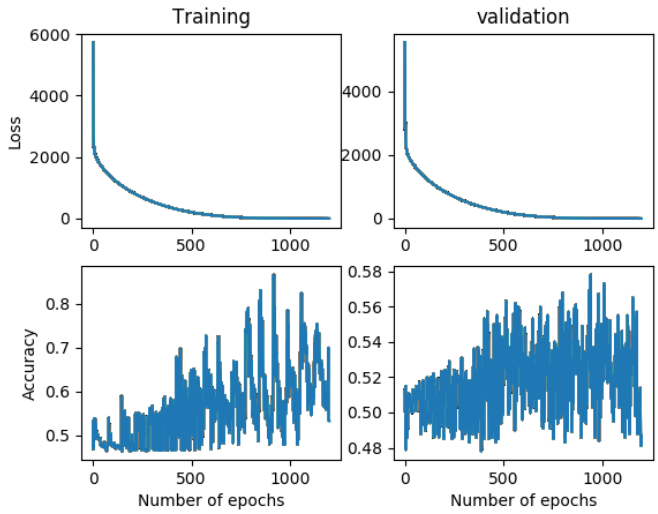


FIGURE 29. Batch Size = 20, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

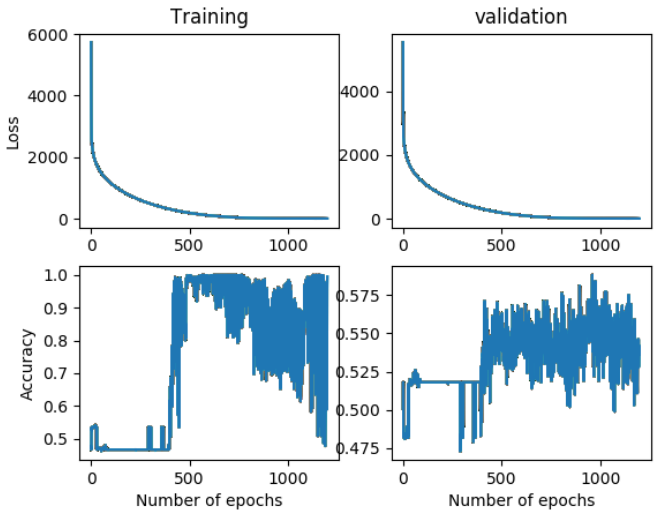


FIGURE 30. Batch Size = 250, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

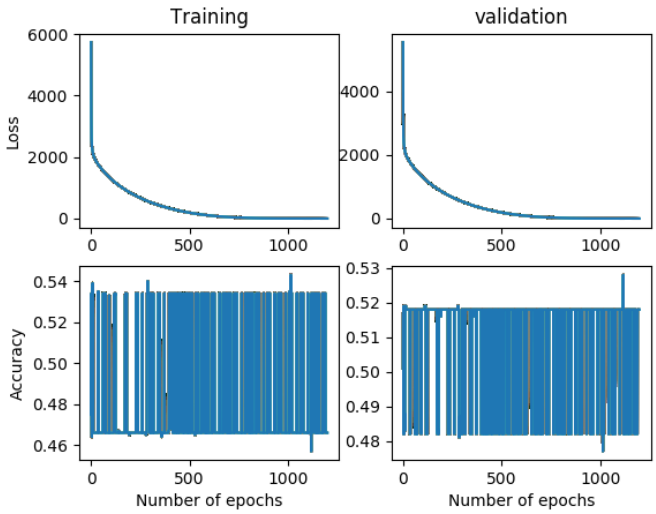


FIGURE 31. Batch Size = 25, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

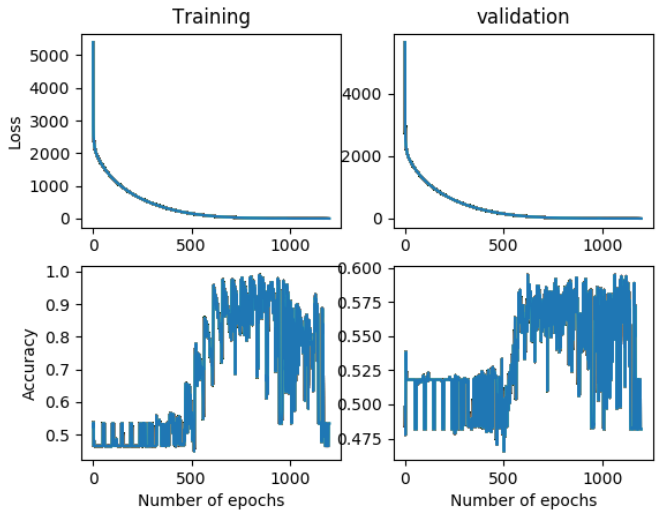


FIGURE 32. Batch Size = 30, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

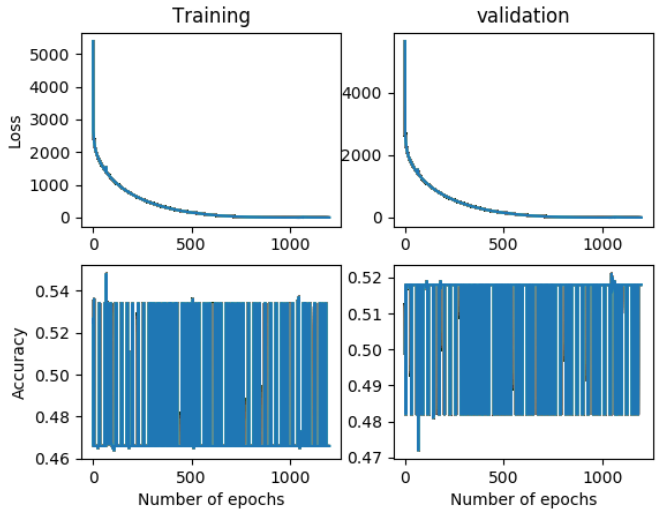


FIGURE 33. Batch Size = 50, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(10) Visualizations.

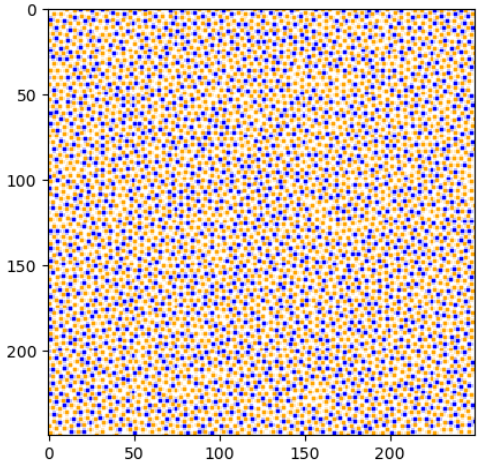


FIGURE 34. Glass original

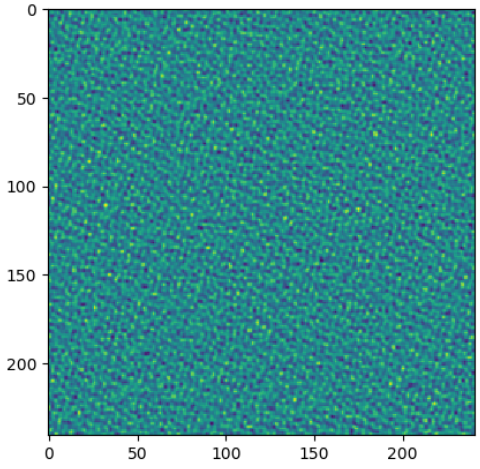


FIGURE 35. Glass channel 1

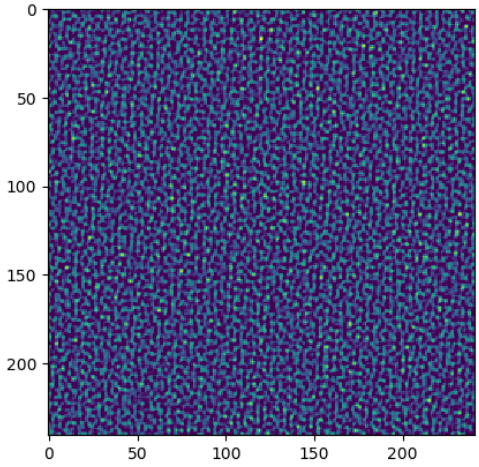


FIGURE 36. Glass channel 2

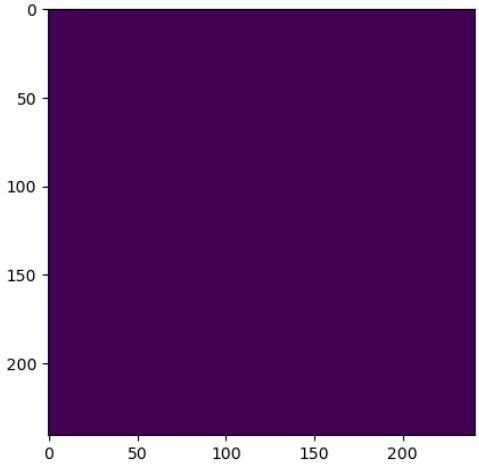


FIGURE 37. Glass channel 3

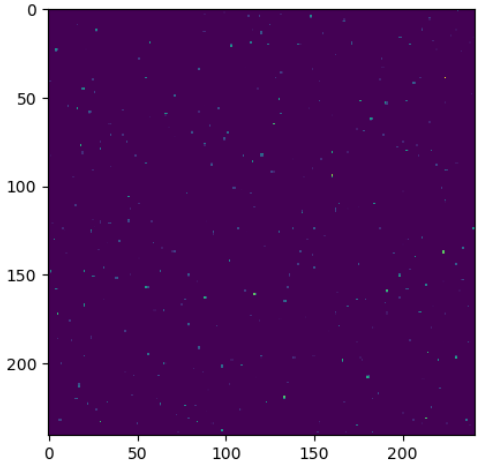


FIGURE 38. Glass channel 4

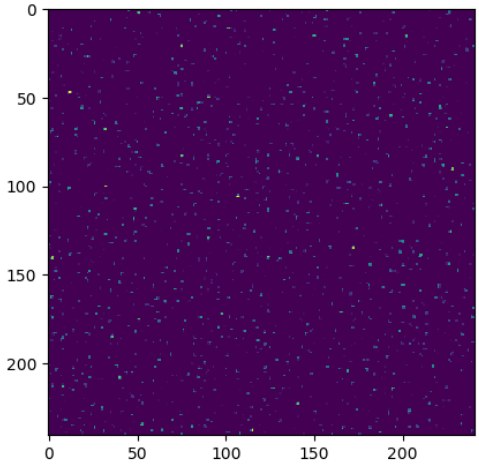


FIGURE 39. Glass channel 5

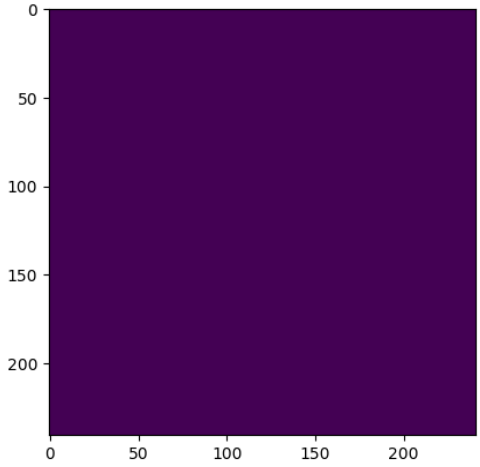


FIGURE 40. Glass channel 6

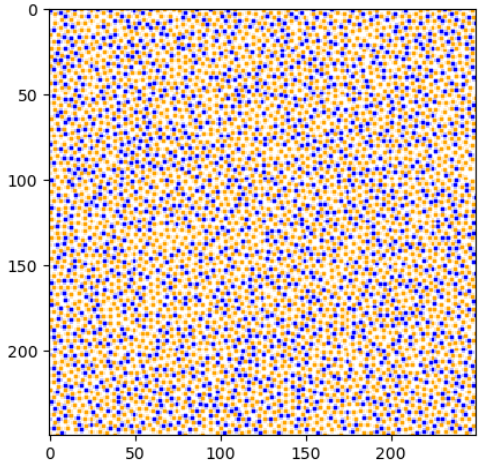


FIGURE 41. Liquid original

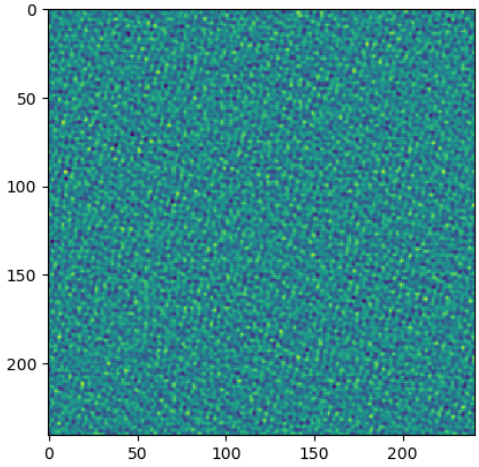


FIGURE 42. Liquid channel 1

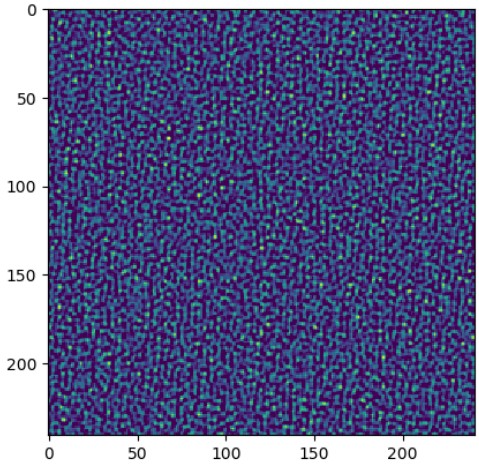


FIGURE 43. Liquid channel 2

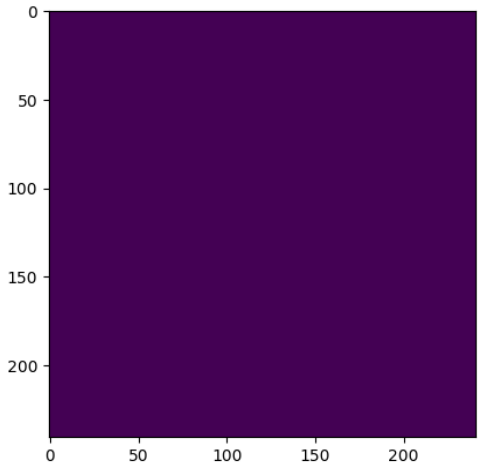


FIGURE 44. Liquid channel 3

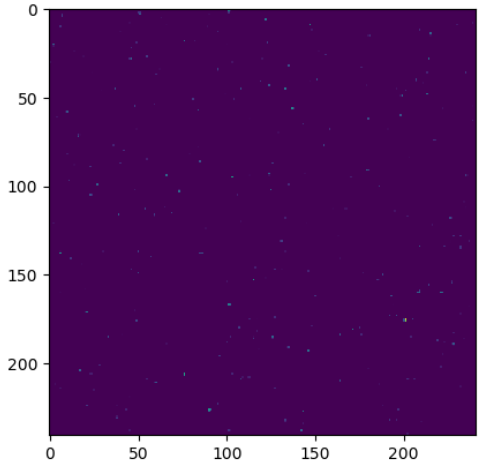


FIGURE 45. Liquid channel 4

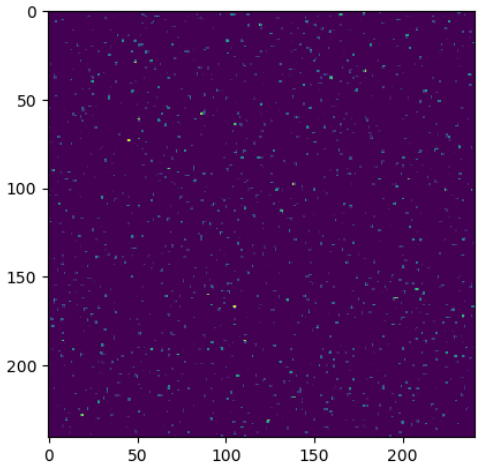


FIGURE 46. Liquid channel 5

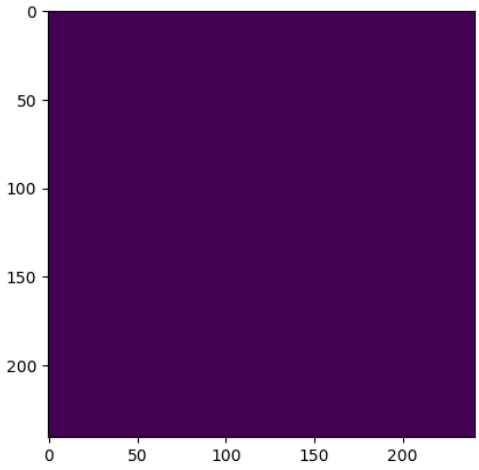


FIGURE 47. Liquid channel 6

2. 12/13/2017

(1) Updated python scripts and merged with GitHub - the recent additions include streamlining the learning rate schedule and data augmentation options. The following is for a standard run on the original endpoint data:

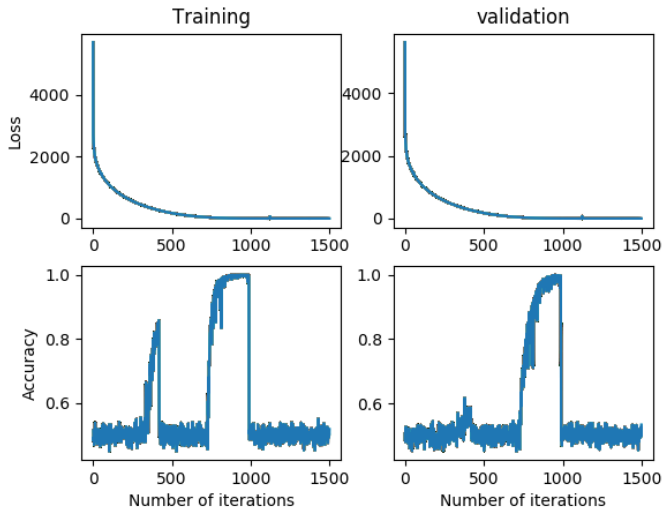


FIGURE 48. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-3, Schedule Length = 550 iterations, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

(2) I then, twice, set the final learning rate to be smaller, at 1e-4:

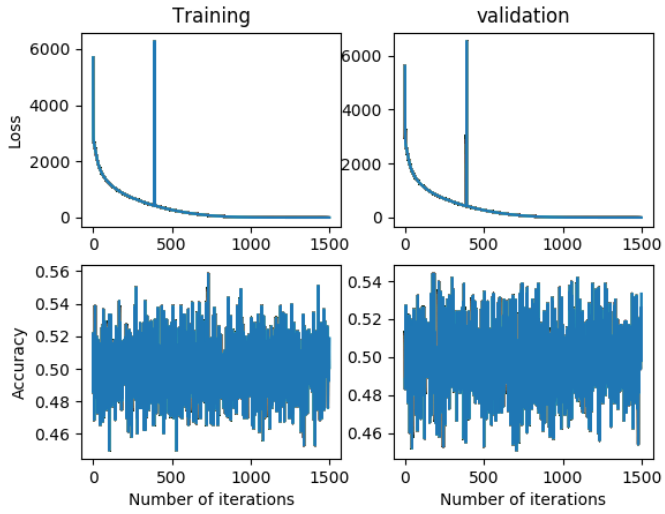


FIGURE 49. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-3, Schedule Length = 550 iterations, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

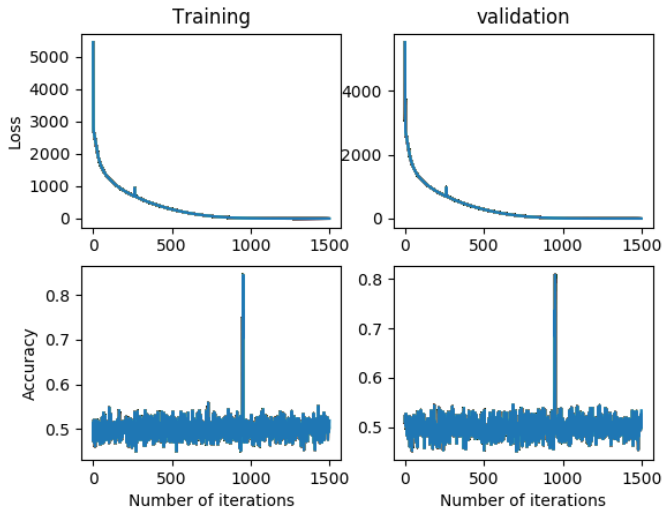


FIGURE 50. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-3, Schedule Length = 550 iterations, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

(3) What is going on here? It seems as though setting the learning rate a magnitude lower really screws things up...
(4) Note: one iteration goes through 10 batches, so if the batch size is 80, then one iteration goes through 800 examples. The training set is 70 percent of the total 20,000 images, so the training set is 14,000 images. Thus, one epoch is 17.5 iterations, or approximately 18 iterations. That means that 1500 iterations is about 83 epochs. Question: how many epochs is typically needed for a binary classification problem? And how long does this typically take?
(5) I also tested the usual hyperparameters on the original endpoint data and turned on the data augmentation, to see if there would be any issues. I got the following training runs:

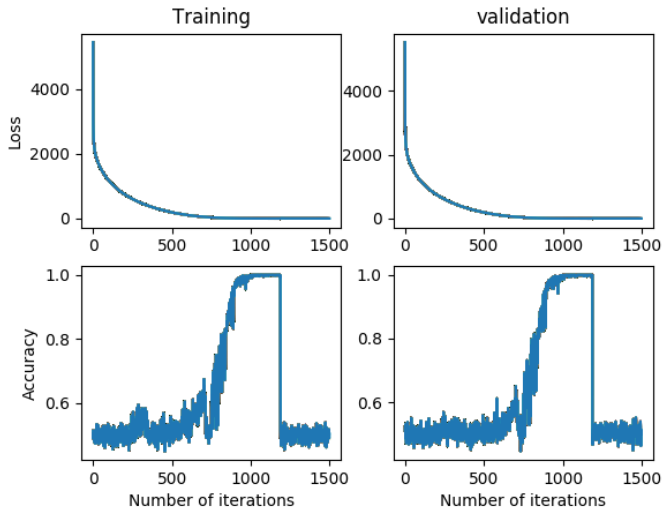


FIGURE 51. Initial Learning Rate = NA, Final Learning Rate = 1e-3, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

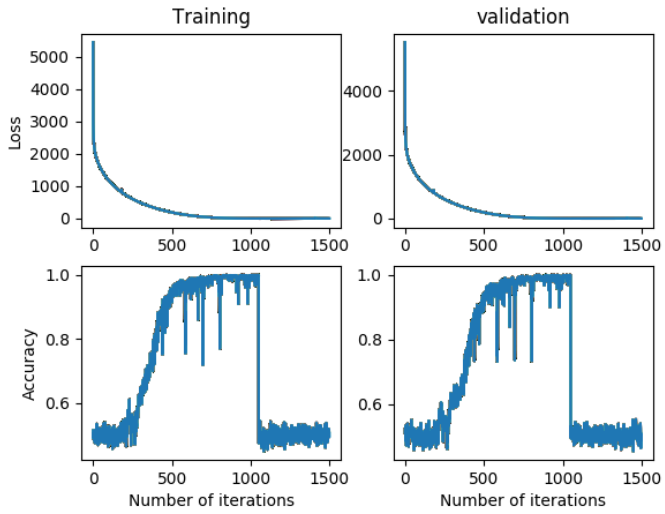


FIGURE 52. Initial Learning Rate = NA, Final Learning Rate = 1e-3, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

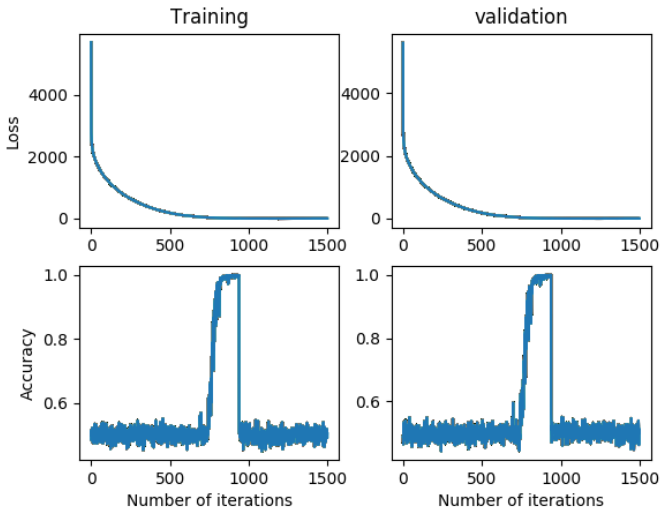


FIGURE 53. Initial Learning Rate = NA, Final Learning Rate = 1e-3, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

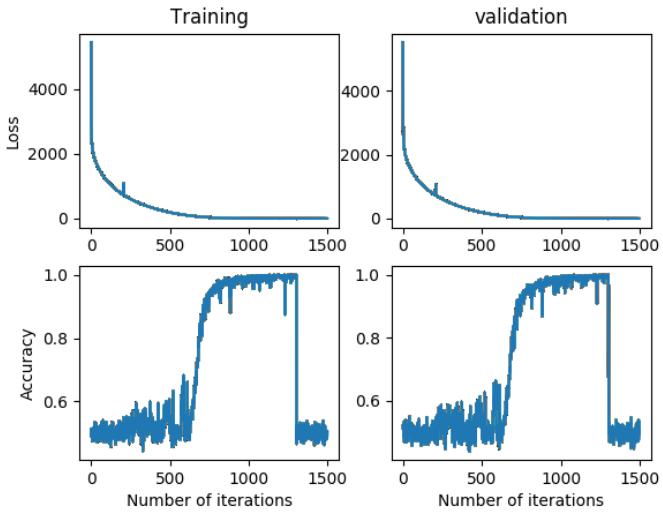


FIGURE 54. Initial Learning Rate = NA, Final Learning Rate = 1e-3, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

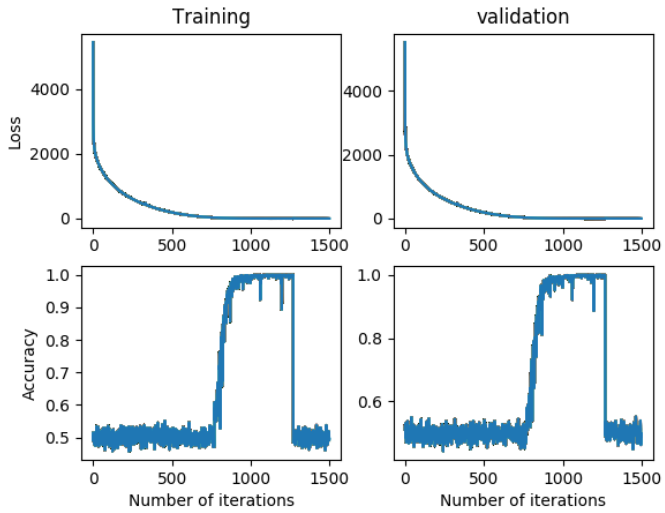


FIGURE 55. Initial Learning Rate = NA, Final Learning Rate = 1e-3, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

(6) I should double check that the dataset augmentation is actually working.

