MACHINE LEARNING GLASSES RESULTS LOG

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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:
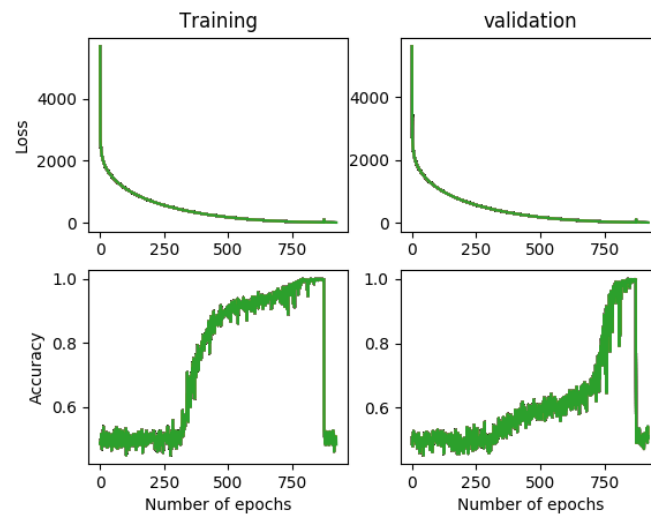

FIGURE 1. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

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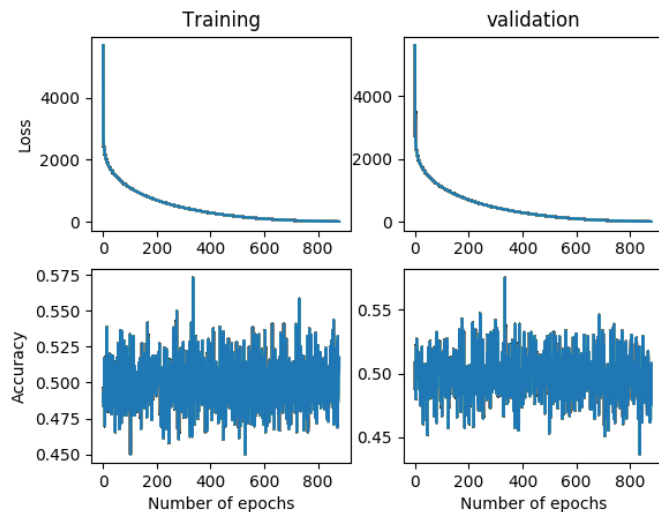
FIGURE 2. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(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
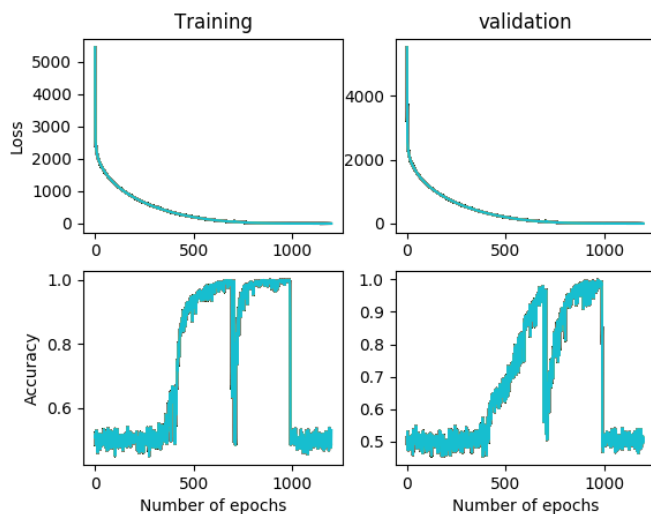