3. 12/22/2017

(1) I am now going to run a series of training runs that will explore the relationship between the learning rate schedule and accuracy. First, let's try the threshold idea. Then, we will try the standard exponential decay idea. Let's try the following. When the accuracy gets to 90 percent, let's decrease the learning rate by an order of magnitude. Let's just run that simple test, say, 8 times, and see what happens!
(2) Initial learning rate = , Final learning rate = ,

4. 12/24/2017

(1) We ran a series of training runs that used a learning rate threshold. The learning rate starts at the initial learning rate. The learning rate changes to the final learning rate whenever the validation accuracy is above 90 percent. This allows the learning rate to go back to the initial learning rate if the accuracy drops below 90 percent. Here are plots showing six tests. These plots demonstrate that the sharp drops in accuracy were, indeed, the result of a learning rate that was too large towards the end of training, since there are no sharp drops in accuracy here:

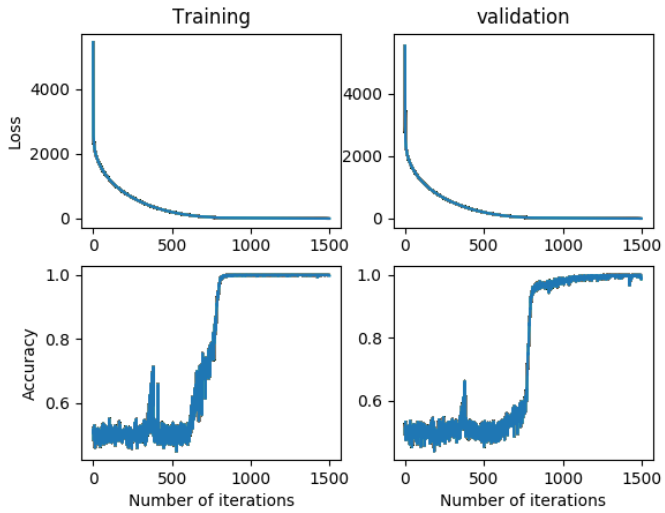


FIGURE 56. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

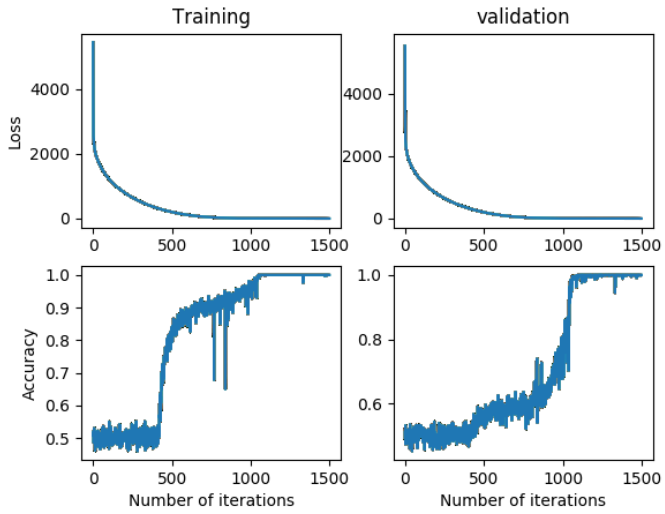


FIGURE 57. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

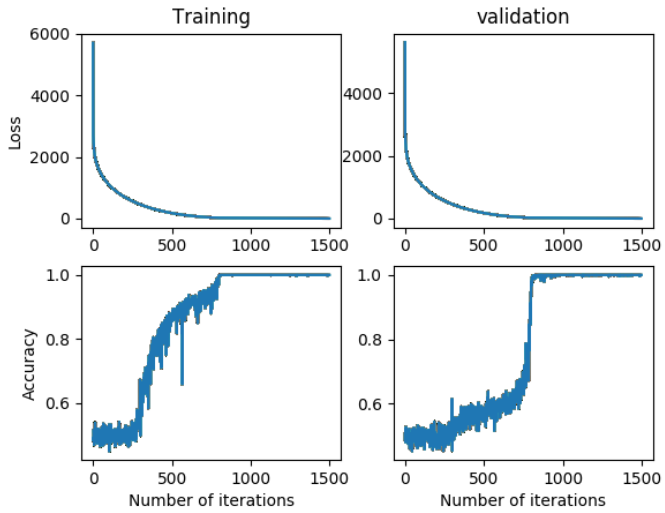


FIGURE 58. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

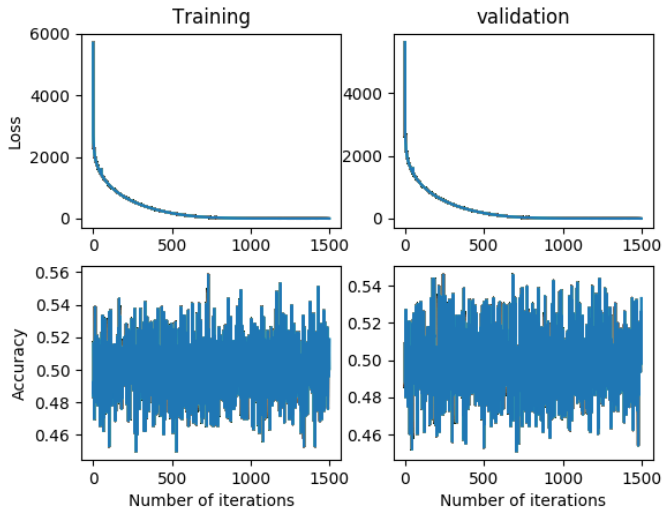


FIGURE 59. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

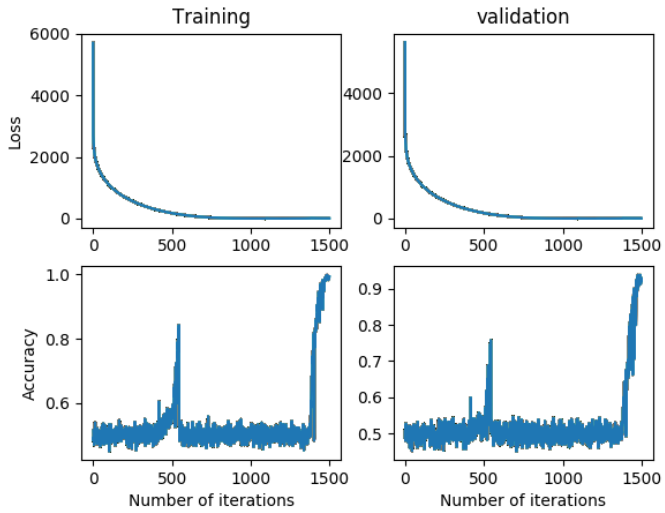


FIGURE 60. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

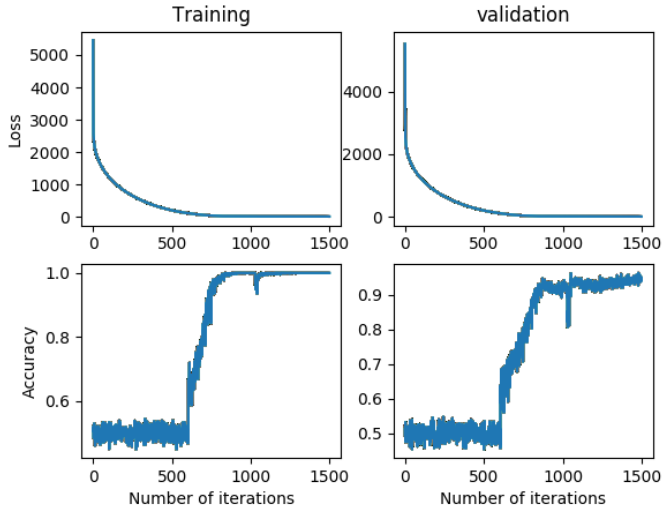


FIGURE 61. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

4.1. **12/29/2017.**

(1) Ran another series of runs that used a similar learning rate threshold just to check that my GitHub had been updated appropriately. This time used only 1e-3 to 1e-4. In one example, the accuracy crashed. Perhaps evidences that smaller learning rates are needed closer to the minimum. For the sake of completeness, these extra runs are reported below:

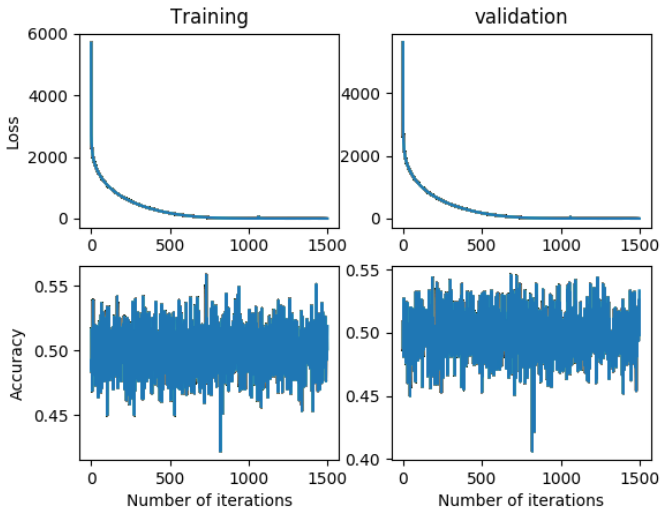


FIGURE 62. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

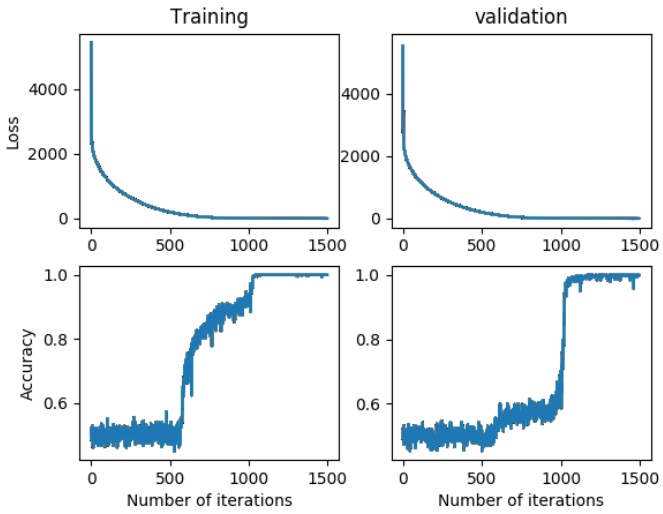


FIGURE 63. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

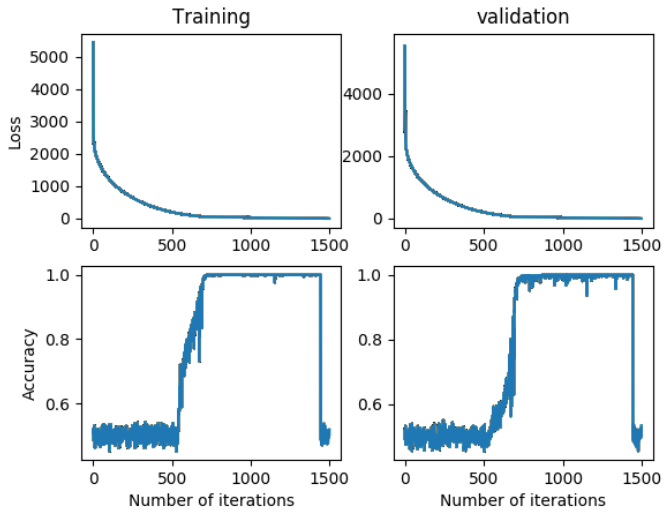


FIGURE 64. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

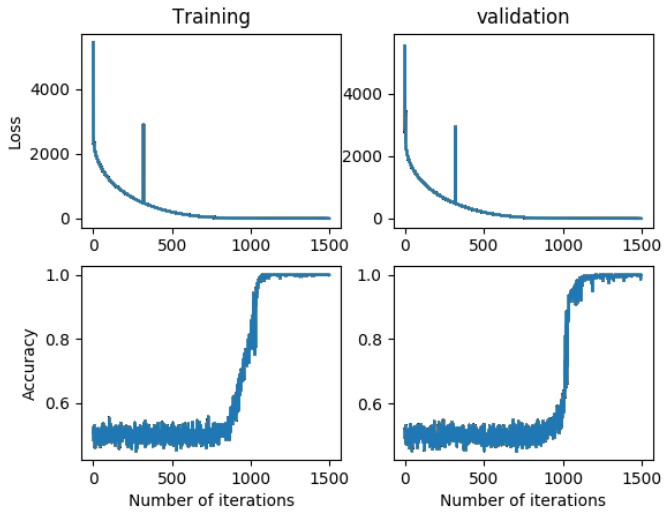


FIGURE 65. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

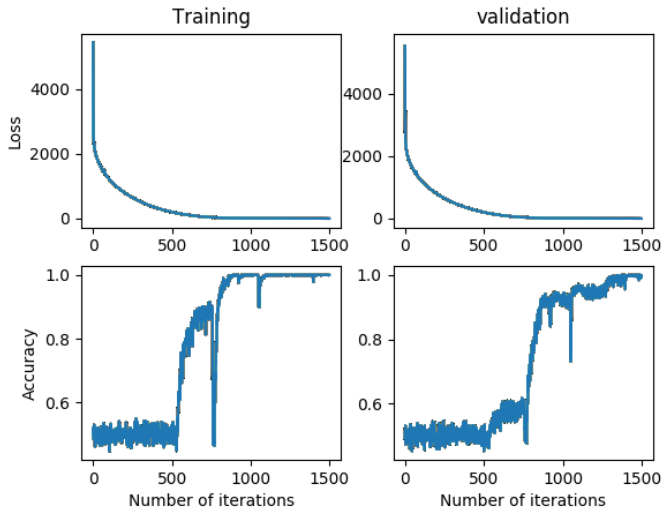


FIGURE 66. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

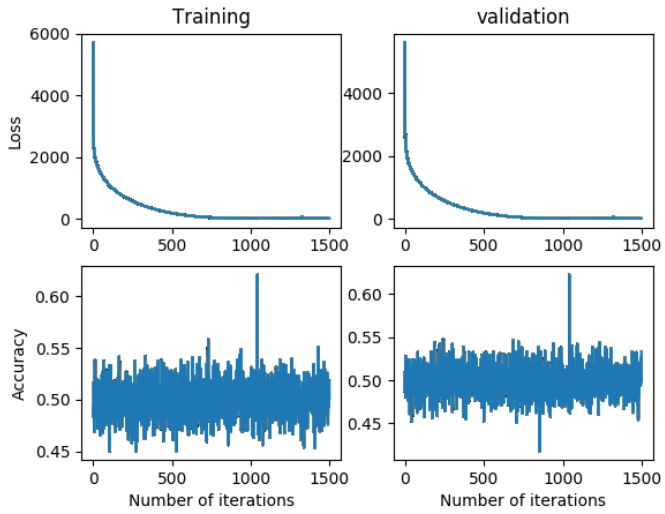


FIGURE 67. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

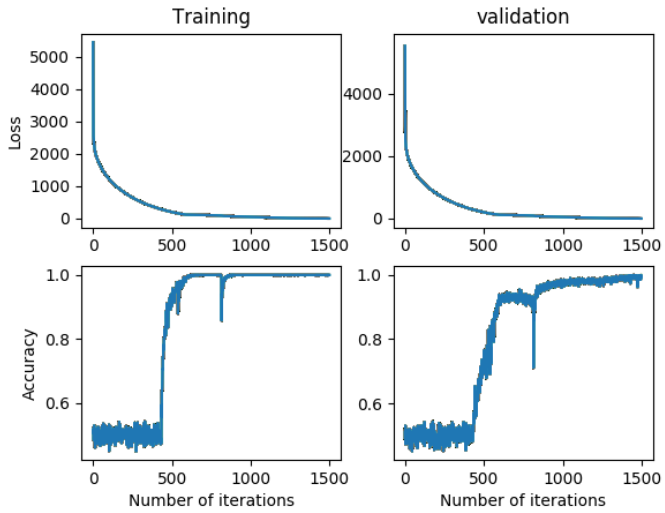


FIGURE 68. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

4.2. **12/30/2017.**

(1) Tested the data augmentation scheme manually. Printed out a series of images and their respective augmented versions that are given when generator.next is invoked, respectively with the data aug option set to false and with the data aug option set to true.

4.3. **1/1/2018.**

(1) Added main_glassliquid_restart.py, a file that can run training starting from a previous saved model. Tested it. Now, let's try to train again on the dataset that consists of glasses and liquids that are each 12 time steps away from the assumed glass transition temperature of 0.21. Previously, the best parameters were batch size 200, learning rate 1e-3, beta 0.01, dropout 0.4. Now, we are going to do a series of simulations using the same parameters, except, first, we are going to include dataset augmentation, and second, we are going to run the simluation at least twice as long. Then, once we get a sense for how these train, we will add in a learning rate threshold step, or even multiple threshold steps if necessary!

4.4. **1/4/2018.**

(1) Realized that I had run on the original endpoint data. So, copied over the folder called "data_12steps" into the current machine-learning-glasses directory, removed the current metadata folder, and created a new metadata folder with this data. Then, set up new training runs again.

5. 1/9/2018

(1) Collected data from the above-mentioned simulations. The training curves are as follows:

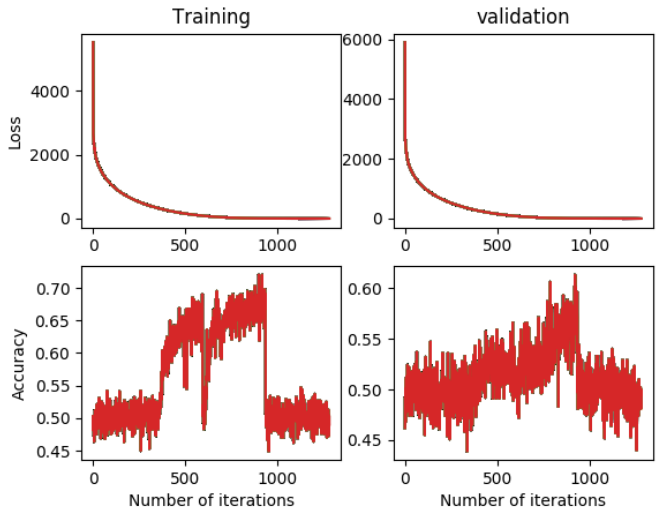


FIGURE 69. Version 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

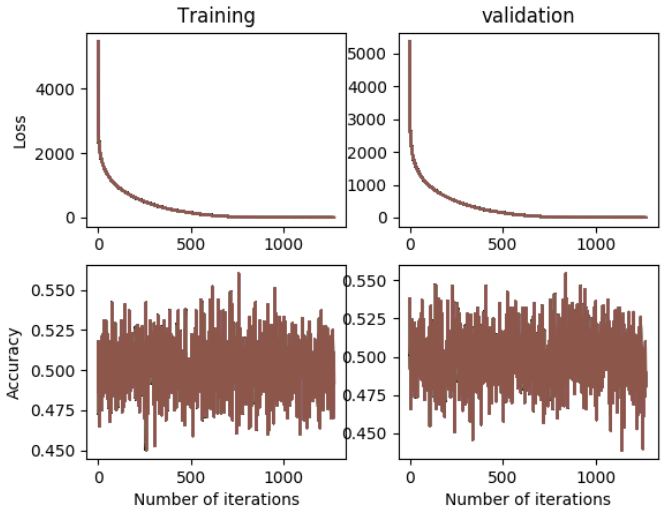


FIGURE 70. Version 2: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

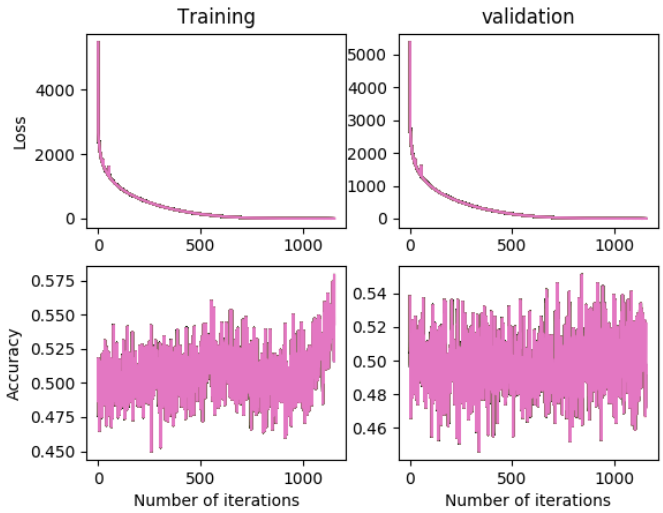


FIGURE 71. Version 3: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

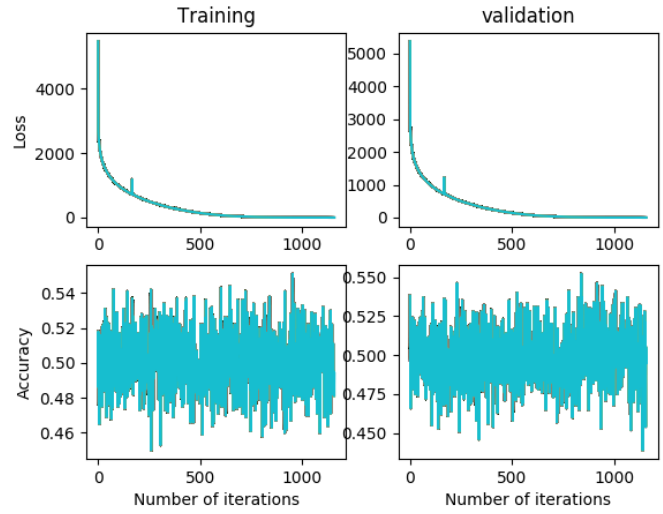


FIGURE 72. Version 4: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

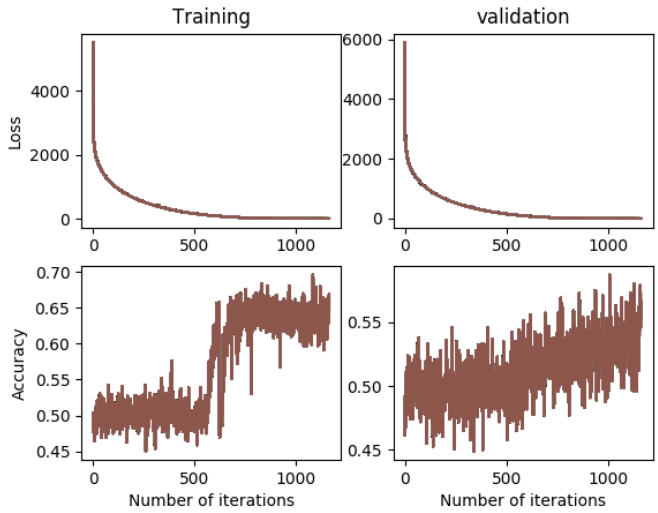


FIGURE 73. Version 5: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

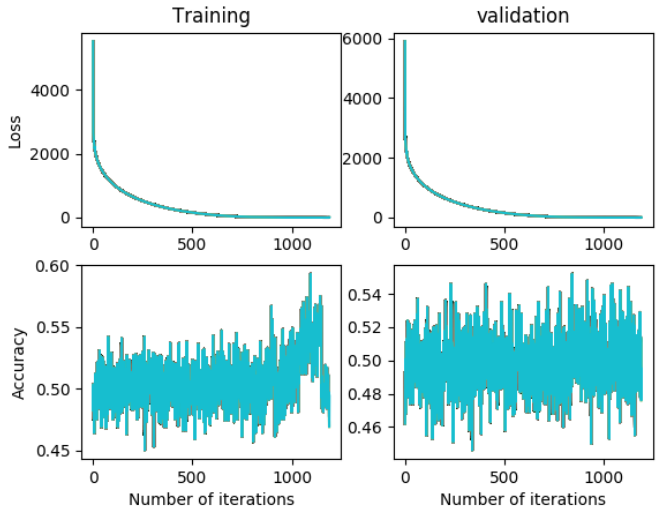


FIGURE 74. Version 6: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

(2) The problem is that my allotted time (36 hours) was not enough, so the simulations terminated early. My program, however, was only set to save the current model at the end of the iterations. So, the current model was not saved, only the best model was saved. So, I went back into the main code and changed it so that the current model is updated and saved at every iteration, in addition to the best

model being updated when necessary. I also included restart capability into the main code (using parsing options), so that there is not a separate restart file.

(3) I am now running 7 new simulations. The first is just a re-do of version1 step 0. The others take version5 step 0 and start from the saved best model as a starting point, using the new restart capabilities of the main code. The first two simulations from this starting point (version5 step2 and version5 step2 trial2) use the original parameters. The next two (version5 step2 trial3 and version5 step2 trial4 use eta_initial=1e-4 and eta_final=1e-5), and the final two (version5 step2 trial5 and version5 step2 trial6) use eta_intial=1e-5 and eta_final=1e-6. We will see how these 7 new runs turn out.

5.1. **1/14/2018.**

(1) Here is the result for the continuations from Version 5 step 0, i.e. Version 5 step 1 trials 1 through 6.

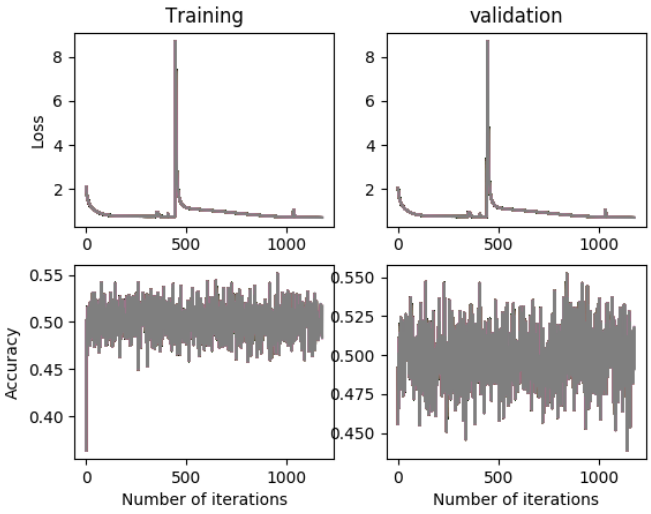


FIGURE 75. Version 5 step 1 trial 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

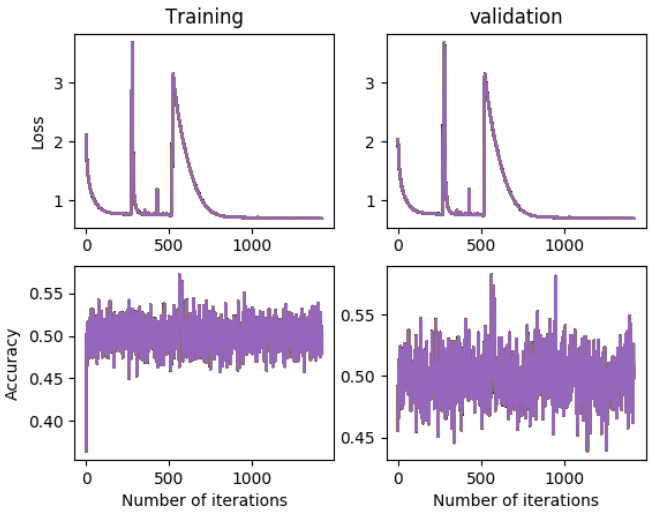


FIGURE 76. Version 5 step 1 trial 2: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

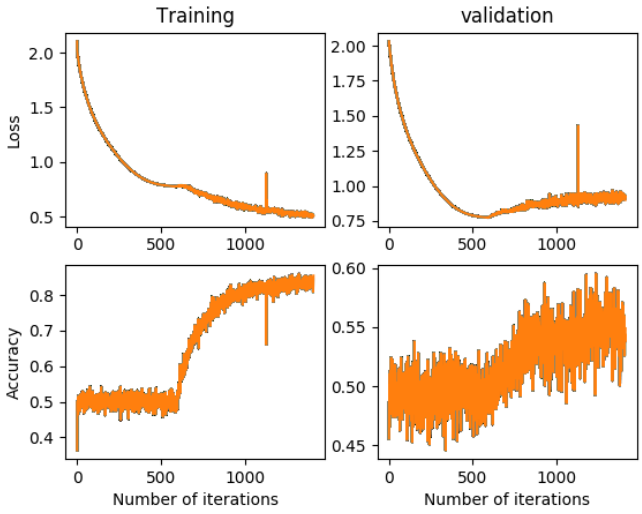


FIGURE 77. Version 5 step 1 trial 3: Initial Learning Rate = 1e-4, Final Learning Rate = 1e-5, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

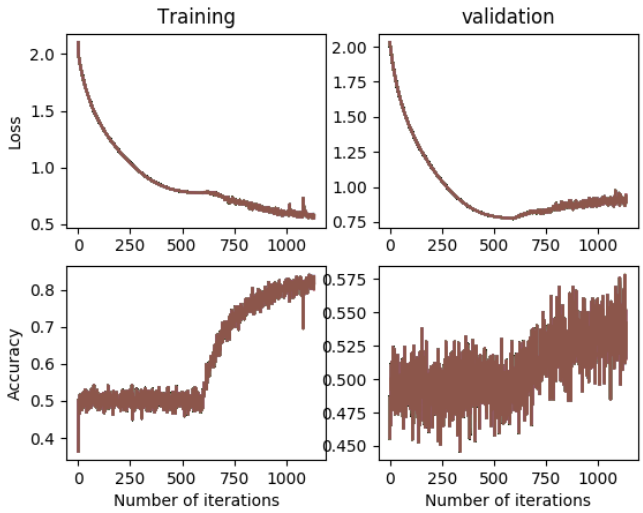


FIGURE 78. Version 5 step 1 trial 4: Initial Learning Rate = 1e-4, Final Learning Rate = 1e-5, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

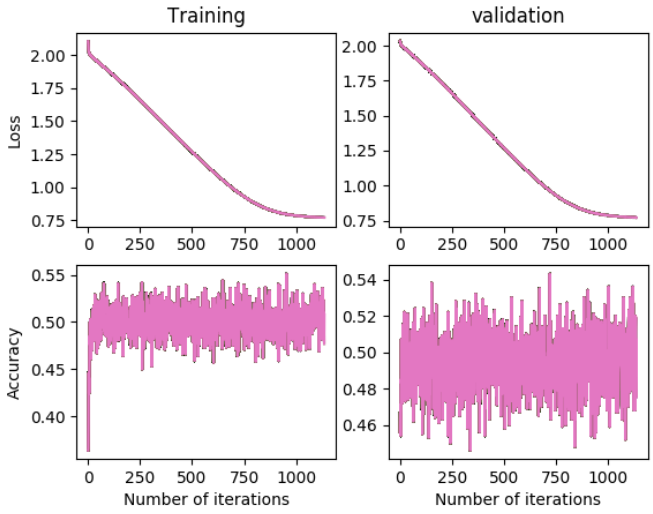


FIGURE 79. Version 5 step 1 trial 5: Initial Learning Rate = 1e-5, Final Learning Rate = 1e-6, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

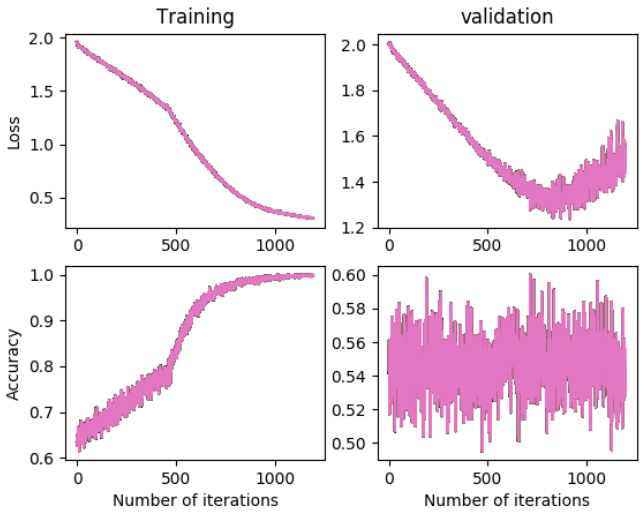


FIGURE 80. Version 5 step 1 trial 6: Initial Learning Rate = 1e-5, Final Learning Rate = 1e-6, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

(2) I am now going to generate new data that is farther away from the assumed glass transition temperature of $T_g = 0.21$. Based on cooling.dat file in the folder N2e7/0, which is the first of 10,000 simulations, this temperature is at the 184th line of the file (0.21575), which is the 183rd time listed. There are 200 times listed in cooling.dat, each one separated by a time length of 100,000 time steps. This is because the total simulation is 2e7, or 20 million. In the folder /project/depablo/kswanson/2017, I open the file make_images_kirk.sh and change the liquid generation number to 500000 and keep the glass generation number at 20000000.

5.2. **1/15/2018.**

(1) After generating the new datapoint, I create a folder called data_liquid5 and transfer it to the git repo. Now, I delete the current metadata folder and create a new metadata folder that contains the data_liquid5 in it.
(2) V1-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(3) V2-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(4) V3-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(5) V4-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(6) V5-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(7) V6-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(8) V7-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(9) V8-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(10) V9-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(11) V10-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.

5.3. **1/19/2018.**

(1) Using timestep 5 (500000) for the liquid and timestep 200 (20000000) for the glass, here are training results:

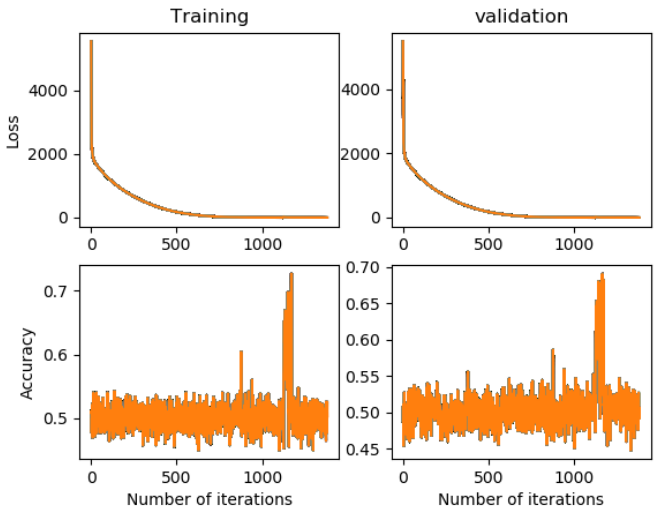


FIGURE 81. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

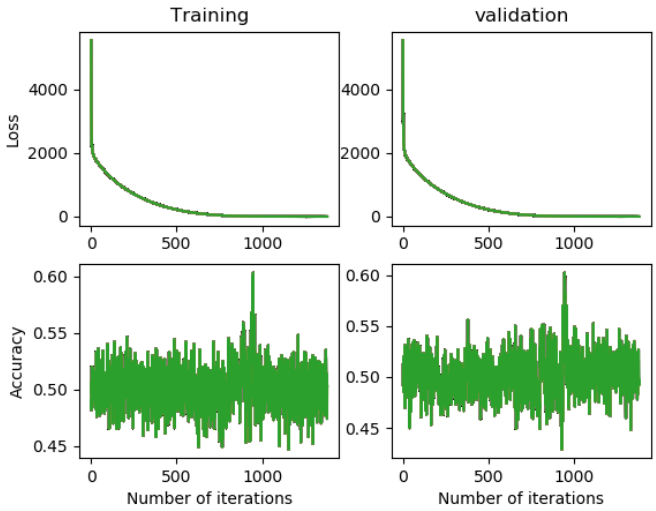


FIGURE 82. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

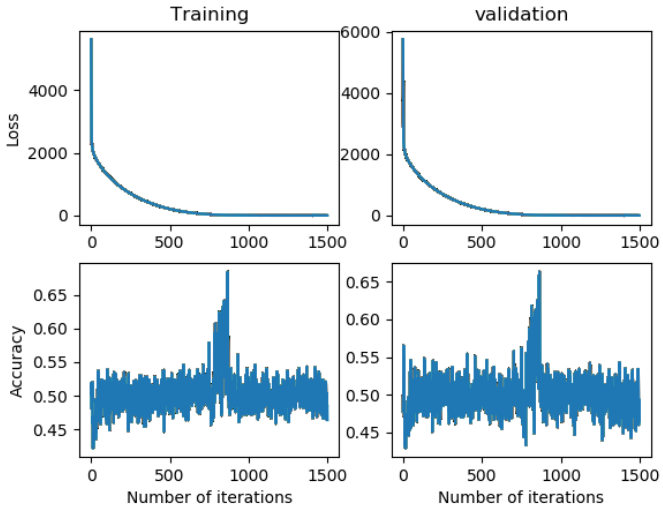


FIGURE 83. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

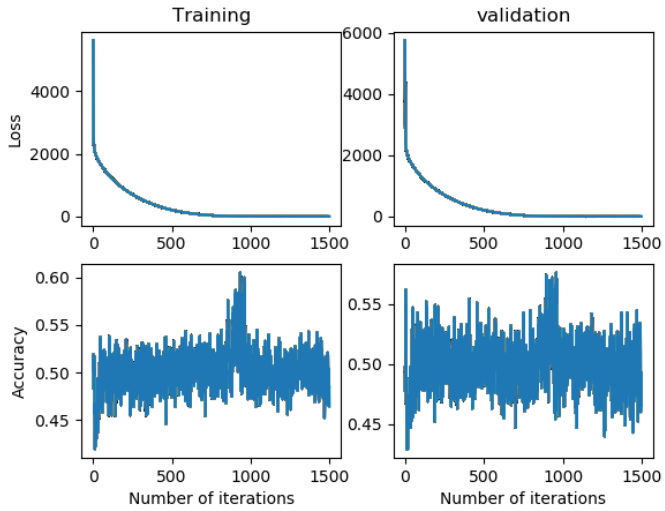


FIGURE 84. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

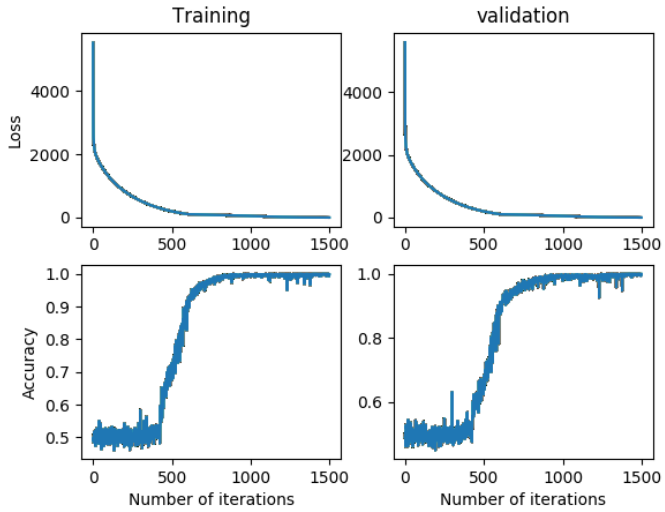


FIGURE 85. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

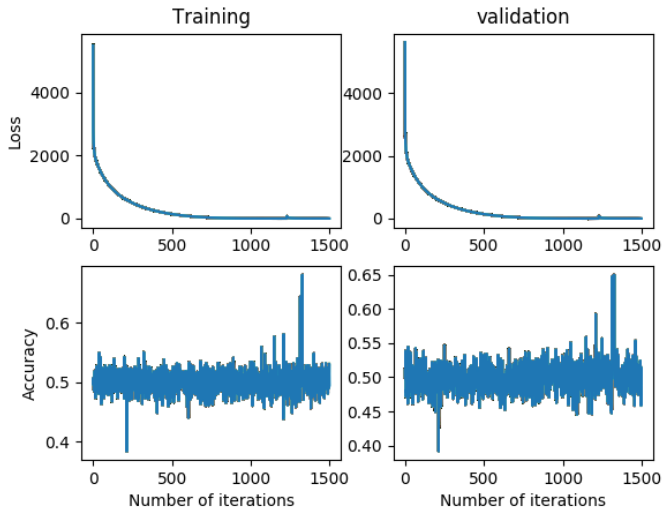


FIGURE 86. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

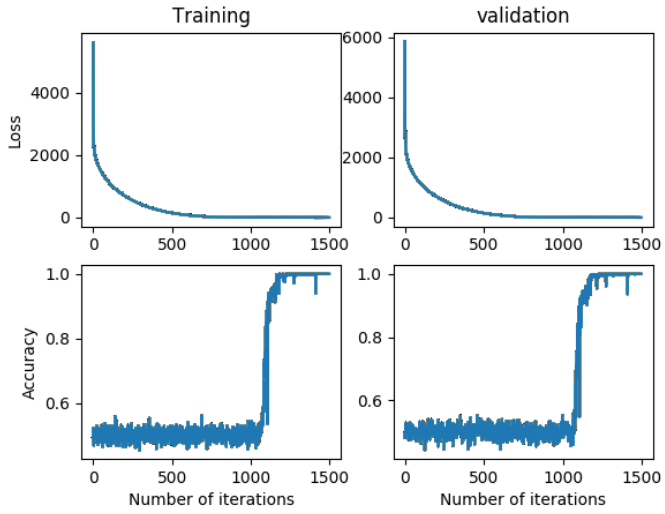


FIGURE 87. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

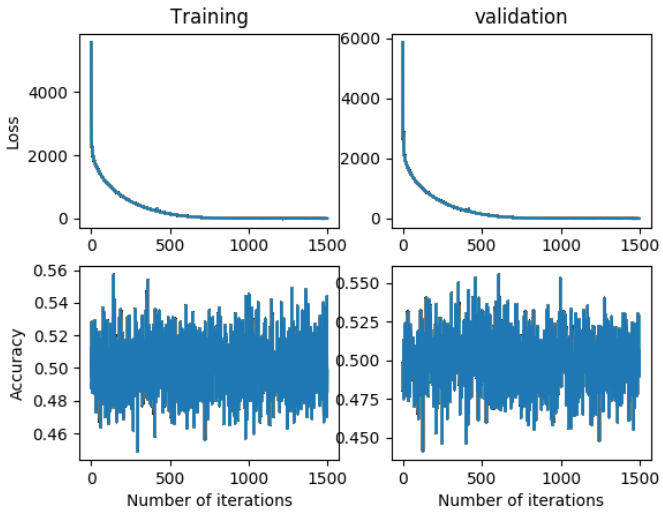


FIGURE 88. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

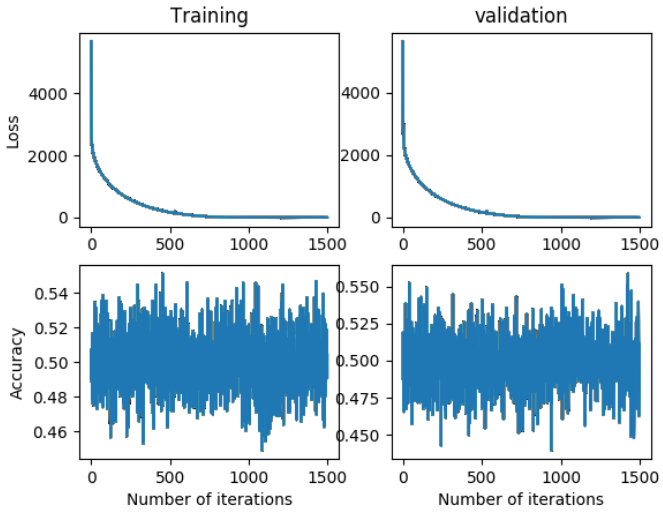


FIGURE 89. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

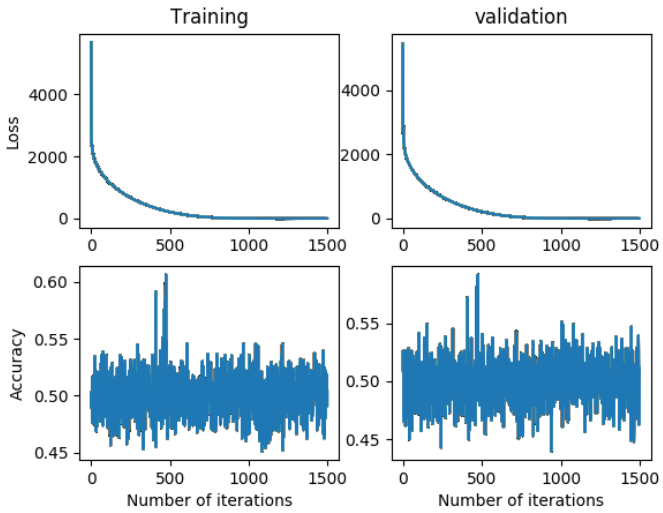


FIGURE 90. Version 10 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

(2) Version 5 Step 1 had a final validation accuracy of 99.7% and a final test accuracy of 99.7333%. Added changes to main_glassliquid.py so that by setting -restart=True and -evaluation=True in the options, and setting -restart_file to the desired filename, one can check the final validation and test accuracy of a given model.
(3) Version 7 Step 1 had a final validation accuracy of 99.8% and a final test accuracy of 99.8333%.
(4) Now I am generating images for liquid timestep 10 (1000000).

5.4. **1/20/2018.**

(1) I am now switching metadata to be from data_liquid10, our new current dataset.
(2) V1-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(3) V2-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(4) V3-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(5) V4-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(6) V5-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(7) V6-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(8) V7-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(9) V8-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(10) V9-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(11) V10-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(12) V11-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(13) V12-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(14) V13-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(15) V14-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(16) V15-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 150, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(17) V16-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 150, L2 beta = 0.01, Dropout = 0.5, data aug = true.