FIGURE 3. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

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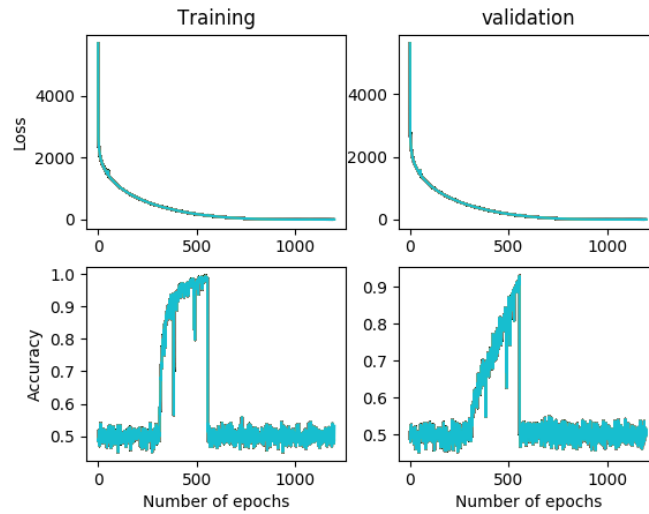
FIGURE 4. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(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.
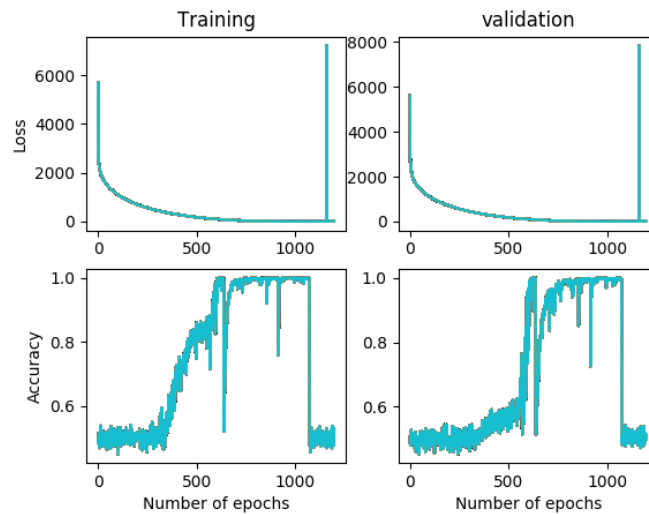

FIGURE 5. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

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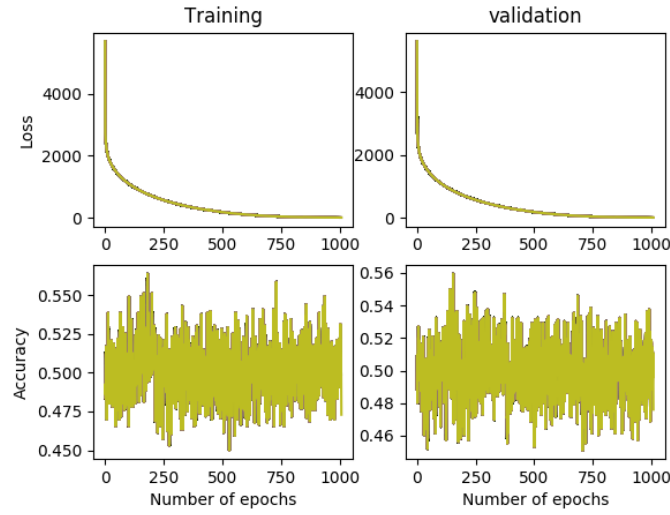
FIGURE 6. Batch Size = 80, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(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 tem-
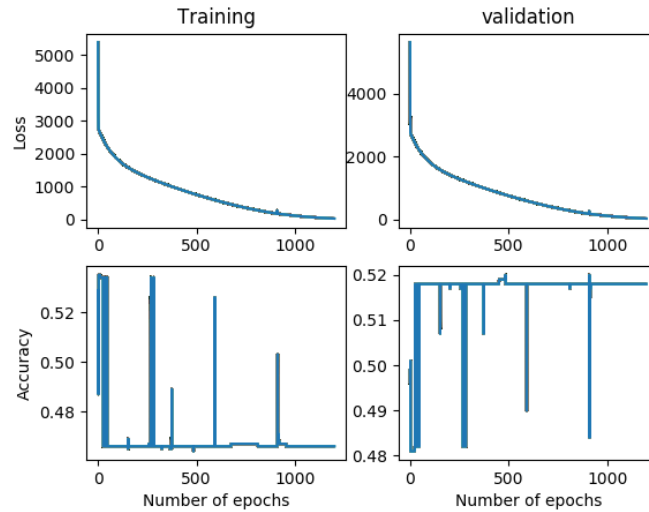   perature of 0.21.