5.5. **1/23/2018.**

(1) Collected results from training runs on the data_liquid10 data. Here they are:

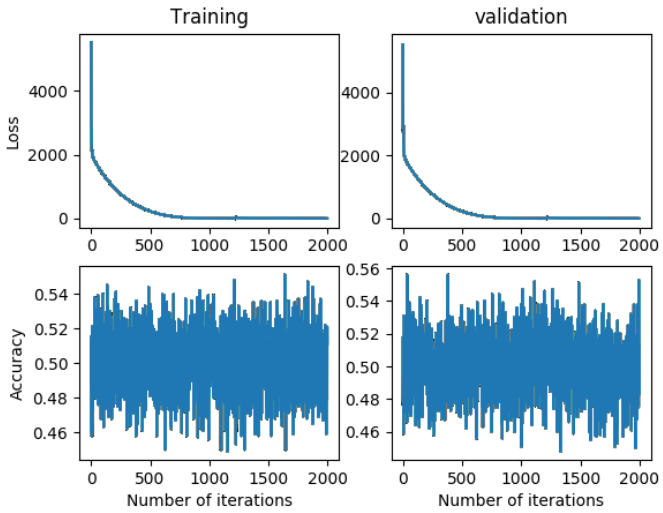


FIGURE 91. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

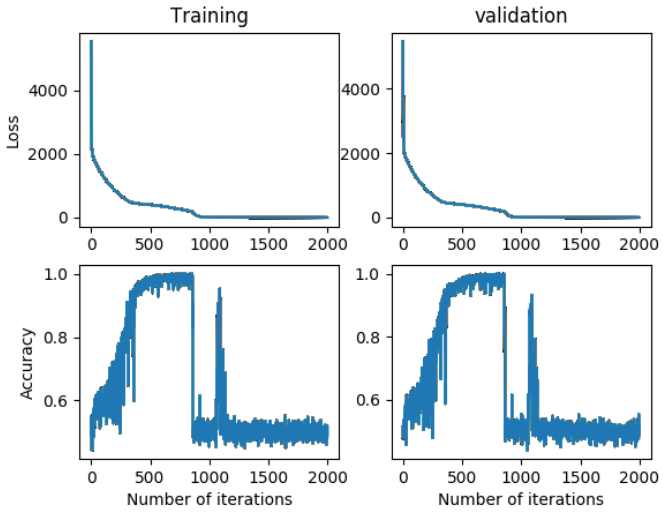


FIGURE 92. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

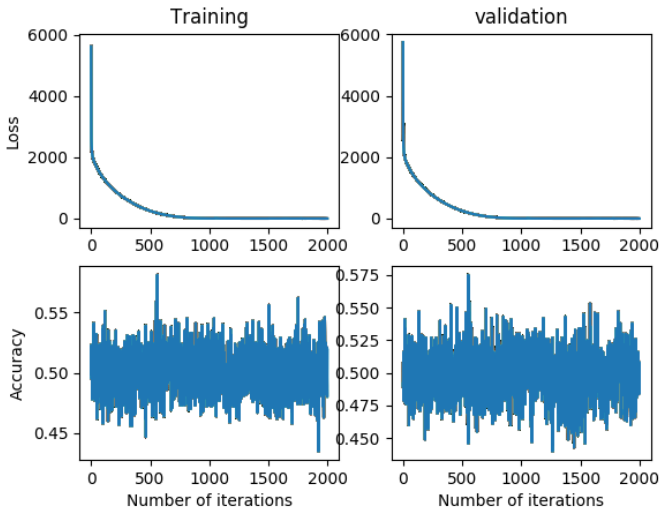


FIGURE 93. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

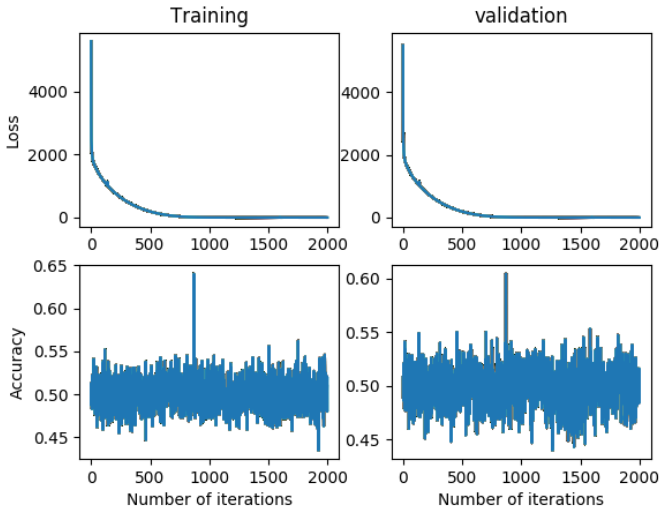


FIGURE 94. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

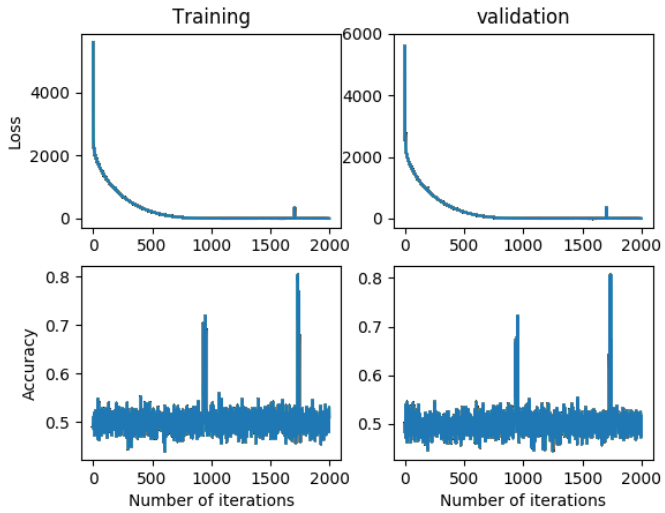


FIGURE 95. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

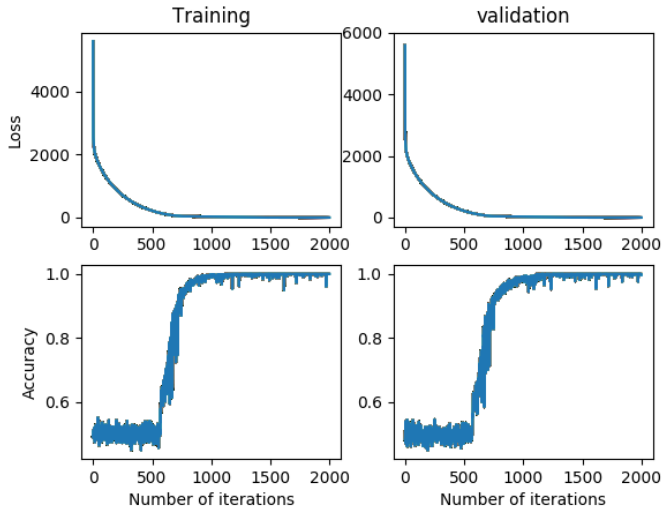


FIGURE 96. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

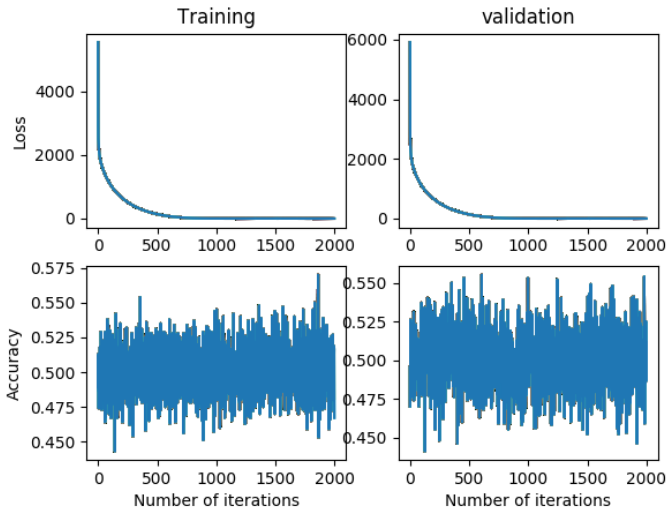


FIGURE 97. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

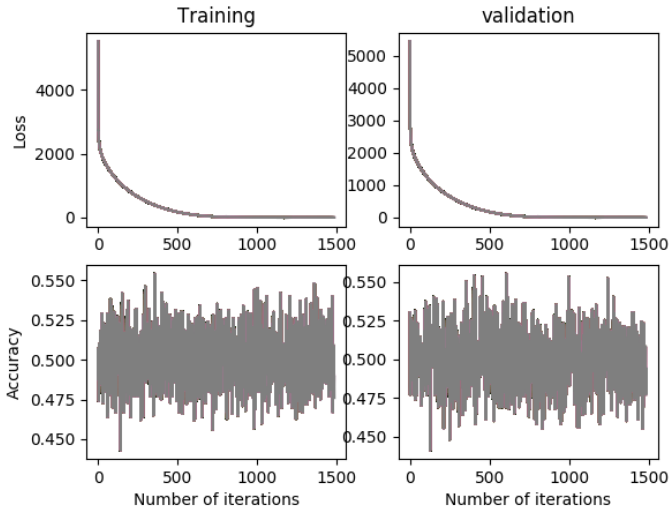


FIGURE 98. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

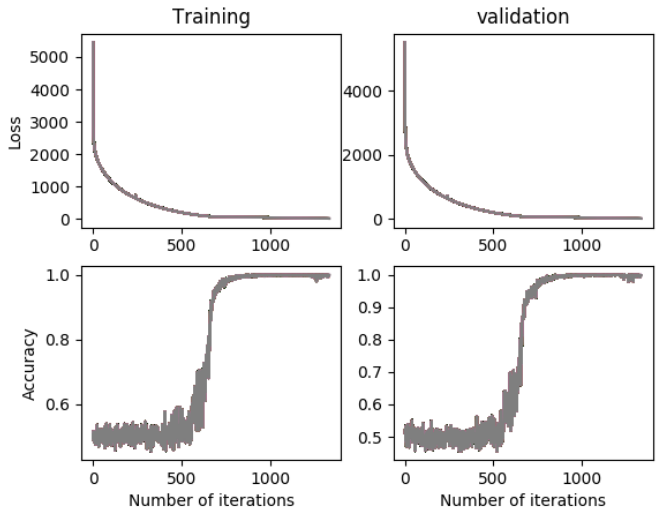


FIGURE 99. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

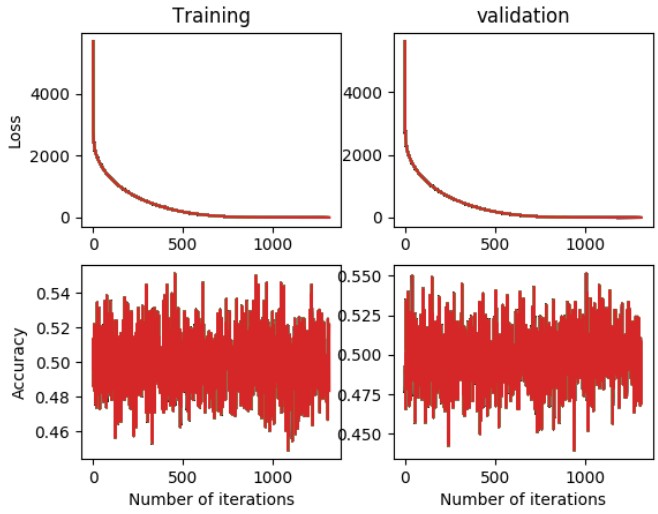


FIGURE 100. Version 10 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

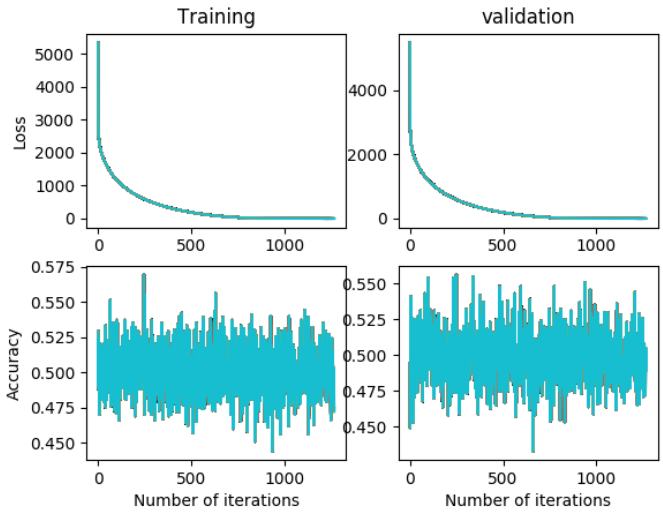


FIGURE 101. Version 11 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

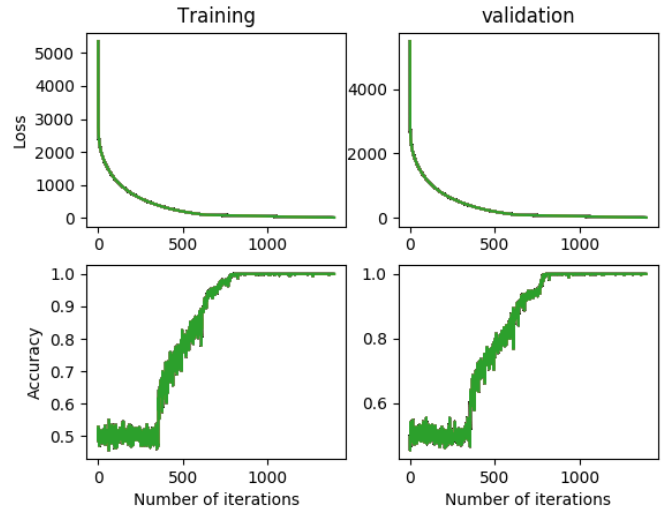


FIGURE 102. Version 12 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

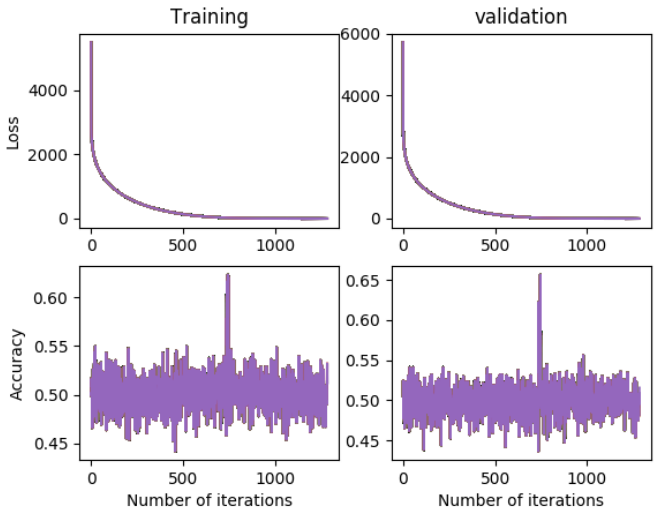


FIGURE 103. Version 13 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true

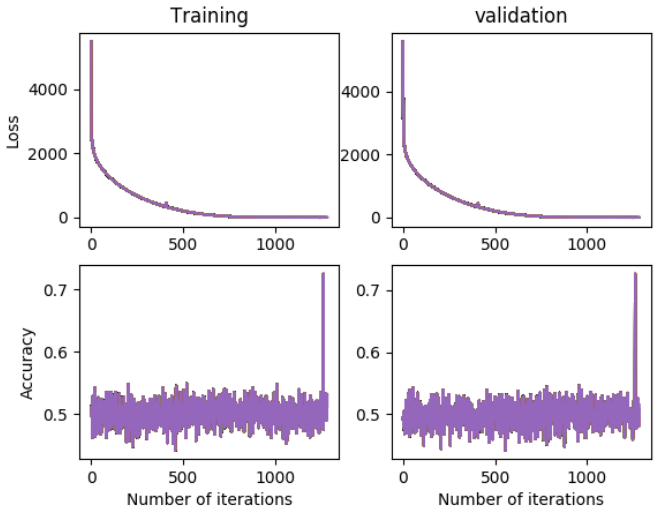


FIGURE 104. Version 14 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true

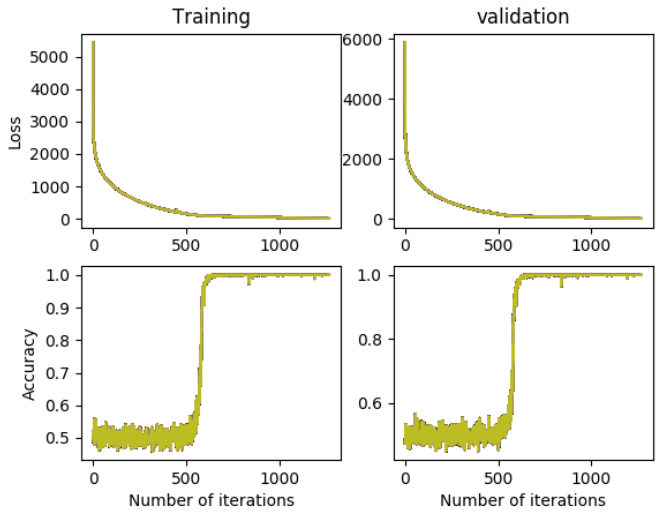


FIGURE 105. Version 15 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 150, L2 beta = 0.01, Dropout = 0.5, data aug = true

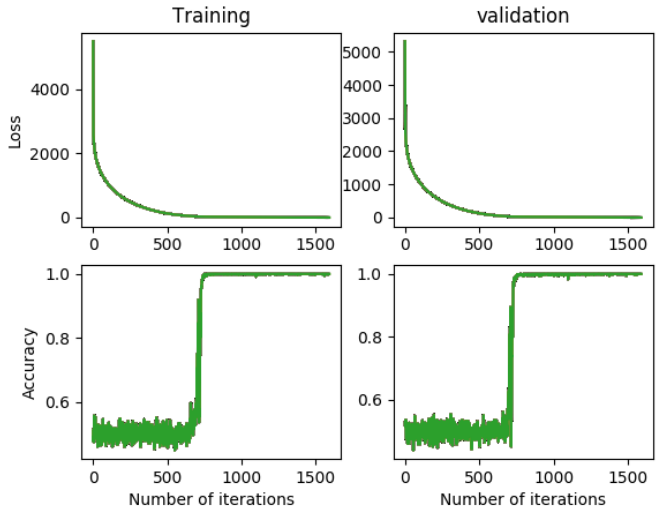


FIGURE 106. Version 16 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 150, L2 beta = 0.01, Dropout = 0.5, data aug = true

(2) Version 16 Step 1 best model had a final validation accuracy of 99.9% and a final test accuracy of 99.9333%.
(3) Now I am going to save this model, and delete the others.
(4) Moved the data_liquid15 file to the working directory. Deleting metadata and creating a new metadata for this dataset.

(5) V1-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(6) V2-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(7) V3-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(8) V4-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(9) V5-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(10) V6-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(11) V7-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(12) V8-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(13) V9-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(14) V10-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.

5.6. **1/23/2018.**

(1) Collected results from training runs on the data_liquid15 data. Here they are:

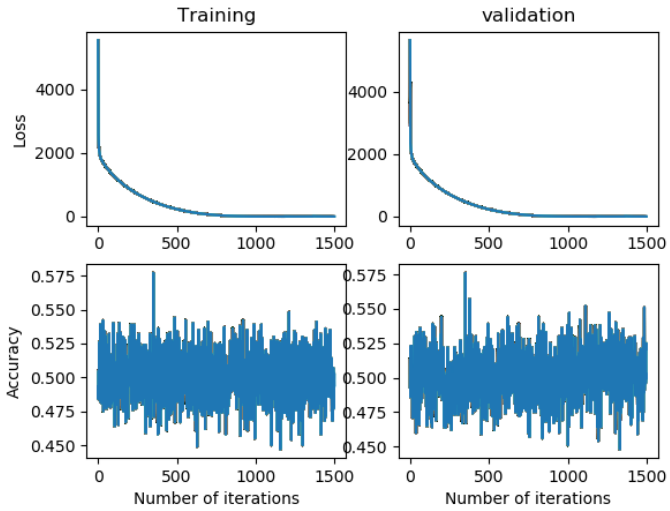


FIGURE 107. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

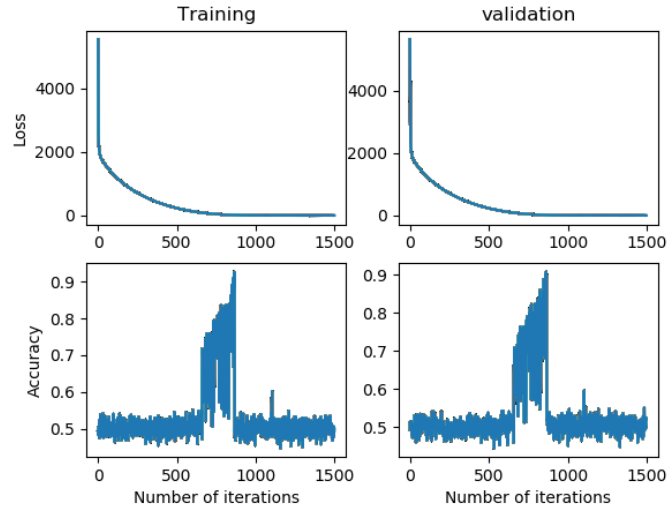


FIGURE 108. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

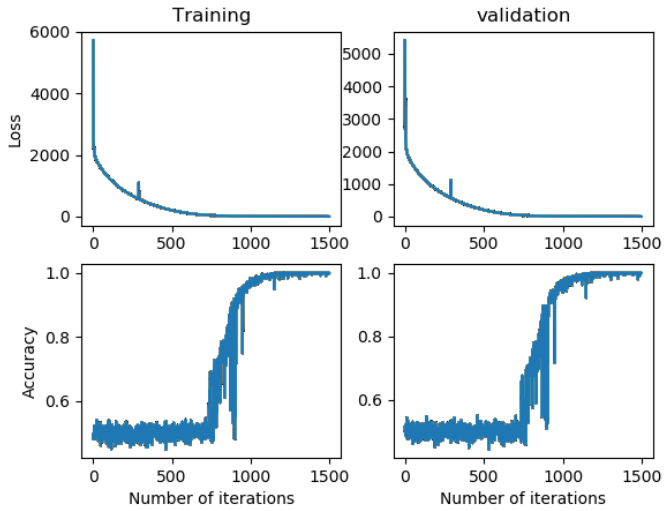


FIGURE 109. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

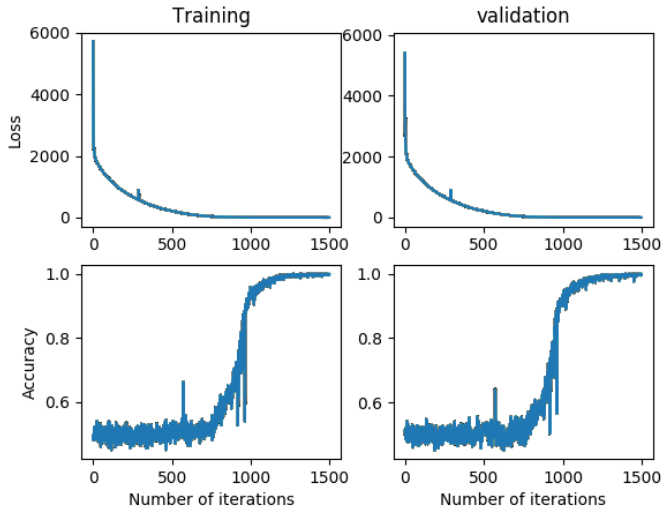


FIGURE 110. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

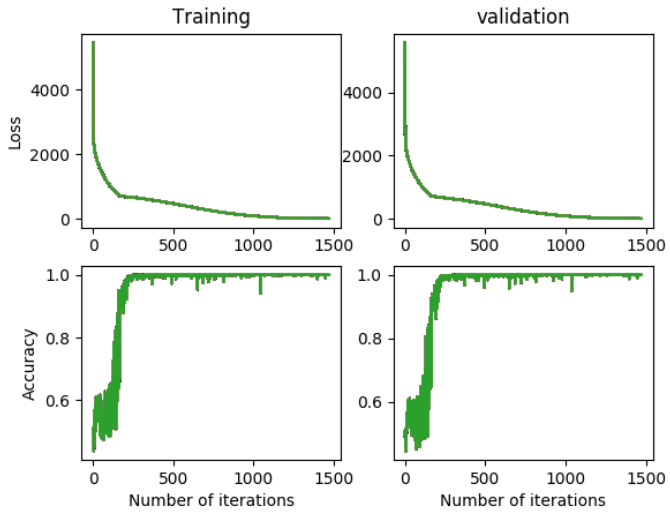


FIGURE 111. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

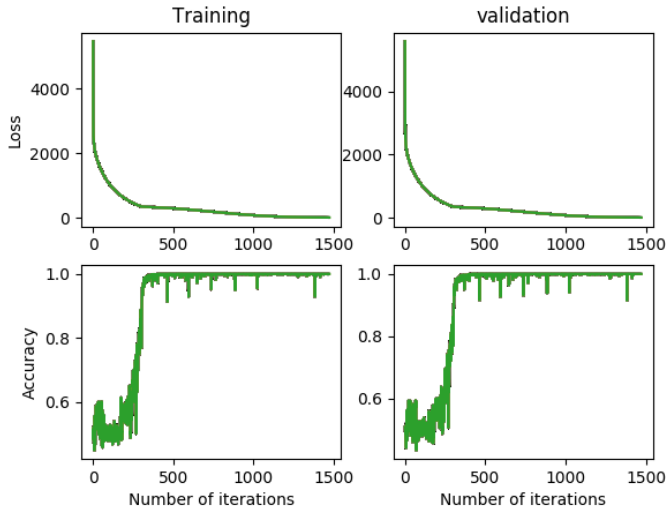


FIGURE 112. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

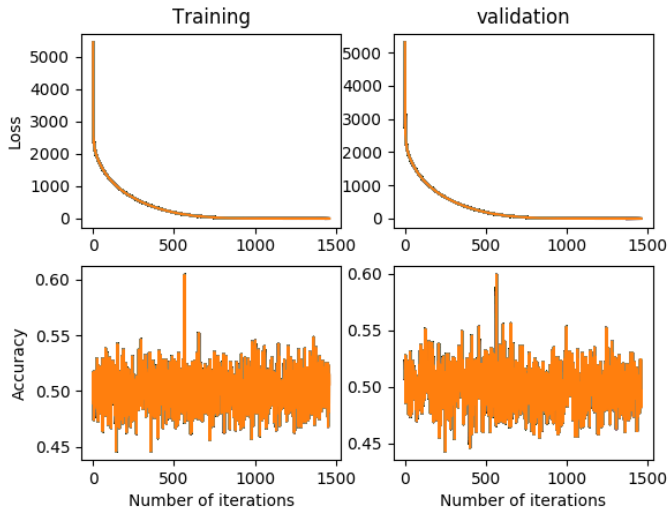


FIGURE 113. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

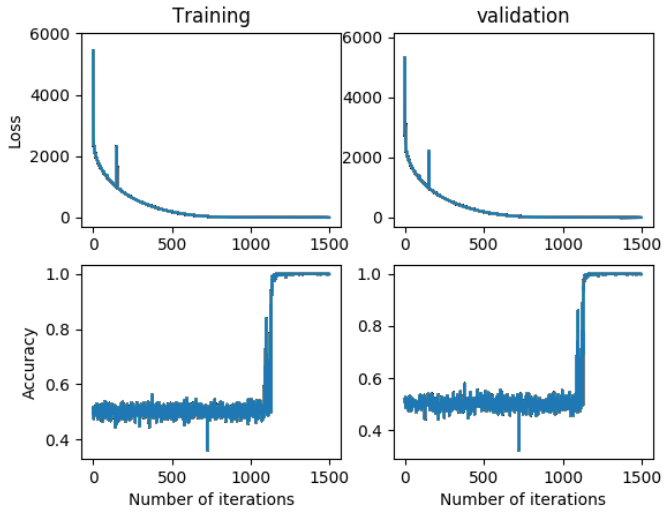


FIGURE 114. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

(2) Version 4 Step 1 had a best model final validation accuracy of 99.7667% and final test accuracy of 99.9333%.
(3) Saving this model, deleting others.
(4) Switching metadata to data_liquid25.
(5) Running same set of versions as before.

5.7. **2/2/2018.**

(1) Collected results from training runs on the data_liquid25 data. Here they are:

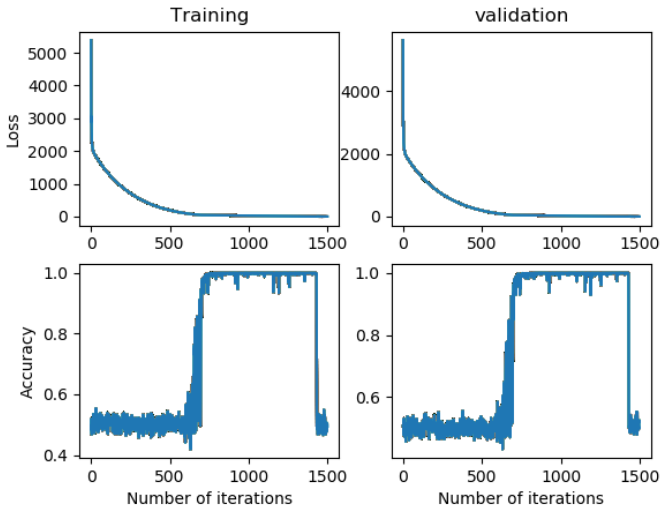


FIGURE 115. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

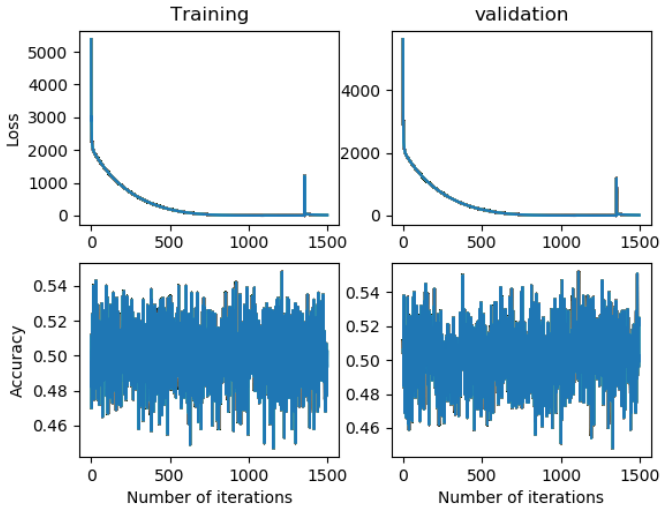


FIGURE 116. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

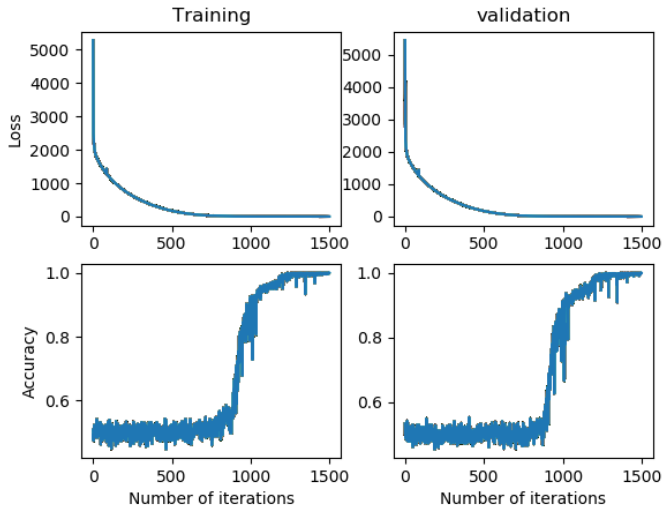


FIGURE 117. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

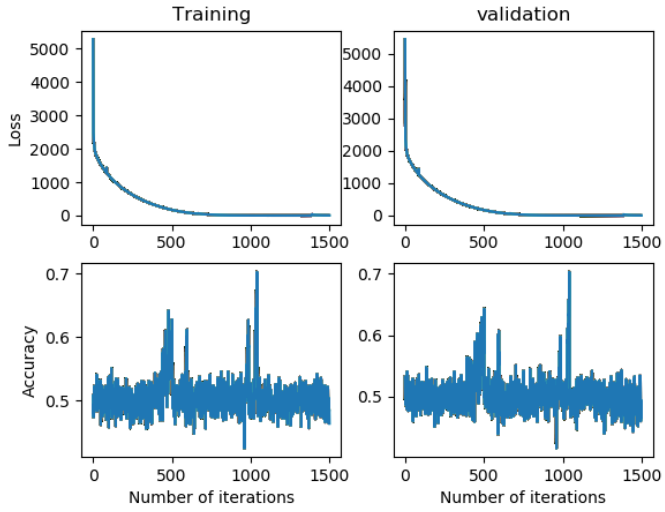


FIGURE 118. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

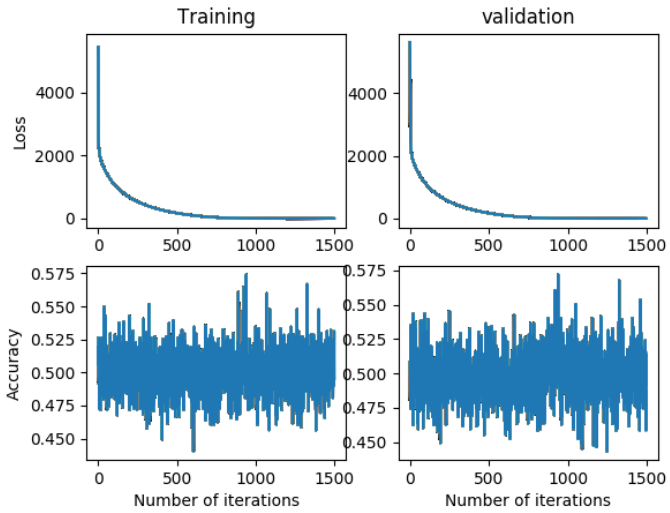


FIGURE 119. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

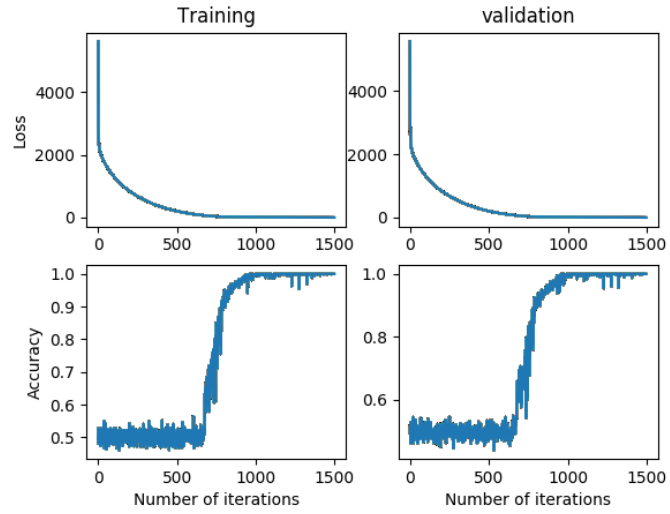


FIGURE 120. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

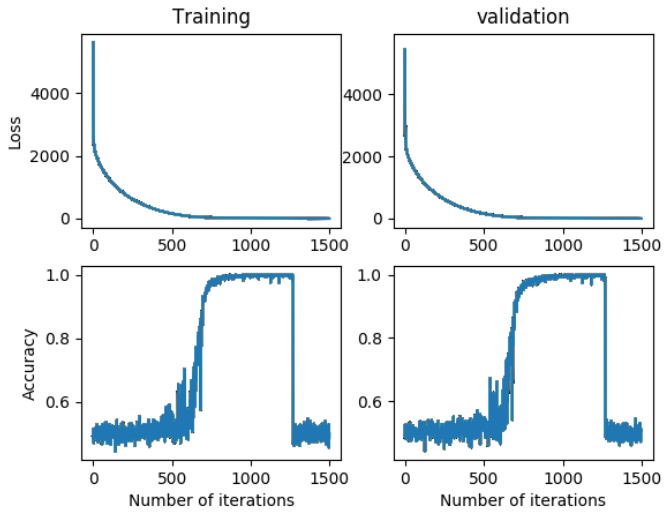


FIGURE 121. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

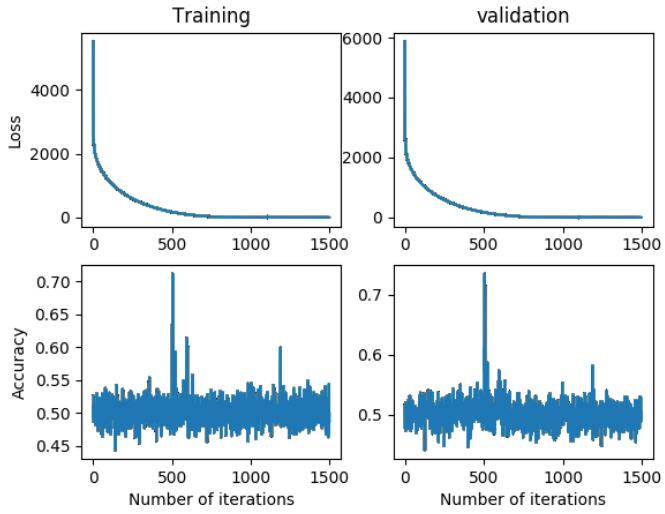


FIGURE 122. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

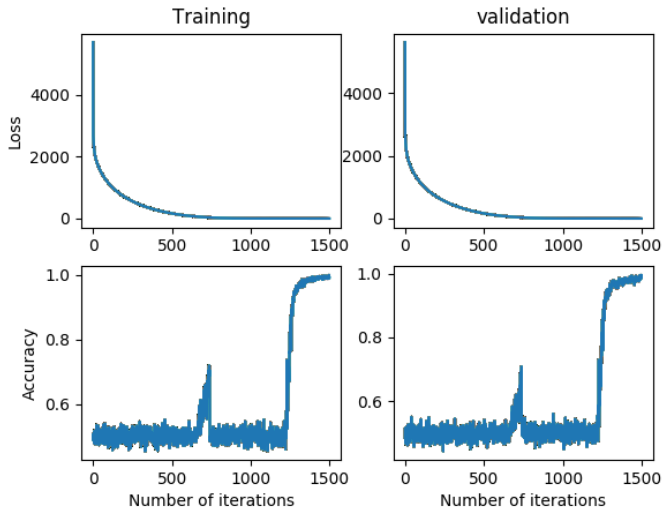


FIGURE 123. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

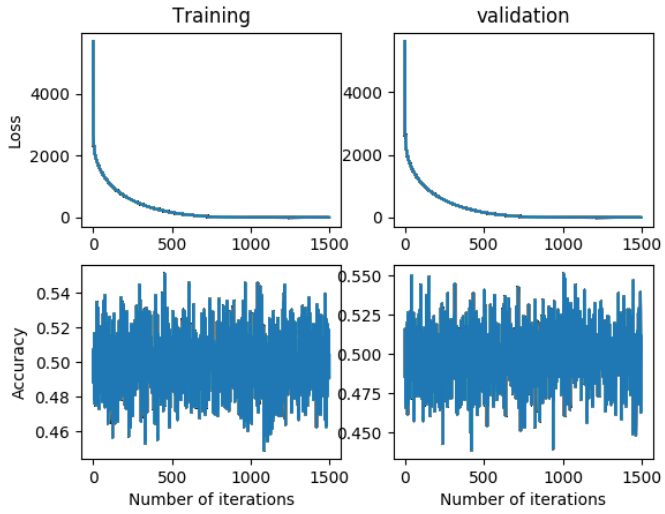


FIGURE 124. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

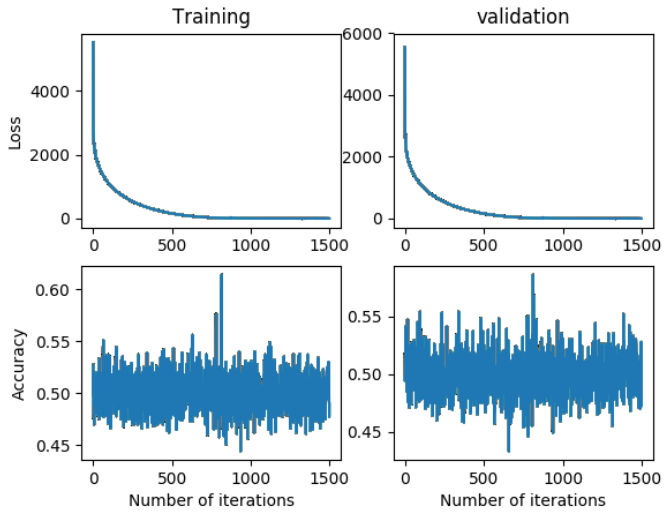


FIGURE 125. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

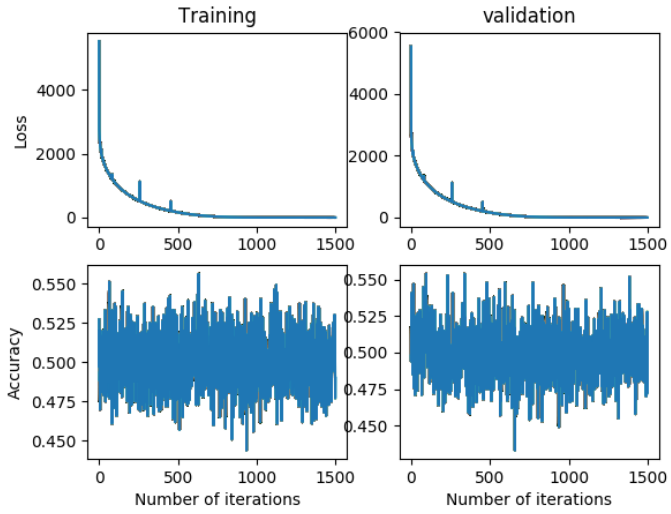


FIGURE 126. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

(2) Version 6 Step 1 has a final validation accuracy of 99.7% and test accuracy of 99.6667%.
(3) Saving Version 6 model.
(4) Just ran the saved data_liquid5_version7_step1_best_model.ckpt on the meta-data from data_liquid25. It had a final validation accuracy of 99.8557% and final test accuracy of 99.6333%. Wow! So how about for the time being, we

just keep running this model on closer and closer liquid data sets to see how well it does...
(5) Changing metadata to be from data_liquid35.
(6) Running the data_liquid5 model as above...this time gets 99.5667% validation and 99.7333% test.
(7) Creating data now for data_liquid45 and data_liquid60.
(8) Ok, now changed the metadata to be from data_12steps. This yields a validation accuracy of 48.2667% and test accuracy of 48.5%. Interesting...so where does it break down? Let's try to find this.
(9) Removing all other models.

5.8. **2/3/2018.**

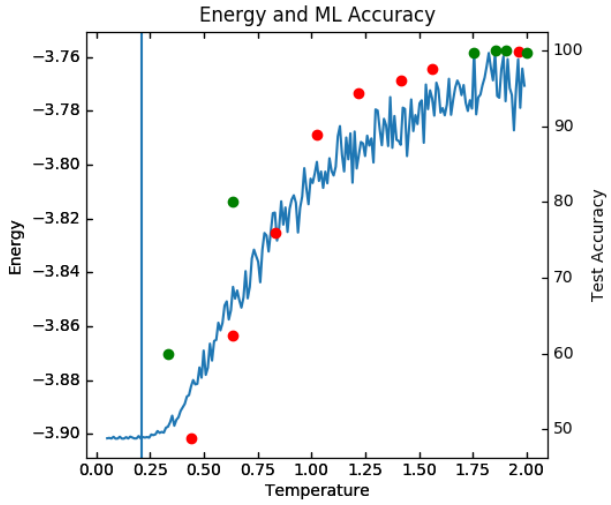
(1) Switching metadata to be from data_liquid45.
(2) Running data_liquid5_version7_step1_best_model.ckpt gives 96.4755% validation accuracy and 97.5466% test accuracy on data_liquid45.
(3) Switching to metadata data_liquid60.
(4) Running data_liquid5_version7_step1_best_model.ckpt gives 96.4446% validation accuracy and 96.0663% test accuracy on data_liquid60.
(5) Switching to metadata data_liquid80.
(6) Running data_liquid5_version7_step1_best_model.ckpt gives 92.8547% validation accuracy and 94.408% test accuracy on data_liquid80.
(7) Switching to metadata data_liquid100.
(8) Running data_liquid5_version7_step1_best_model.ckpt gives 90.0206% validation accuracy and 88.8201% test accuracy on data_liquid100.
(9) Switching to metadata data_liquid120.
(10) Running data_liquid5_version7_step1_best_model.ckpt gives 76.8569% validation accuracy and 75.9367% test accuracy on data_liquid120.
(11) Switching to metadata data_liquid140.
(12) Running data_liquid5_version7_step1_best_model.ckpt gives 60.5473% validation accuracy and 62.3961% test accuracy on data_liquid140.
(13) Switching to metadata data_liquid160.
(14) Running data_liquid5_version7_step1_best_model.ckpt gives 47.7124% validation accuracy and 48.7964% test accuracy on data_liquid160.
(15) Switching metadata to data_liquid140 and running training again, using the same stuff as before.

5.9. **2/19/2018.**

(1) New idea on MPNN. Modified Josh's code, "plot_config.py", and renamed it "coord_config.py". This new file eliminates the plotting function, and instead outputs a text file with the raw (x, y, z) atomic coordinates of a given configuration. Added this file to GitHub.
(2) Currently running the (x, y, z) coords program on Midway to generate these files for the endpoints of the simulation (i.e. at 20,000,000 and 100,000) for Shubhendu.

5.10. **2/22/2018.**

(1) Here is a plot showing progress to date:



(2) What I sent to Josh and Shubhendu in email: I have a few new results. Attached to this email is a plot I put together a few minutes ago. The blue curve is the value of the inherent structure energy as a function of temperature (values on left axis) taken from one example simulation. The vertical blue line is the assumed glass transition temperature for the 2D Kobb-Andersen glass, which is at 0.21 (from Dan's vapor-deposited paper). The dots show various machine learning accuracies I have achieved (values on the right axis). I'll explain the red dots first, then the green dots.

Red dots: I created a data set where the glass images were derived from timestep 20,000,000, or temperature = 0.05 and the liquid images were derived from timestep 500,000, or temperature = 1.95125. Temperature = 0.05 is the farthest we can go into the glass regime with our data. I then trained the CNN on this data set and achieved a test accuracy of 99.8%. I saved this model. Then, I used this model to predict whether images were glass or liquid on seven other data sets. Each of these data sets uses the SAME glass images, i.e. images from temperature = 0.05, but uses liquid images from temperatures that are increasingly close to the glass transition. The results are shown as red dots. So, the red dot at temperature = 0.635 and accuracy = 62.3961%, for example, means that this model achieves approximately 62.3961% accuracy when tested on liquid images derived from temperature = 0.635.

Green dots: These dots represent CNNs that have been trained exactly at that data point. So, the green dot at temperature = 0.33275, for example, represents the test accuracy of a CNN that has been trained on liquid images taken from that exact temperature, 0.33275, with glass images again taken from temperature = 0.05.

It looks nice, but what if we're just learning a much more complicated way of calculating the inherent structure energy?

(3) After speaking to Josh, these are the steps we decided that we need to take, using CNNs:
(4) Classify glass vs liquid:
    Improve model accuracy using data across the liquid regime
    Calculate T_g rigorously
    Calculate the potential energy instead of the inherent structure energy
    NEW classify between two liquids? (Added 3/6/2018)
(5) NEW idea: identify the phase transition temperature by stepping across into the glass regime until the classification accuracy gets really low. (Added 3/8/2018)
    Generate supercooled liquid data at the same energy as the glass
    Generate artificial 5-fold patterns
    Generate 3D data for classification
(6) Classify liquid-cooled versus vapor-deposited glasses:
    Generate data
(7) Other tasks?
    Classify low density vs high density water
(8) We also have an answer as to why the CNN learning to classify liquid versus glass, irrespective of what it is learning (i.e. potential energy, inherent energy, geometry, or anything else). From the viewpoint of the CNN, we know nothing about the material that is being given to the CNN other than the geometric configuration of particles. We don't know whether interactions are pairwise or more complicated, we don't know how the material operates, other than that we have been able to train the CNN on labelled materials, where the labelling could be based on some macroscopic rather than microscopic property. And yet, the CNN is still able to take just this raw structure information, no dynamics, and still tell the difference between a glass and a liquid. So it is able to classify these materials with high accuracy based on nothing but structural atomic configurations. This is interesting.
(9) So, based on these above steps, I will first start by running more training to improve green dot accuracy.

5.11. **2/27/2018.**

(1) Logging results now that should have been logged a while ago. This is the training results for data_liquid140.