FIGURE 7. Batch Size = 100, Learning Rate = 1e-4, Beta = 0.01,
Dropout = 0.5
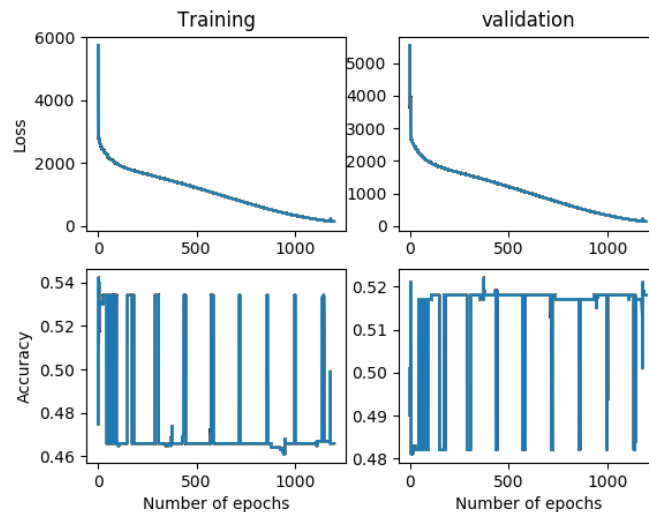
FIGURE 8. Batch Size = 10, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5
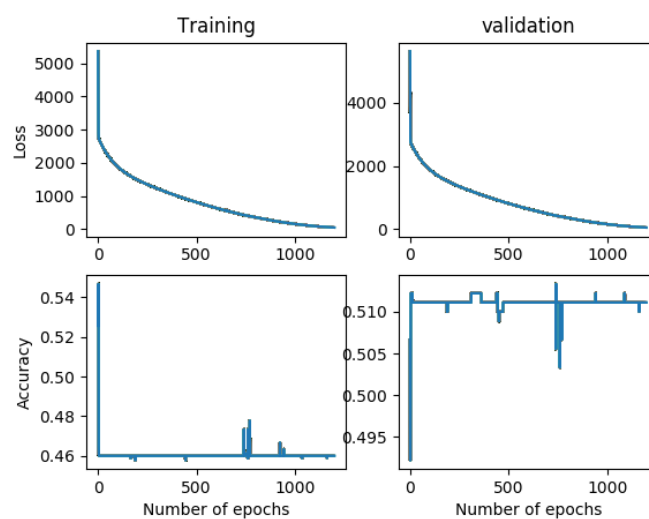

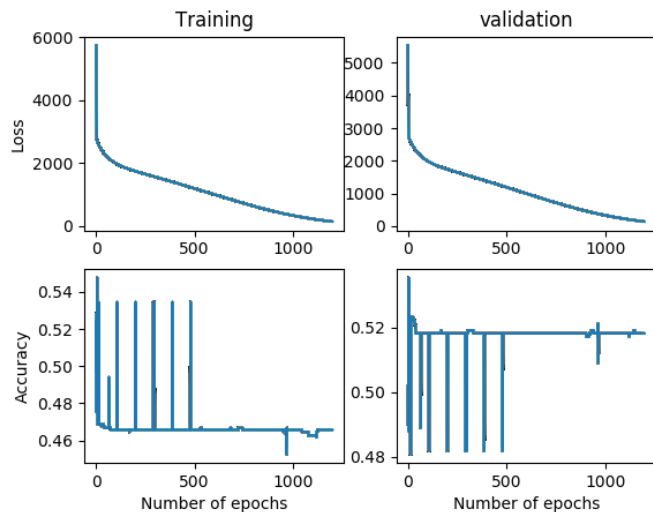FIGURE 9. Batch Size = 150, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