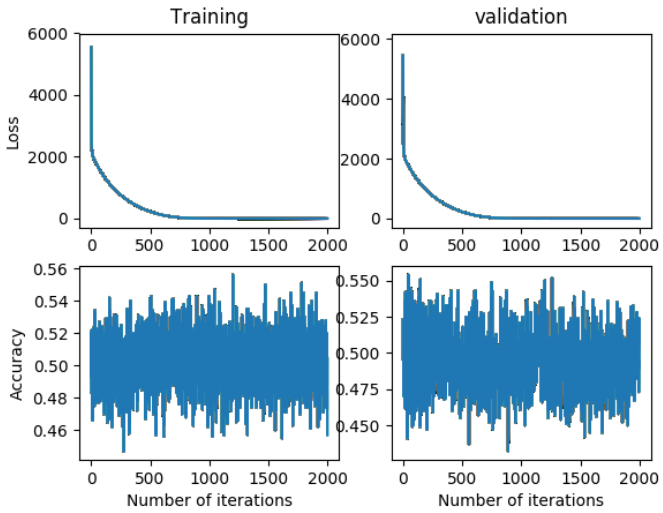


FIGURE 127. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

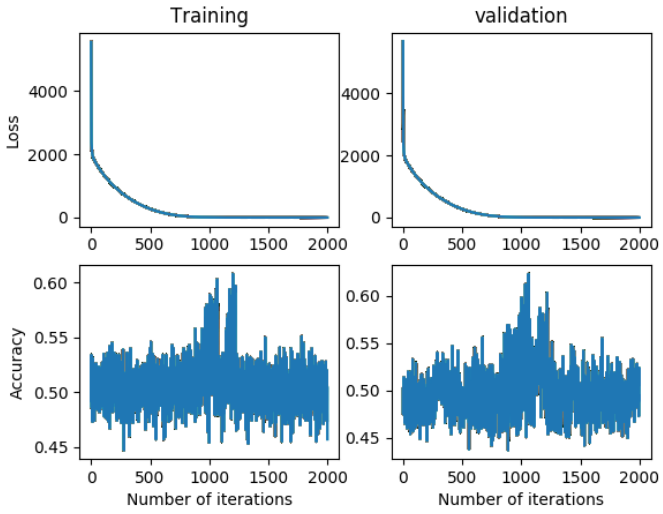


FIGURE 128. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

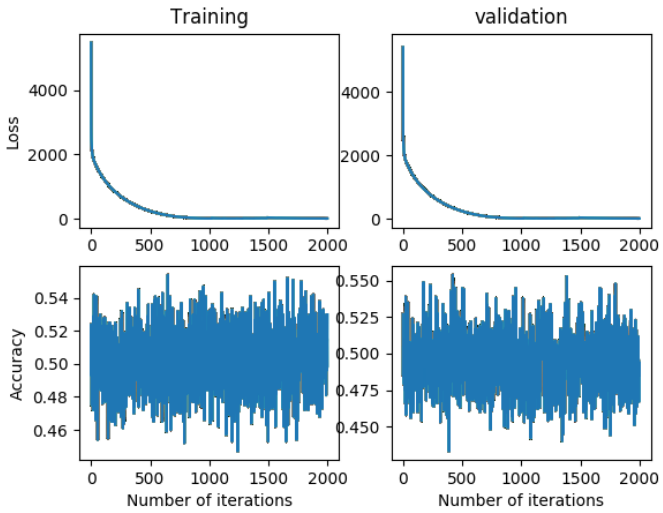


FIGURE 129. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

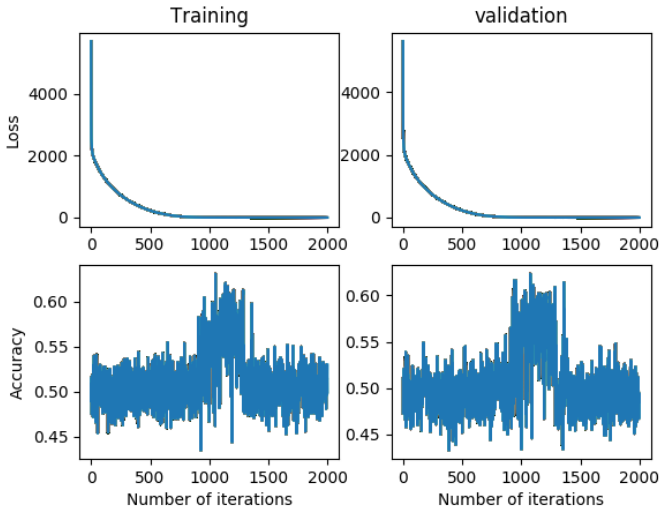


FIGURE 130. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

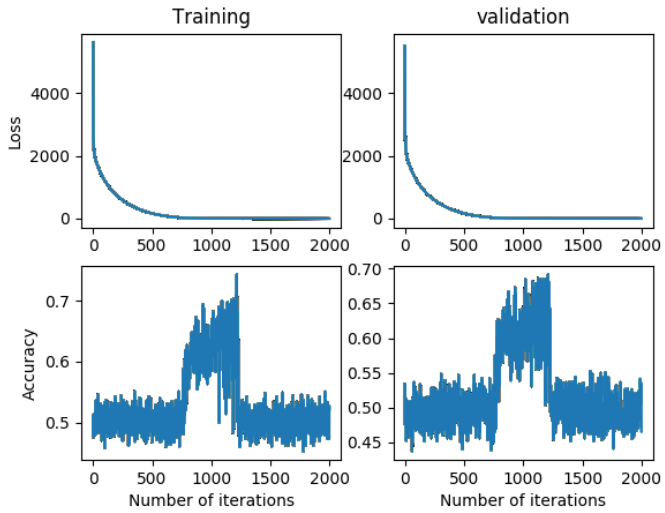


FIGURE 131. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

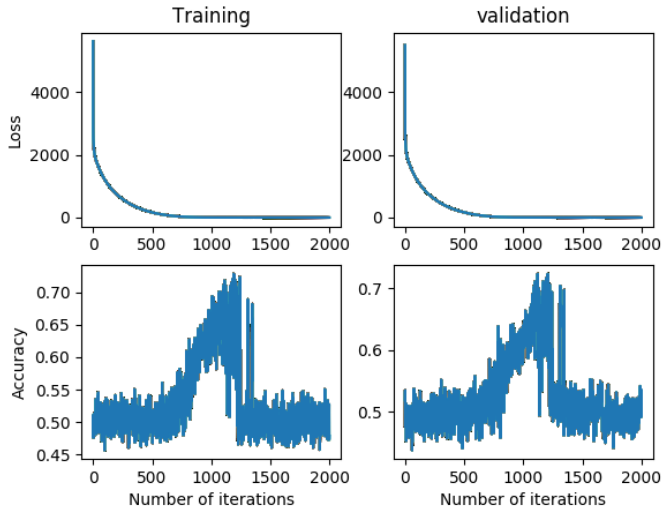


FIGURE 132. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

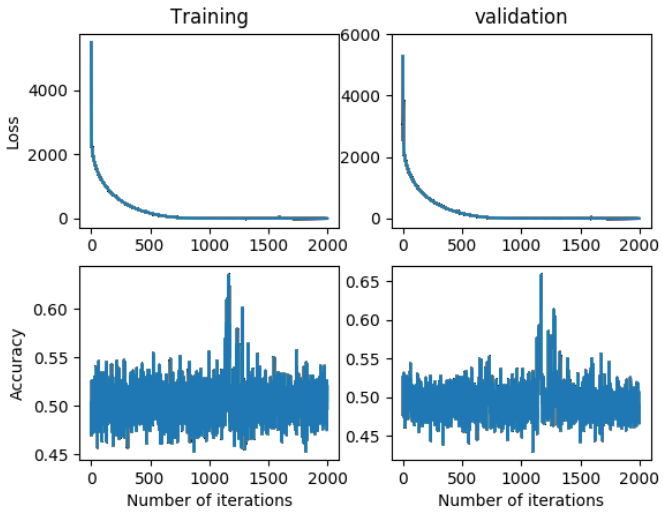


FIGURE 133. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

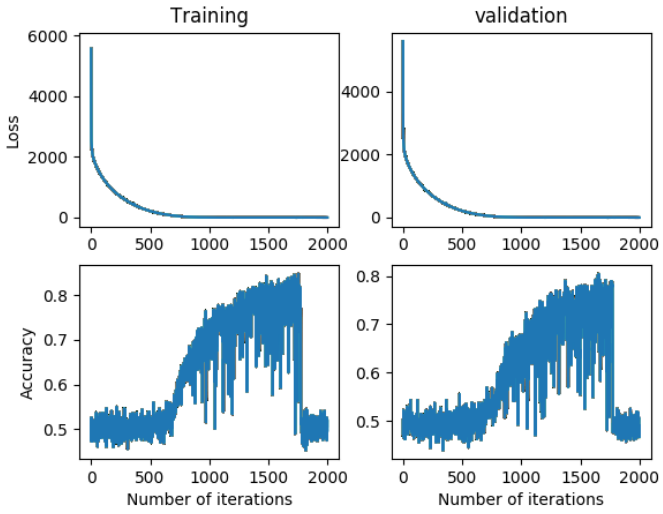


FIGURE 134. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

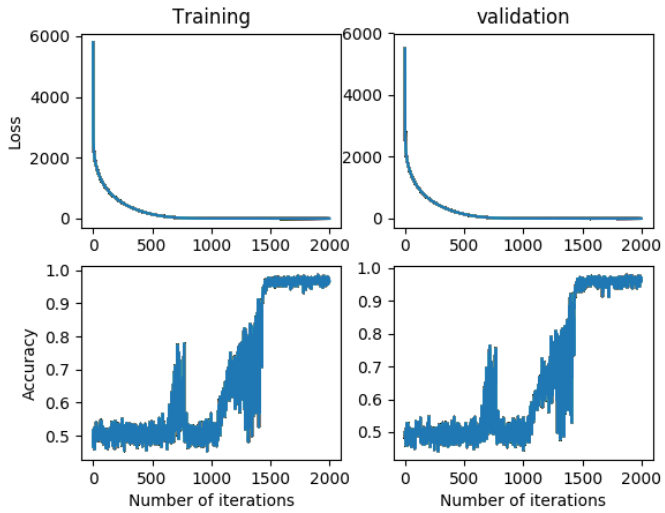


FIGURE 135. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

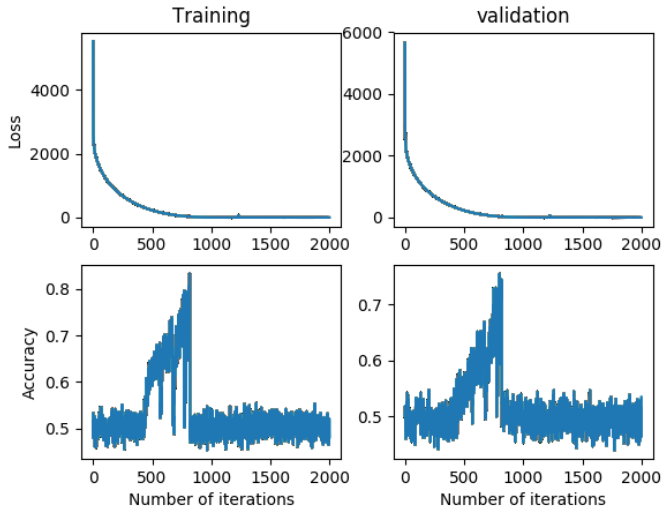


FIGURE 136. Version 10 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

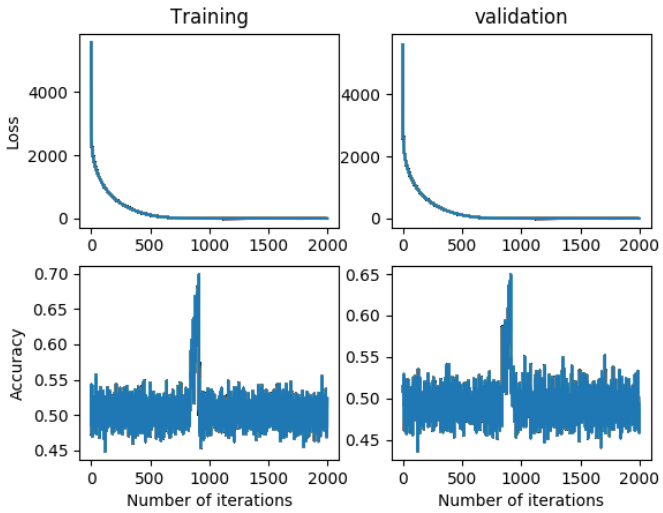


FIGURE 137. Version 11 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

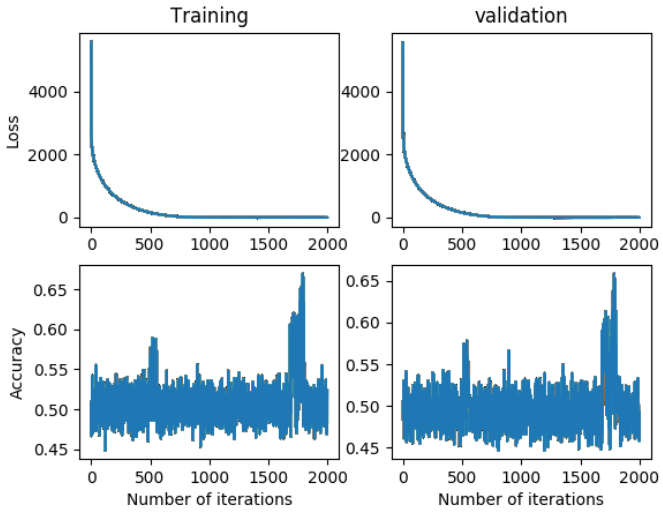


FIGURE 138. Version 12 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

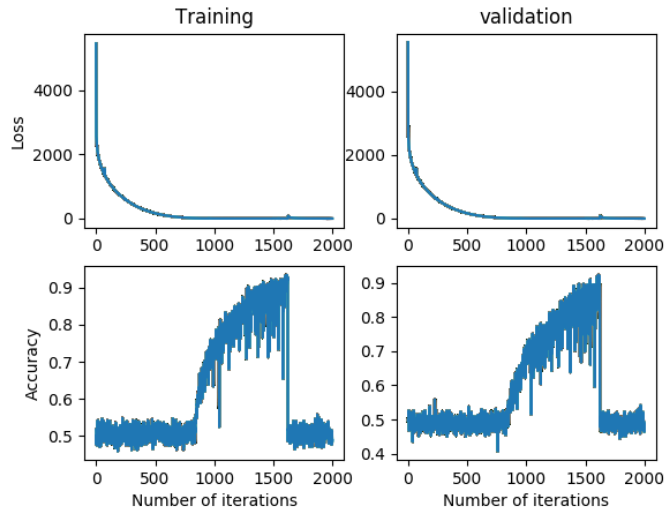


FIGURE 139. Version 13 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true

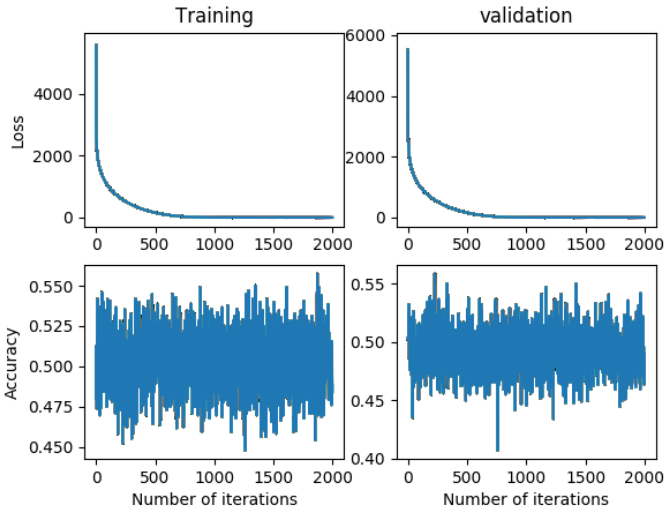


FIGURE 140. Version 14 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 130, L2 beta = 0.01, Dropout = 0.5, data aug = true

(2) Version 9 Step 1 has a final validation accuracy of 96.2847% and test accuracy of 96.3194%.
(3) Saving Version 9 Step 1 model. Deleting other information.
(4) Now I want to find the true average glass transition temperature for the simulation data that we have. What I will do is construct an average cooling.dat plot, i.e. a plot that averges the data from all 10,000 cooling.dat files that we have.

Then, I will estimate by eye (or using some slightly more quantitative method for sake of argument) what the true average glass transition temperature is. We anticipate that it is higher than 0.21.

5.12. **3/6/2018.**

(1) Wrote a program called plot_average_cooling data, which I moved to the 2017/N2e7 directory. It collects the data from all 10,000 cooling.dat files and averages them across each temperature, so that we obtain an average cooling curve that is representative of the simulations:

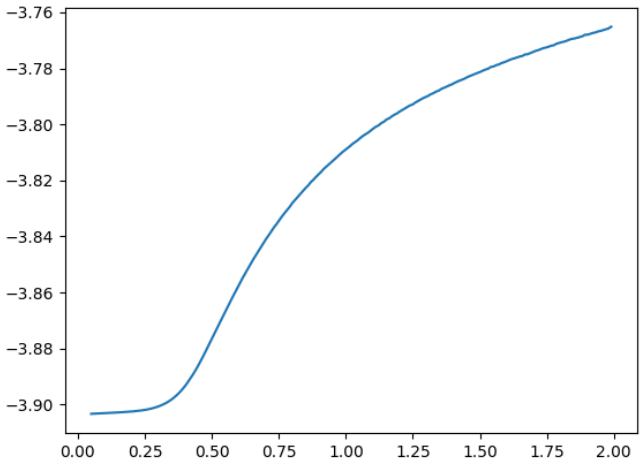


FIGURE 141. Averaged cooling.dat data

(2) Estimated the kink in inherent structure energy by finding the intersection of two lines, using points (0.05, -3.9033) and (0.245, -3.902) for the glass data and points (0.44, -3.8876) and (0.557, -3.8654) for the liquid regime. The result is a glass transition at around 0.37. Removing the data_12steps result, as this is actually stepping over the new glass transition, here is a new plot of our results:

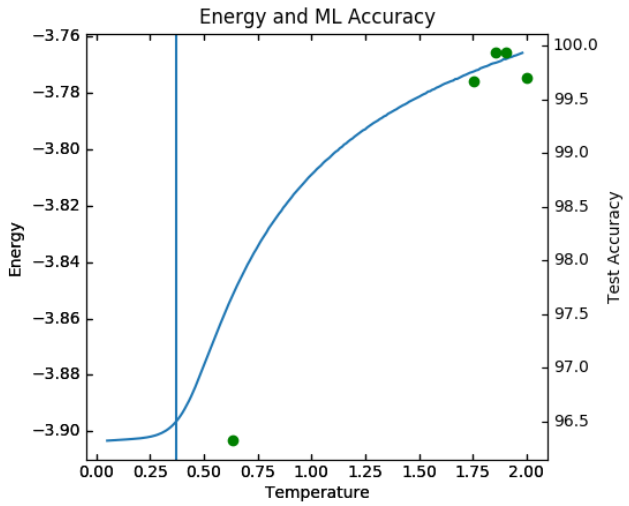


FIGURE 142. Updated results plot

(3) Switching to data from data_liquid155, which corresponds to T = 0.479.
(4) Now running the same versions as before.
(5) PROBLEM: How is this any different from distinguishing between two liquids at different energies/temperatures? SO we should try to classify between two liquids!!! Added to the to do list above.

5.13. **3/7/2018.**

(1) Read sections of papers (now on Box) on MPNN, meeting with Shubhendu tomorrow.
(2) Still running training on 155.
(3) Looked into simulating new liquids that will be at the same inherent structure energy as the glass, but ran into issues with the batch scripts as written - emailed Josh for assistance.

5.14. **3/8/2017.**

(1) New idea: identify the phase transition temperature by stepping across into the glass regime until the classification accuracy gets really low.
(2) Reading https://arxiv.org/pdf/1802.09876.pdf. Suggests that networks with one layer are not only sufficient, but more interpretable.
(3) Analysis of activation of neurons. Previously, for Ising model, only 1 layer with 3 neurons needed. Plotting weight matrices of each neuron. Look at activations as a function of five-fold symmetry??

5.15. **3/9/2018.**

(1) We will be implementing MPNN using: https://github.com/priba/nmp_qc
(2) First instruction is to install requirements using pip install -r requirements.txt
(3) On Midway 2, /home/swansonk1 directory, error in installing torch: "PyTorch does not currently provide packages for PyPI"

(4) For the time being, I will try this on my laptop instead. Actually, my desktop, which has cuda installed.
(5) Again, pip install -r requirements.txt failed, so for torch, i.e. PyTorch, I used the command conda install pytorch torchvision -c pytorch from pytorch.org.
(6) Successfully installed all packages in the requirements.txt file.
(7) Downloaded the qm9 dataset.
(8) Following Sec. 6 on https://arxiv.org/pdf/1704.01212.pdf, the input feature for our particles will be a one-hot encoding of either particle A or particle B. The adjacency matrix will be a raw distance feature matrix, where the entries are one-dimensional and indicate the euclidean distance between the pair of atoms.
(9) Tried running python main.py, but saying no module rdkit.
(10) So, went to http://www.rdkit.org/docs/Install.html and conda installed. Now I can create an environment as described. However, torch no longer works inside the environment. Need to investigate how environments work, then.
(11) Opened the rdkit environment. Then re-installed PyTorch as above.
(12) No module named networkx. So, pip install networkx within the rdkit environment. Same thing for joblib and tensorboard_logger.
(13) Tried running main.py. Got error, 'Graph' method has no attribute 'nodes_iter'. Found this solution: https://stackoverflow.com/questions/33734836/graph-object-has-no-attribute-nodes-iter-in-networkx-module-python. Trying it now by replacing with nodes() in datasets/utils.py, specifically on line 28 in the qm9_nodes function.
(14) Also removing edges_iter on line 54. Issue seems to be that the new version of networkx has mismatches.
(15) Having some more issues with GPU compatibility. PyTorch says my GPU is too old. Also, there are more inscruitable errors. So, I am going to uninstall networkx and install the version that should be compatible with this model, networkx version1.11. Used pip install networkx==1.11.
(16) New error with .expand in line 174 of m_mpnn. Stack suggests that this has to do with bug in new version of PyTorch: https://github.com/pytorch/pytorch/issues/2491. So, like networkx, I am going to find the versin of PyTorch that was latest when the last commit for this program was made.
(17) Found that the most recent version of PyTorch prior to the last commit on MPNN May 29, 2017, was the version v0.1.12: https://github.com/pytorch/pytorch/releases, on May 2, 2017. So, I am installing this version using conda install pytorch=0.1.12 -c soumith. This lets me download without cuda: http://pytorch.org/previous-versions/. Hopefully this will get rid of the GPU problem? If not, we'll turn to Midway.
(18) Ok, this works! I was just able to run, in the demos folder, demo_qm9_mpnn.py. Now, I am going to go through this and try to understand what's going on. If necessary, I will add comments to this code file.
(19) The data is transformed into special data objects via the Qm9 class in the datasets folder. Each object of this class has four main attributes: the graph, the nodes, the edges, and the targets. The graph is the adjacency matrix that describes connections between atoms in the molecule. It is real symmetric and is a numpy matrix. The nodes are given as a list of features for each particle. The edges

are described by a dictionary, where (1, 2): [distance, one-hot enconding of bonding] is the format. Finally, the target properties are given as a list as well.

(20) We would probably choose our adjacency graph to take into account only a certain number of nearest neighbors as "bonded." Then, we would just need to make sure that the graph is **connected**. That is the only requirement of the scheme, which can then later be optimized.

5.16. **3/13/2018.**

(1) Modified the coords_config.py file so that it outputs atom type, x-coordinate, and y-coordinate insetad of x, y, z.
(2) Produced a sample file from the file N2e7/0 at time 100,000
(3) Wrote a script adjacency_matrix.py to compute the adjacency graph and relevant information for MPNN input. It works generally, but the loops appear to be inefficient. Next time, I will have to look into using matrices, as well as ensuring that the matrix is **connected**.

5.17. **3/14/2018.**

(1) Added some funcionality to adjacency_matrix. Found functions that could be used for matrix manipulations, namely euclidean_distances from sklearn and arr.argsort() for numpy arrays. Also found that you can load txt into numpy array using np.loadtxt().

5.18. **3/15/2018.**

(1) Created graph_reader.py, which returns grpah information from an input glass/liquid data file in less than 7 seconds. Used matrix operations rather than only loops to increase computational efficiency.
(2) Tomorrow, I need to go to RCC to check how to make the MPNN code work on Midway, and I also need to implement a check for connected graphs.
(3) Downloading results from data_liquid155.

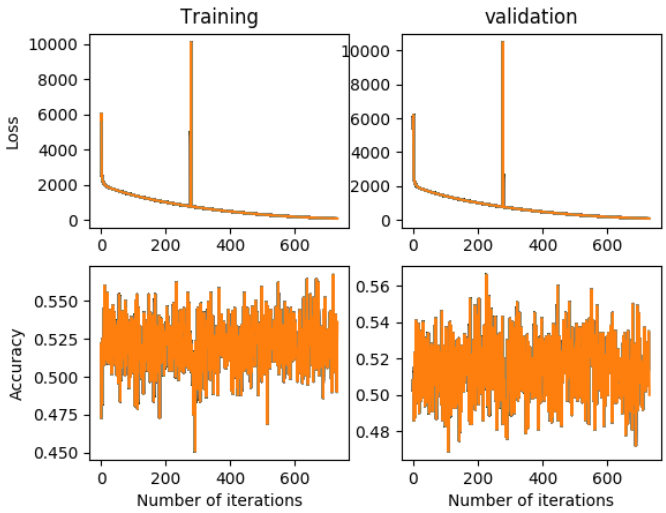


FIGURE 143. Version 1 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

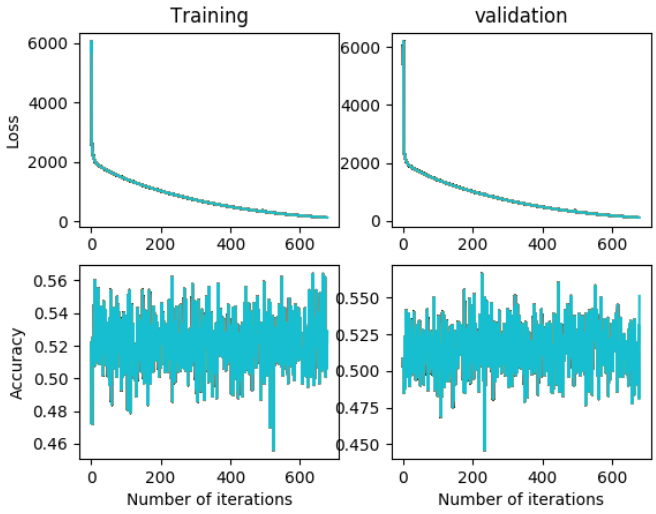


FIGURE 144. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

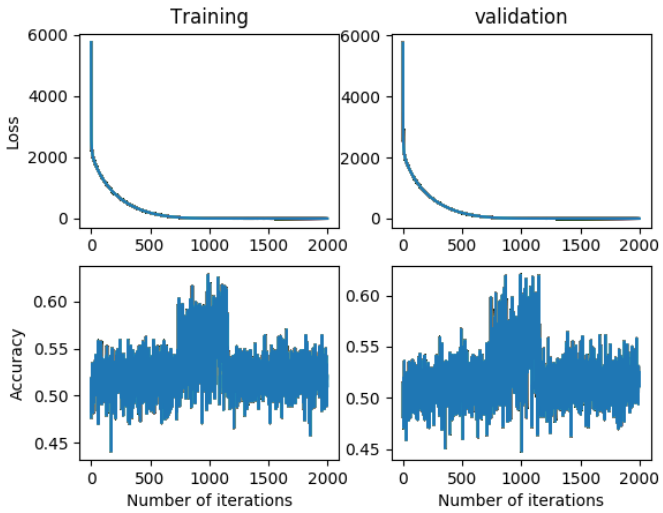


FIGURE 145. Version 3 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

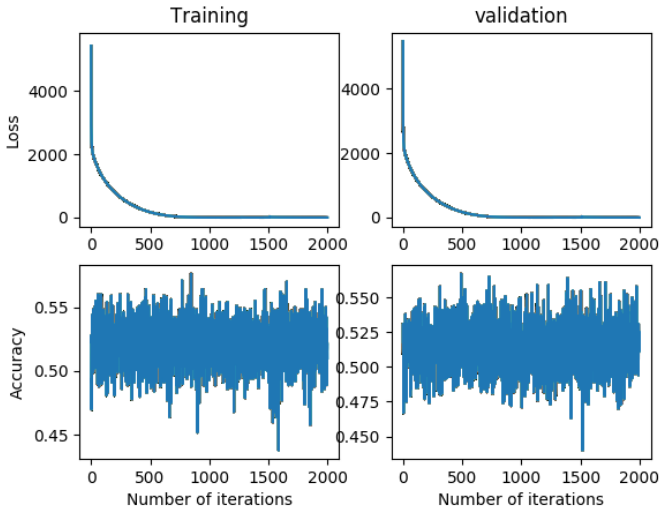


FIGURE 146. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

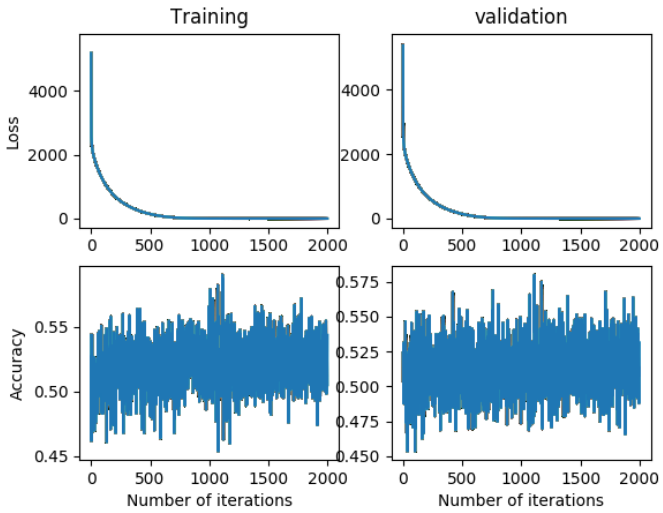


FIGURE 147. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

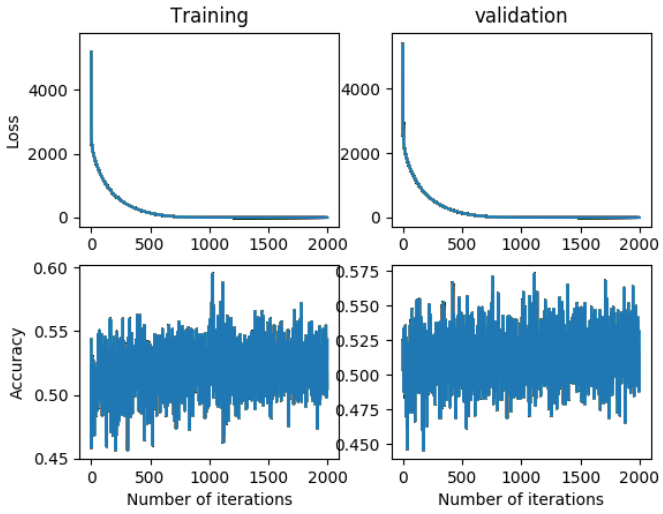


FIGURE 148. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

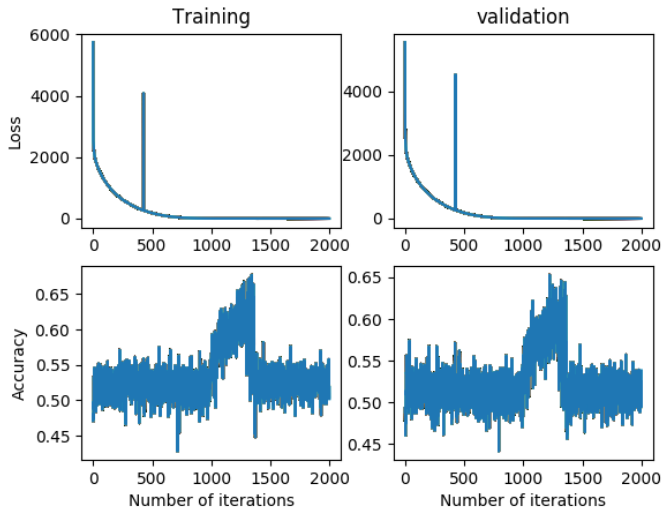


FIGURE 149. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

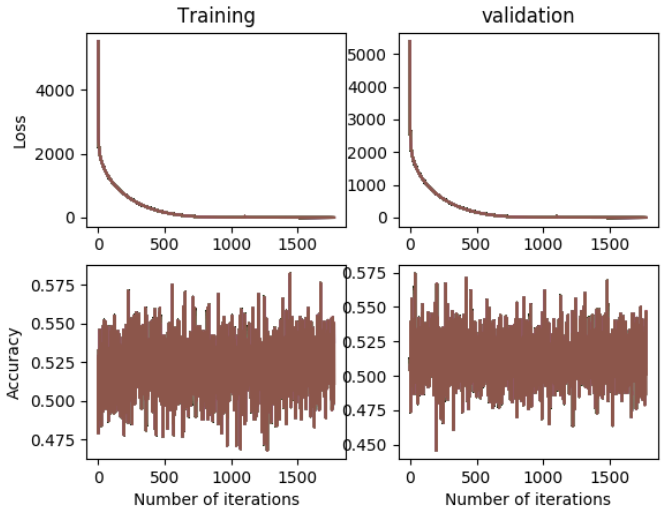


FIGURE 150. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

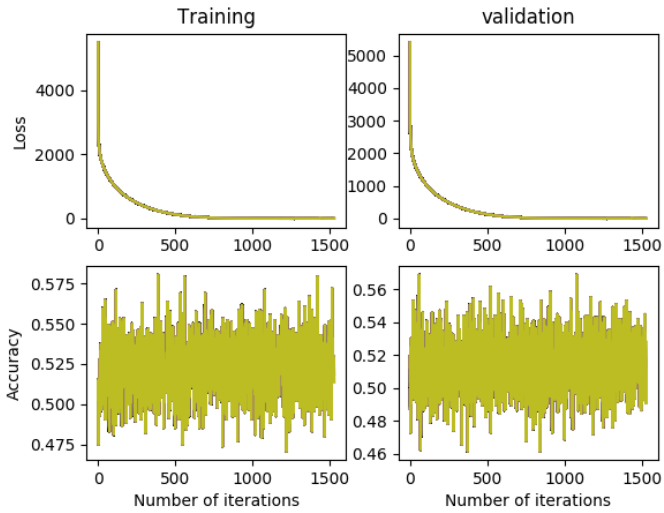


FIGURE 151. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

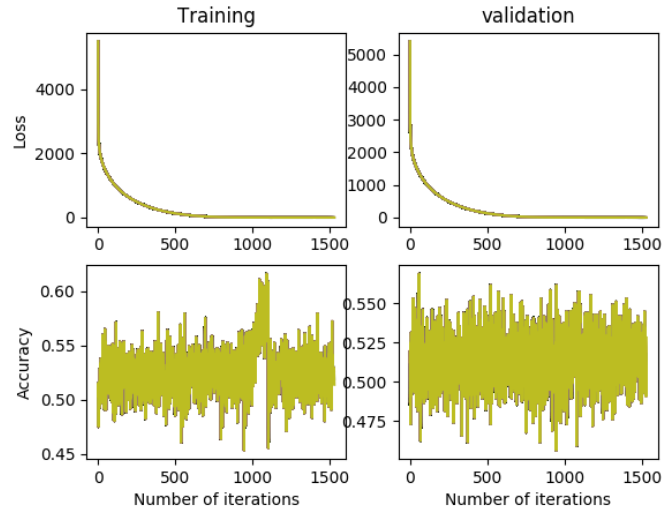


FIGURE 152. Version 10 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

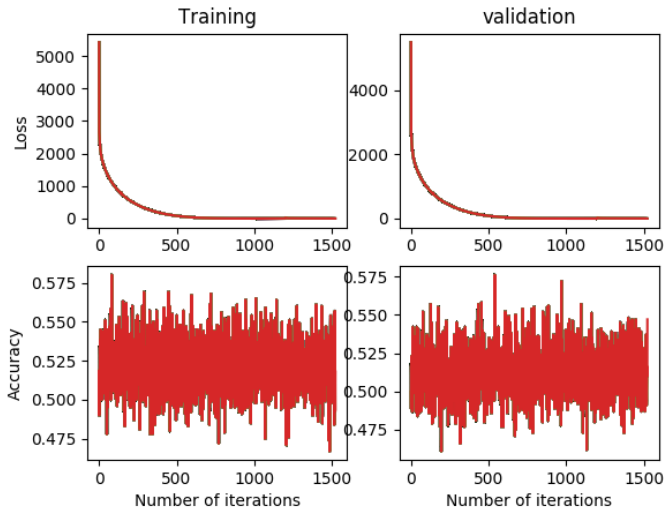


FIGURE 153. Version 11 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

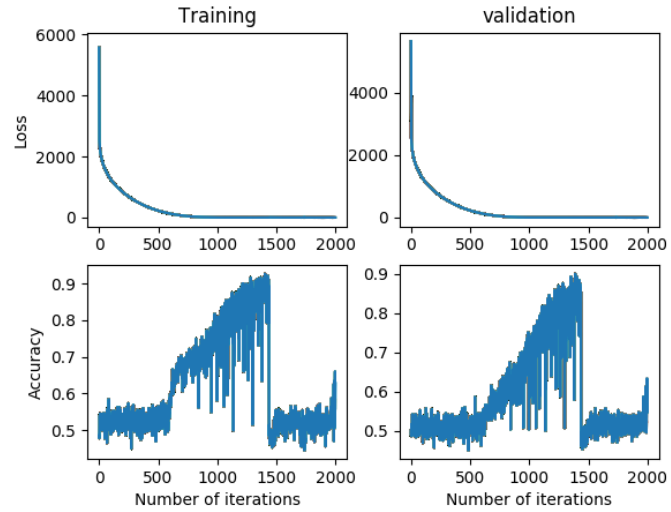
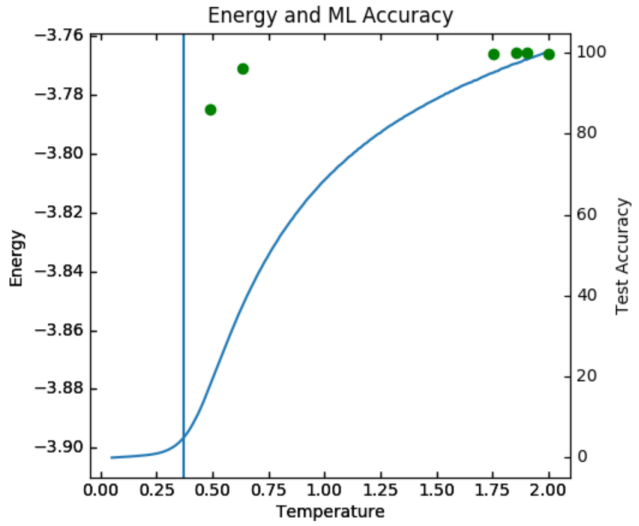


FIGURE 154. Version 12 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

(4) Version 12 Step 1 has a final validation accuracy of 86.9408% and test accuracy of 86.1111%. These could have probably been improved using a lower learning rate threshold.
(5) Saving Version 12 Step 1 model. Deleting other information.
(6) Updated accuracies:



5.19. **3/21/2018.**

(1) The functions that manipulate graph data in demo_qm9_mpnn.py, which is the demo I am currently working off of, use classes and objects. So, I wrote graph_reader_class.py based on graph_reader.py, which defines a GlassyData class that can be used to construct the graph information (adjacency matrix etc.) for a text file with glass/liquid coordinate information.
(2) I saved this file on the workstation in the nmp_qc folder. I then added a line in demo_qm9_mpnn.py that says from graph_reader_class import GlassyData.
(3) I saved a single file example in a folder called glass, within the data folder, whose filename is glass.00000.txt.
(4) I then used train_ids = [files[i] for i in idx] and data_train = GlassyData(root, train_ids, 7) to try printing data_train[0][0][0] etc..
(5) In order for this to work, I had to pip install sklearn within the rdkit environment.
(6) Then, it worked!
(7) Next, I need to move the data to the local machine, then write a demo script that is strictly for glass/liquid data.

5.20. **3/26/2018.**

(1) Added "len" attribute to graph_reader_class.py. Moved all data to local workstation, and wrote demo script that is strictly for glass/liquid data.
(2) No issues yet on local machine.

5.21. **3/27/2018.**

(1) Added more functionality to demo_glasses_mpnn. Need to reduce dataset size to 500 in each class and move this crap to Midway so we can get better computing power/GPUs!

5.22. **3/28/2018.**

(1) Installed pytorch version 0.1.12 onto Midway 2 home directory. Found in the data file, data_coords_endpoints that there is an empty file called "loading".

(2) Copied data_coords_endpoints to home, removed "loading" file, and truncated it so that there are 600 glass files and 600 liquid files.
(3) There appears to be an accuracy function in datasets/utils.py
(4) module load Anaconda3, then source activate my-rdkit-env
(5) Went into project directory. Did the usual rdkit command. Then, removed networkx from its location based on teh error message that was being given. Then pip installed using –user flag networx version 1.11 as well as joblib and tensorboard_logger. Also downloaded appropriate version of PyTorch as usual. Seems to work.
(6) Had to pip install sklearn –user in /project/depablo/kswanson
(7) At last, it appears to be working!
(8) Problem on workstation: once I add the line, output = model(g, h, e), the process gets killed. So, perhaps I've reached the limit for what my local workstation can do?
(9) Turning to Midway, here are the following outcomes: if I go onto depablo-gpu, then within the train function, I get an error that starts like THCudaCheck FAIL file=/py/conda-bld/pytorch_1493672080115/work/torch/lib/THC/THCCachingHostAllocator.cpp line 258 error=11 : invalid
(10) When I try to run on the log-in node, I get AssertionError: Found no NVIDIA driver on your system. Please check that you have an NVIDIA GPU and installed a driver from http://www.nvidia.com/Download/index.aspx.
(11) I am hoping that if I can find the appropriate way to use torch/PyTorch on Midway, then I will be able to solve this. So, I need to go to RCC next time I work on this to resolve this problem.
(12) ALSO, next time, I OUGHT TO WORK ON MAKING NEW LIQUID SIMULATIONS!!

5.23. **3/30/2018.**

(1) Finally fixed the issue with new liquid simulations. Can't start seq 0 10, must start seq 1 10, because otherwise the program just sleeps. So, I am now running a cooling rate of N2e6, 10 examples. Once they are done, I will look at their average cooling inherent structure energy and determine if I have achieved a lower transition temperature, etc., from which I can determine exactly what data I want to generate and collect.

6. 4/2/2018

(1) Spoke to Igor at RCC, PyTorch not available on Midway. Sent him an email to work on it.

7. 4/3/2018

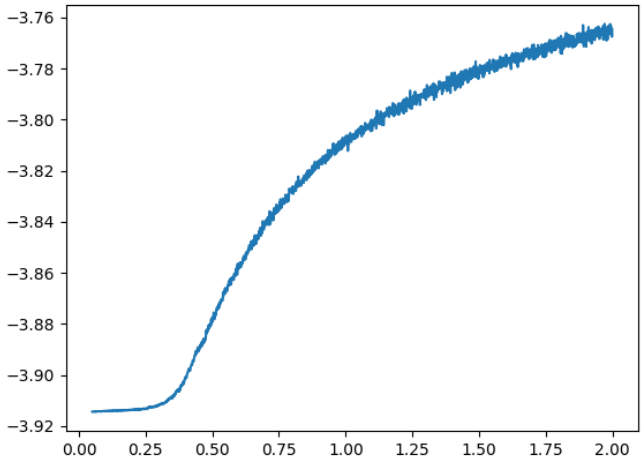
(1) A decrease of the cooling rate leads to a decrease of the glass transition T_g. Josh says 2e8 corresponds to a lower cooling rate, 2e6 to a higher one. So, 2e8 must be related to the number of timesteps necessary to get to T = 0.05, hence more steps, lower rate. So, I am now running 20 examples each of rate 2e8,

2e9, and 2e10 to check whether this measurably changes the cooling rate to be below the glass transition.

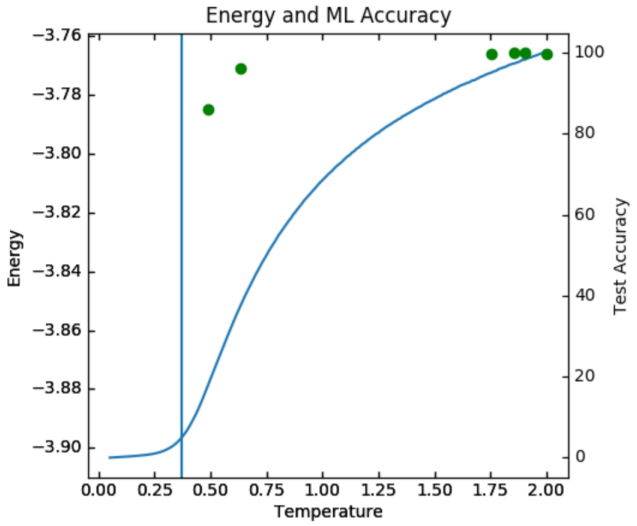
(2) Now I'm going back to MPNN to see if I can get this to work on Midway.
(3) In an email, Igor from RCC says: try sinteractive -p gpu2 –gres=gpu:1, module load cuda/8.0, module load Anaconda/5.0.1, check "which python" and it should show /software/Anaconda3-5.0.1-e17-x86_64/bin/python. If not, module purge, repeat second two steps.
(4) Logged on. Ran demo_glass_mpnn.py, and it gets inside the train function, prints one or two things, then screen connection is terminated.
(5) I am going to test this with the qm9 dataset, just to see if it can do normal training not on my glass/liquid shit. So, let's try that.

8. 4/9/2018

(1) The N2e8 data finished running. It computed 20 examples, and using the average cooling data python script, I computed the average cooling curve of these 20 simulations:



Compared to the N2e7 cooling curve,



this curve does not look markedly different. In fact, using a rough approximation by looking at the intersection of linear approximations to the glassy and liquid regimes, the glass transition is around 0.4, barely different from 0.37.

(2) So, instead I will try a faster cooling rate, such as N2e5, and see if I can shift the curve to the right. There will probably be issues with the cooling.dat file, but we will first just try to run the simulation to see what happens and then diagnose the error.
(3) Try to distinguish between two glasses in the glass regime, try to train on aggregated liquid data....
(4) Now, working on MPNN on Midway. Was able to go into the data folder in nmp_qc and download the qm9 dataset using the command "python download.py qm9". Now, let's try one of the standard demos on this dataset to see if that at least works on Midway.

8.1. **4/10/2018.**

(1) Downloaded qm9 dataset successfully. Had to pip install wget in environment. Also, now able to do "python demo_qm9_mpnn.py" and it appears to be running completely fine.
(2) Running this program takes about 4775MiB/11439MiB on midway2-gpu01
(3) Error occurs when running the enumerate(train loader) line...
(4) Checking capabilities of demo_glass_mpnn.py versus demo_qm9_mpnn.py. I want to make sure that they are the same at least up until data_train etc. by checking exactly what data is being stored and showing that the data types and structures are the same.
(5) For a single datapoint, data_qm9_mpnn.py prints a 'numpy.matrixlib.defmatrix.matrix', 'list', 'dict', and 'list'.
(6) For a single datapoint, data_glasses_mpnn.py prints a 'numpy.ndarray', 'list', 'dict', and 'numpy.ndarray'.
(7) Ok, well here is a point of dissimilarity, so we should make sure to enforce perfect similarity at this point before moving on.

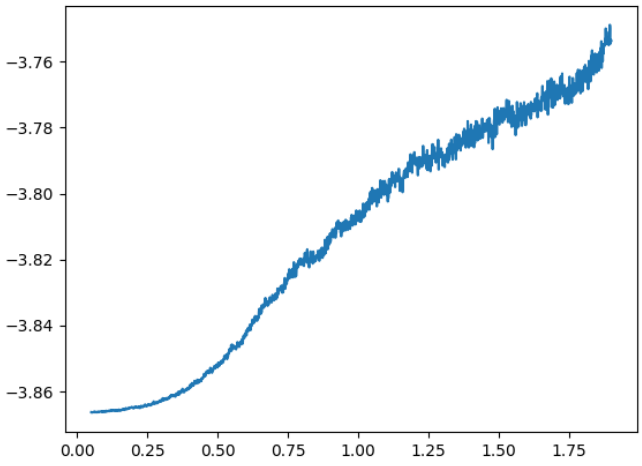
(8) Went into the file graph_reader_class.py and added np.matrix for the adjacency matrix and list() for the target. Now, we also get 'numpy.matrixlib.defmatrix.matrix', 'list', 'dict', and 'list' for the output. Dissimilarity resolved.
(9) Screen still closes when I try to enumerate(). Fuck.