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

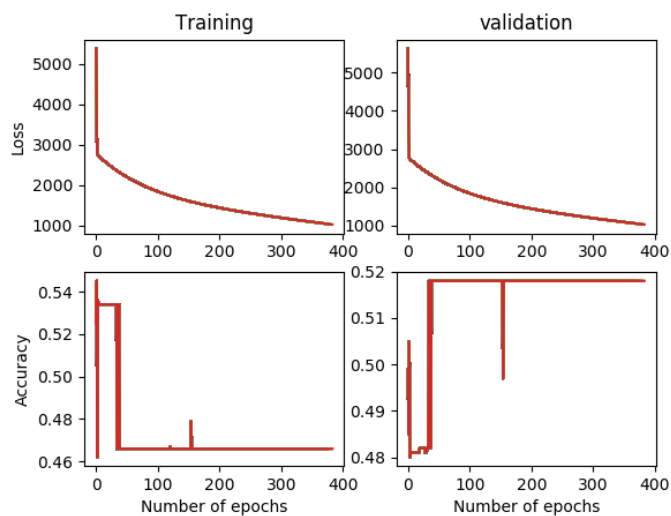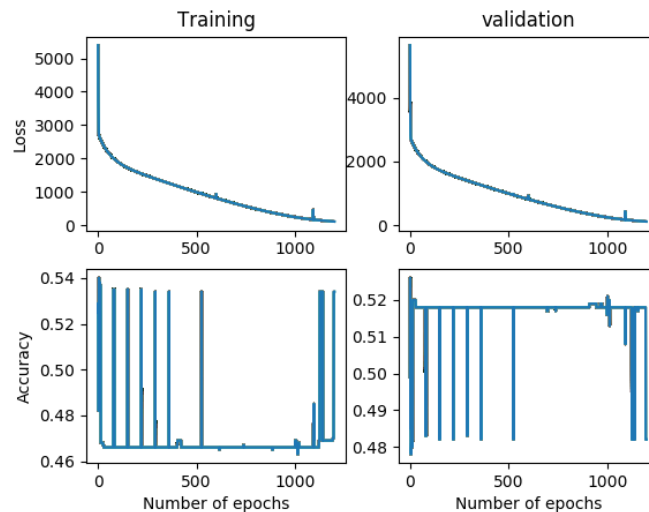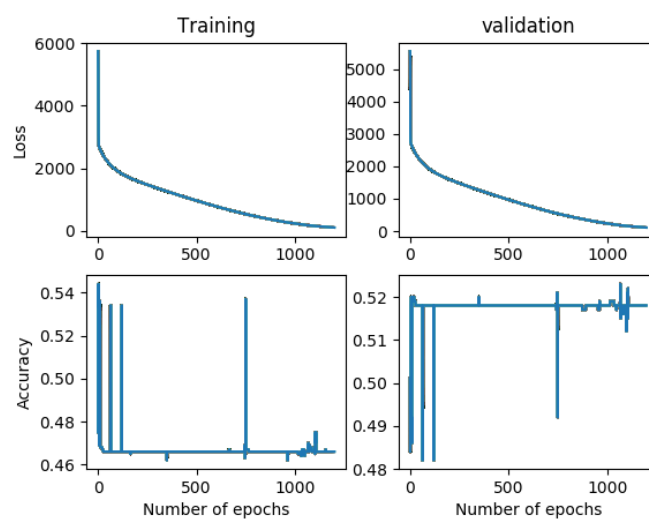FIGURE 16. Batch Size = 80, Learning Rate = 1e-4, Beta = 0.01, Dropout = 0.5