8.2. **4/11/2018.**

(1) Making a new directory, 2e5-working-directory, to run N2e5 simulations. They require having a seed with different variables set so enough cooling.dat information is printed, i.e. in in.analyze-glass and in.make glass set variable freq equal some number less than variable tend.

8.3. **4/12/2018.**

(1) Here is the cooling curve for the 2e5 data:



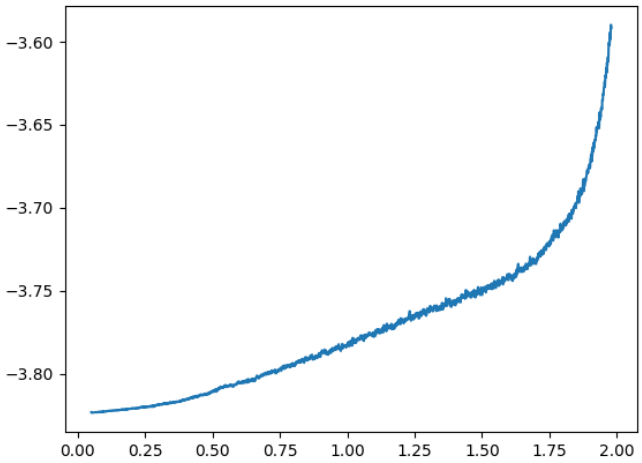
(2) Something looks weird, so let's run examples for 2e6 and also for 2e7 just to have a complete comparison with what I'm doing with my current files. Then, we can play around to get things better.
(3) Created 2e6 folder and set the freq variable to 1000. Running 20 simulations.
(4) Created something similar for 2e7 folder and set freq variable to 10,000. Running 10 simulations.
(5) Finished these, need to download the images. Change plot so it cuts off initial drop to make plot more reasonable. Running 2e4. Looks like kink is less distinct. Message Josh for advice...how determine transition temperature??

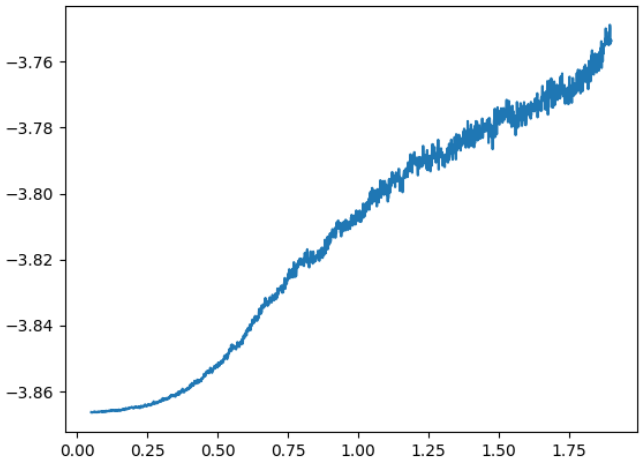
8.4. **4/13/2018.**

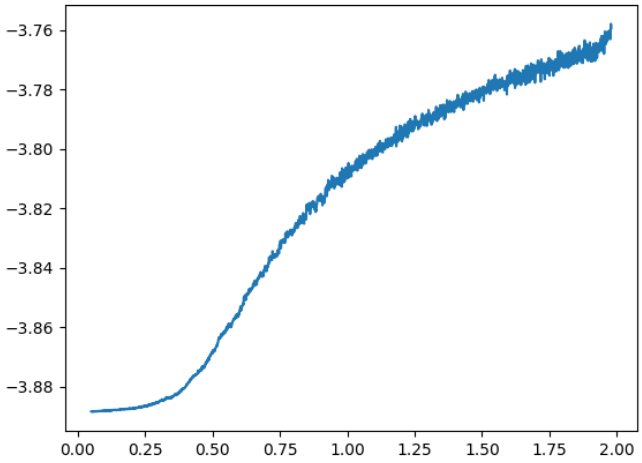
(1) Beginning collection of images for glass data_164 T = 0.401, data_174 T = 0.3035, data_184 T = 0.206, data_194 T = 0.1085. We will use the best model from data_155 to see how that model does as we cross the glass transition temperature. In this sense, it's kind of an artificial dataset, since the liquids are not actually liquids but are glasses. WE SHOULD ALSO try training the model on the ENTIRE liquid curve. Maybe that's what I can set up on Monday.

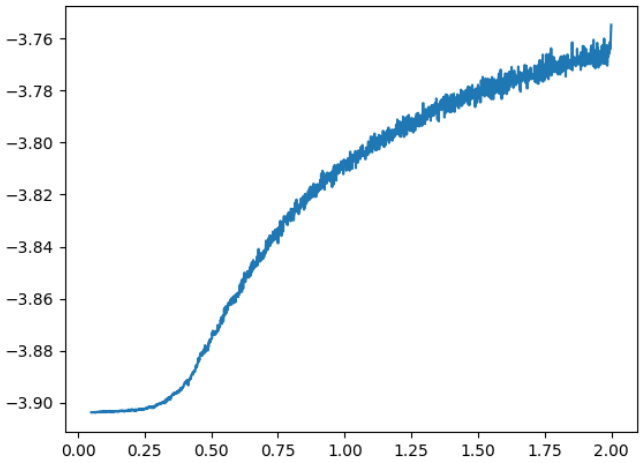
8.5. **4/16/2018.**

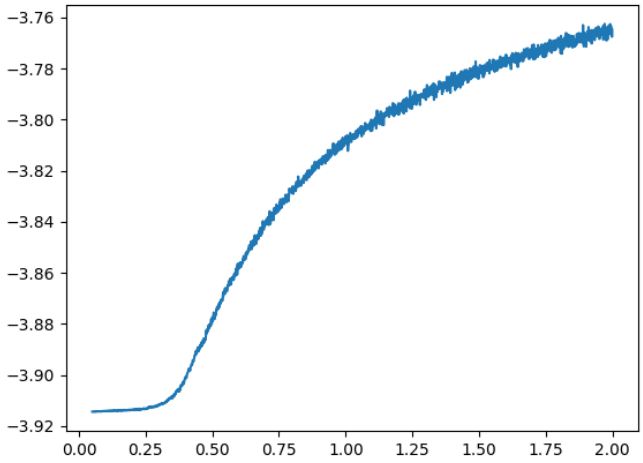
(1) We now have representative cooling curves for 2e4, 2e5, 2e6, 2e7, and 2e8, respectively:






−3.76
−3.78
−3.80
−3.82
−3.84
−3.86
−3.88
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00


−3.76
−3.78
−3.80
−3.82
−3.84
−3.86
−3.88
−3.90
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00



(2) Let's throw out 2e4, since the curve looks pretty different from the others, and start with 2e5.
(3) Wrote a python script, Tg_calculation.py, which I used to compute approximate Tg values:

$$\begin{aligned} &\text{2e5} \quad T_g \approx 0.385279666197 \\ &\text{2e6} \quad T_g \approx 0.374750431427 \\ &\text{2e7} \quad T_g \approx 0.340983034936 \\ &\text{2e8} \quad T_g \approx 0.290198100183 \end{aligned} \tag{8.1}$$

For the glass points that determine a line in the glass regime, I used temperatures 0.05 and close to 0.20015, and for the points in the liquid regime I used temperatures close to 0.50045 and 0.80075. Because 2e5 and 2e8 appear to have a different enough T_g, I will now generate 10,000 simulations for both 2e5 and 2e8. I will re-compute the glass transition temperatures after this, to confirm their values. I will then take the midpoint temperature, around T = 0.338, and take configurations from 2e5 that will correspond to glass and configurations from 2e8 that will correspond to liquid. I will then train the network to see if I can distinguish between them.
(4) Created folders 2e8-folder and 2e5-folder. For 2e8, changing the in.make-glass and in.analyze-glass in seed to have variable freq equal 1000000. For 2e5, changing to 1000. Running 500 simulations for each. Also, removing the sleep command, as it is unnecessary automation.
(5) Tried running main_glassliquid.sbatch to test the performance of the best model from data_liquid155 on other datapoints, but getting error, "No such file or directory." Not sure what is going on. Emailed Igor to figure it out.
(6) Tested the best version from data_liquid155 on other datasets. Accuracy at least 90% for anything lower than 155, then gradually decreases down to 80, 70, 60, finally 45% for data_liquid194. Not a sharp cutoff though.

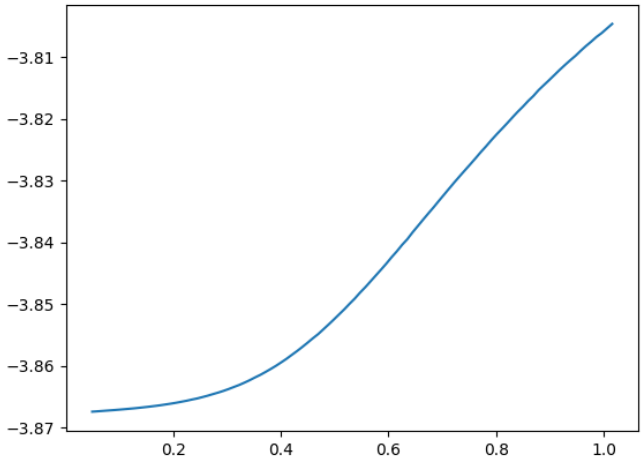
(7) Inherent structure energy of -3.66 will be a glass for 2e5 but a liquid for 2e8. That is what we want to compare. We will start first by evaluating the data_liquid155 model on this. We would also try training across the curve. And then training directly on 2e5 versus 2e8.

9. 4/18/2018

(1) Evaluate current model on a different cooling curve, say 2e5 or 2e6.
(2) Construct artificial geometries, tuning separation between particles, to feed into trained network.
(3) Talk to Daniel about his configurations.
(4) Compare 2e5 and 2e8 when it's done.
(5) Choose a smaller subsection of the 4320 to do MPNN with....LOL WHY DIDN'T I DO THIS BEFORE AHHAHA

10. 4/23/2018

(1) Looking at the cooling curves again, the glass at energy -3.866 for cooling rate 2e5 is still a liquid for cooling rate 2e7, for which we already have data. So, we already have FULL data to do this, haha great.
(2) First, let's construct a complete average cooling curve for cooling rate 2e5:



(3) Now, let's recalculate the estimated glass transition temperature. We get:

$$\text{2e5} \quad T_g \approx 0.380974669843 \tag{10.1}$$

which is similar to previous value.
(4) Now, we will evaluate the current model on 2e5. We will construct a dataset that is composed of glass around T = 0.05 and liquid around T = 0.8. Specifically, we will choose T = 0.05, which corresponds to energy -3.867438353 and T = 0.80075, which corresponds to energy -3.82253291198. Generation of 10,000 images of each is currently running.

(5) We will also need data from 2e7 that corresponds to energy -3.867438353. Based on the average cooling curve for 2e7 data, T = 0.54725 (i.e. simulation step 14800000) has an average energy of -3.86698027516. So, we will compute 10,000 images at this temperature. This is running now.

11. 4/24/2018

(1) The image processing for 2e5 is complete. We now have 10,000 images of glass and liquid, where glass is at T = 0.05 and liquid is at T = 0.80075. We will now evaluate the version 12 best model at 155 on this and see what accuracy it obtains.
(2) Moving the folder containing 2e5 images, called data_liquid_2e5123, to /project/depablo/kswanson/r learning-glasses.
(3) Changing metadata to be from that folder.
(4) Evaluating, we get validation accuracy of 89.3311% and test accuracy of 89.1304%. This is good news!
(5) Now, let's move on to glass versus supercooled liquid.
(6) Constructed a folder called data_supercooled, which contains the image data from T = 0.05 for cooling rate 2e5, labelled glass, and the image data from T = 0.54725 for cooling rate 2e7, labelled liquid.
(7) Switching metadata to be from data_supercooled.
(8) Able to classify with 87.2148% validation and 85.2013% test! Excellent.

12. 4/26/2018

(1) We are now going to return to MPNN to crush it. Start by reducing our dataset so that each configuration file only consists of 20 atoms. Let's see if our algorithm can at least process that.
(2) Copy coords_config.py to coords_config_restricted.py. Change line 60 so that we only range over 20 atoms. Let's try to use this now to construct a new dataset. Modifying make_coords_kirk.sh on Midway 2 in the 2017 folder so that it executes the new restricted coords file.
(3) Generated this dataset with about 200 total glass + liquid samples, each with 20 atoms. Let's try our MPNN code on this shit.
(4) Ok, gpu2 is busy. In the meantime...
(5) Removed a lot of files from Download folder. Followed instructions to get my-rdkit-env and associated packages on my laptop (desktop is, like, broken or something).
(6) Downloaded the 20 atom data file from Midway. Modifying graph_reader_class.py.
(7) Doesn't work, because no NVIDIA driver.

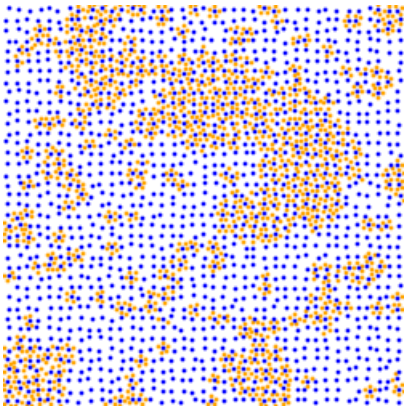
13. 4/30/2018

(1) Took demo_glass_mpnn_working.py and graph_reader_class_classification.py and moved to Midway. On midway2, gpu2, do module load cuda/8.0, module load Anaconda3/5.0.1, then python filename –no-cuda. It works! Time to see how large of a graph we can process on Midway.

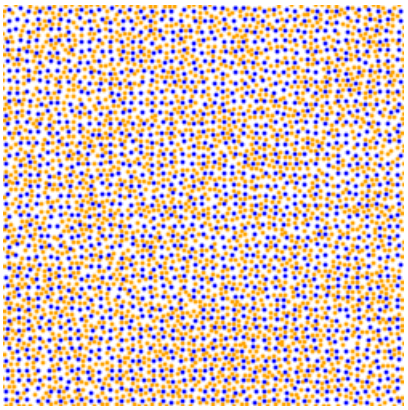
(2) So, moving data_coords_endpoints_restricted100 to the data/glass folder. Have to change the graph reader class to support 100 sized data instead of 20.
(3) Ok, getting 'bus error' or 'screen terminated'. Let's try backing it off to 25, and incrementally move here to find the breaking point. Then we will check with RCC to see what the issue is, and move on from there.
(4) System I. On Midway 2 gpu 2, we do: sinteractive –partition=gpu2 –gres=gpu:1. Then, we do module load cuda/8.0, module load Anaconda3/5.0.1, source activate my-rdkit-env. Then, we do python demo_glasses_mpnn_classification.py –batch-size=. So, we are using cuda. We are experimenting with different datasets. Each dataset has approximately 100 glass and 100 liquid configurations. The difference between the datasets is the number of atoms in each configuration. Also, we are using the change g, h, e, target = next(iter(train_loader)) instead of enumerate(train_loader), which appears to work better. The So far, we have gotten up to: size 20 batch size 100, size 25 batch size 100, (batch sizes not really representative), 100 batch size 20, (we'll do batch size 20 from now on), 200 with batch size 20.
(5) Noticed that 10624 MiB / 11438 MiB was the memory usage in this process. So, my guess is that a similar problem is occurring as before with TensorFlow. We need a command that will restrict memory usage on the GPU to allow growth. This is probably why I am getting kicked off/it is complaining about memory problems.
(6) From the developer: i think measuring GPU memory usage via nvidia-smi might be misleading (and might be the issue). We use a caching allocator and a few tricks, so we cant use nvidia-smi's reporting. https://discuss.pytorch.org/t/using-volatile-true-for-prediction-uses-more-gpu-memory-than-volatile-false/8330
(7) Let's test the volatile thingy?
(8) Use multiple GPU nodes in parallel?

14. 5/15/2018

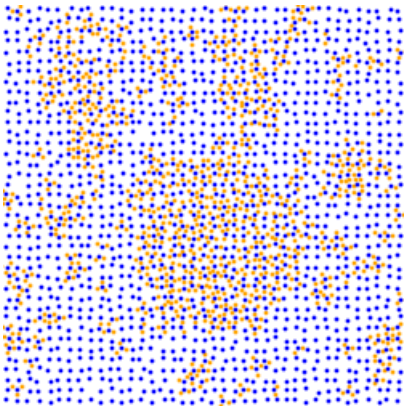
(1) Was not writing stuff in the log for a while. So there will be some kind of discontinuity here.
(2) The first thing we want to do is to generate 100 examples of the new, filled out, artificial five-fold symmetry images. The python script we are working from is called artificial-geometries.py. This is running now.
(3) We are also running something similar, but for three-fold symmetry. Once these are done, we will render the images and test.
(4) Finally, to test another hypothesis we have, we will construct images that have no symmetry or clustering at all. We will simply leave that part out. We will create a new python file called artificial-geometries-liquid.py for this task. This is running now as well on Midway.
(5) This is what the clusters of 5-fold symmetry look like:

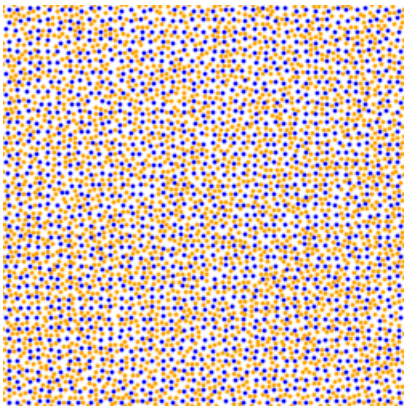


(6) This is what the filled out picture might look like:

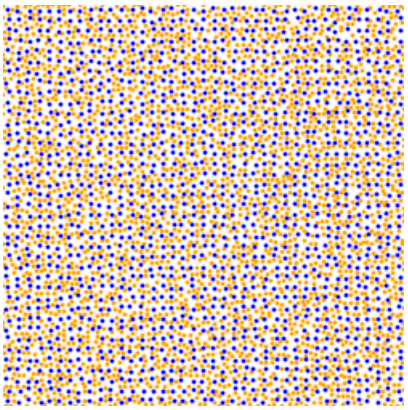


(7) This is what the clusters of 3-fold symmetry look like:





(8) With zero symmetry, i.e. random placement only, we have:



(9) POTENTIAL IDEAS: Don't fill in the cluster area with any more extra particles. Save that for the other regions. For the artificial liquid, i.e. zero symmetry, adjust the blue particles more so that they clump a bit.

15. 5/16/2018

(1) Potential problem: Midway 2 gpu2 is not giving expected accuracies. On data_supercooled, for example, it's showing the inverse of 86% accuracy. Wondering if there is some kind of memory issue going on here. Tried using depablo-gpu but getting the following error: kernel version 384.69.0 does not match DSO version 367.44.0 – cannot find working devices in this configuration. Emailed Igor and awaiting information.
(2) Also, turned the 0 symmetry, 3 symmetry, and 5 symmetry files into images.

16. 6/11/2018

(1) We are going to start by cleaning up the code for generating artificial images via Shubhendu. We will then move on to trying Josh's idea. We could also train a CNN on small subsets in parallel with MPNN on small subsets. See the smallest subset that MPNN can train on with a batch size of 20. We should also pitch the current results to Prof. Skinner to see what he thinkgs about publishing without interpretation.

17. 6/22/2018

(1) From a while ago. We discovered that labeling from the function create_one_hot_mapping was inconsistent. So, when checking accuracy, one must make sure to manually assign the correct labeling after checking what the correct labeling is. For the data_liquid155_version12_step1_best_model.ckpt, the correct labeling is liquid as [1, 0] and glass as [0, 1].
(2) So for now, we are going to do a manual assignment. Updated this on main_glassliquid.py and on GitHub.
(3) Now, we have an issue where the program is getting killed. Tried ./filename for saver, but still it just gets killed. What is going on with the saver? Restoration seems to go ok, but then the accuracy evaluation just fails.

18. 6/25/2018

(1) Current To Do List:

Get the singularity container to work on depablo-gpu nodes, since this is the only tool we currently have left

Overlay the glass cooling curves to show when the depart each other, as Skinner mentioned

Train on glass versus supercooled liquid at the same energy, or glass versus glass at the same energy, in order to get a better percentage

Deal with the question of whether rendering the plots using the blue and orange dots screws with the data

Train on PVD versus liquid-cooled data in order to show a complete story

Try Josh's Monte Carlo scheme

Use TensorBoard, Try Keras

Implement MPNN on subsets, train CNN on subsets

Implement MPNN + pooling as Shubhendhu suggested to analyze the entire image

Read de Pablo + Ediger papers

Understand why PVD versus liquid cooling structure analysis was important for Dan's paper

Coordinate system independent necessary? Ask Alexei

Analyze spherical harmonics

Check out Nick's DeepChem suggestion (MPNN implemented there?)

Run full 2e8 data in order to have that full dataset

Ask Shubhendhu example of how the network

Read papers on machine learning!!! Start with all of the papers Shubhendhu has sent recently.....

(2) Just ran the following on midway-13b-18 (i.e. depablo-gpu) from the /project/depablo/kswanson/mac
learning-glasses directory, and it printed final validation accuracy 0.862784 and final test accuracy 0.863454 on data_supercooled:
sinteractive –partition=depablo-gpu –gres=gpu:1 module load singularity singularity exec -B /project:/project –nv /software/src/singularity_images/tf_1.8.0.simg python main_glassliquid.py -eta_initial=1e-3 -eta_final=1e-4 -eta_threshold=0.90

-batch_size=1 -iterations=1500 -beta=0.01 -keep_probability=0.5 -filename="artificial-eval" -training_data_aug=False -restart=True -evaluation=True -restart_file="data_liquid155_version

(3) Now, we will go back to MPNN and see how large we can go in terms of number of particles. Goal is to get at least 100, perhaps up to 300, with batch size 20.
(4) Problem. We are trying the following command, from Igor's email a while ago: module load singularity singularity shell –nv /software/src/singularity_images/PyTorch_cuda_9.0.sin python demo_glasses_mpnn_classification.py –batch-size=5 from /home/swansonk1/nmp-qc/demos. It says no module named rdkit. So, tried source activate my-rdkit-env, but this is not possible. Only works after module load Anaconda3. But then after source activate, I try the module load sinularity stuff and I still get the rdkit error. I'm not sure how I got this stuff to work before. But perhaps I need to load this environment in singularity itself, in other words, after I do module load singularity, I THEN need to install the rdkit environment. So, we will try this tomorrow morning. If this does not work, and we have exhausted all other combinations, we will email Igor.

19. 6/26/2018

(1) Starting where we left off yesterday.
(2) In /home/swansonk1, tried module load Anaconda3, then conda create -c rdkit -n my-rdkit-env-test rdkit. It appeared to download and install all relevant packages. Source activate my-rdkit-env-test, then pip list shows that the packages are indeed installed, apparently.
(3) Tried module load Anaconda3, module load singularity, source activate my-rdkit-env-test, singularity shell –nv /software/src/singularity_images/PyTorch/cuda_9.0.simg python demo_glasses_mpnn_classification.py –batch-size=5, but got the error /usr/local/Anaconda3-5.1.0/bin/python: /usr/local/Anaconda3-5.1.0/bin/python: cannot execute binary file. Then tried module load Anaconda3, module load singularity, source activate my-rdkit-env-test, singularity exec –nv /software/src/singularity_images/PyT python demo_glasses_mpnn_classification.py –batch-size=5 and got the error ModuleNotFoundError: No module named 'rdkit', even though the virtual environment definitely contains rdkit.
(4) Tried simply downloading using conda install the PyTorch version I did on local machine a long time ago, only using module load Anaconda3 and no singularity. Then just ran python demo_glasses_mpnn_classification.py –batch-size=10, but the program crashed after "Check cuda."

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E-mail address: swansonk1@uchicago.edu

INSTITUTE FOR MOLECULAR ENGINEERING, UNIVERSITY OF CHICAGO, 5640 S ELLIS AVE, CHICAGO, IL 60637