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

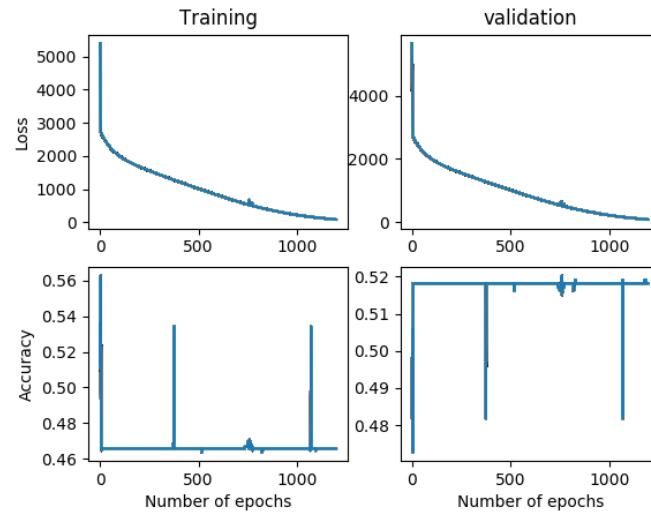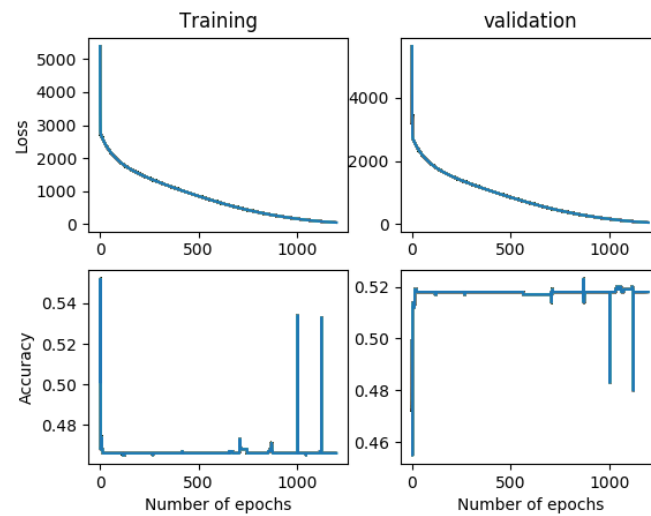FIGURE 18. Batch Size = 10, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

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
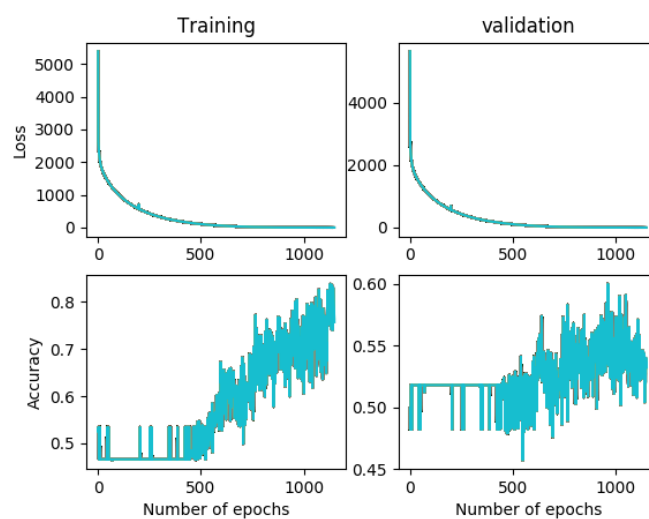
FIGURE 21. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.1
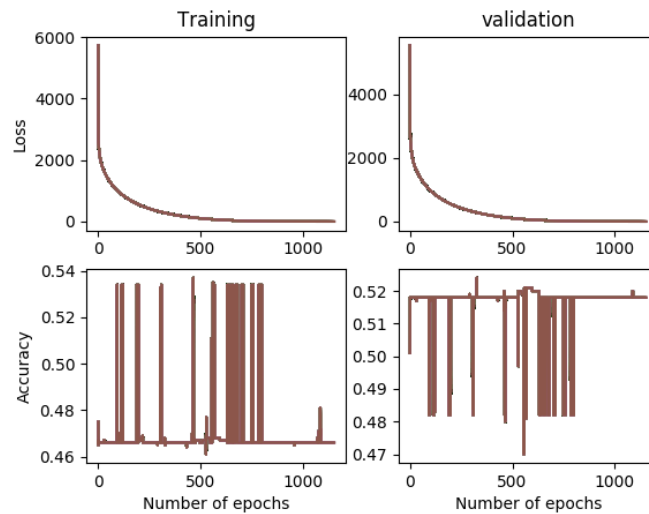
FIGURE 22. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.2
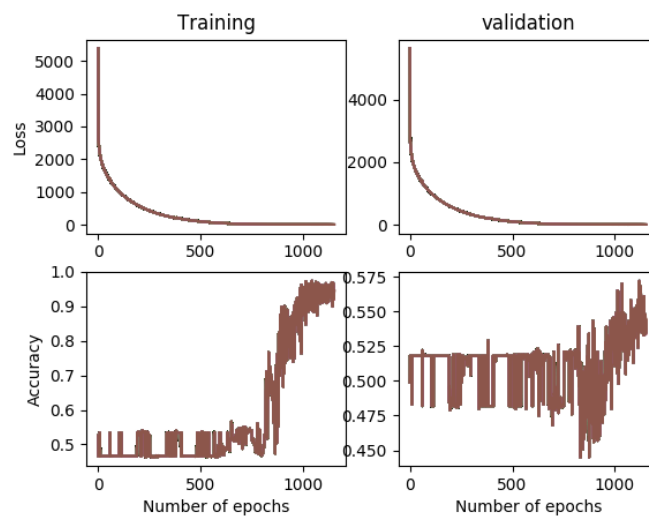
FIGURE 23. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.3
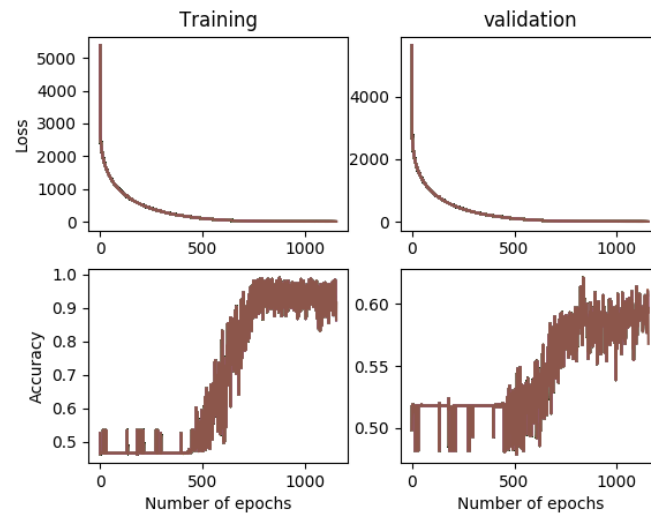
FIGURE 24. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4
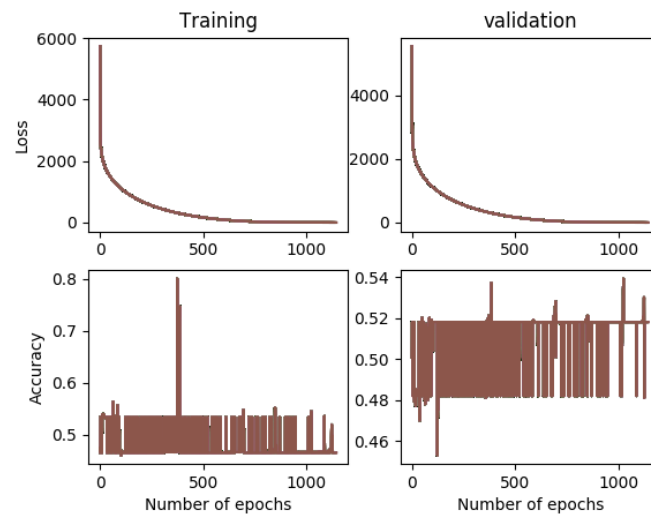
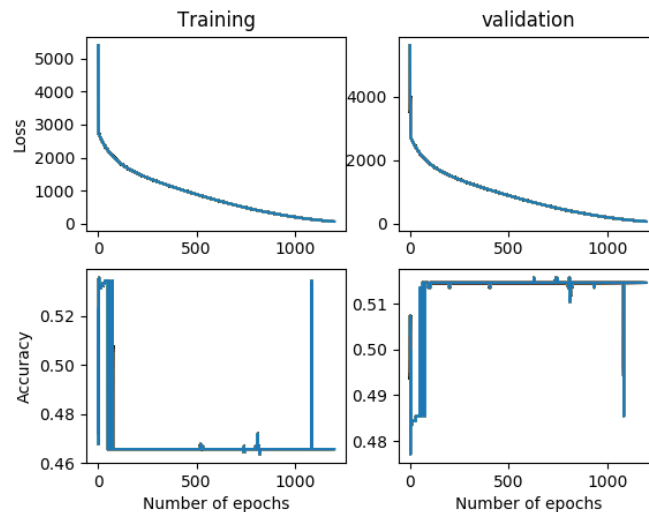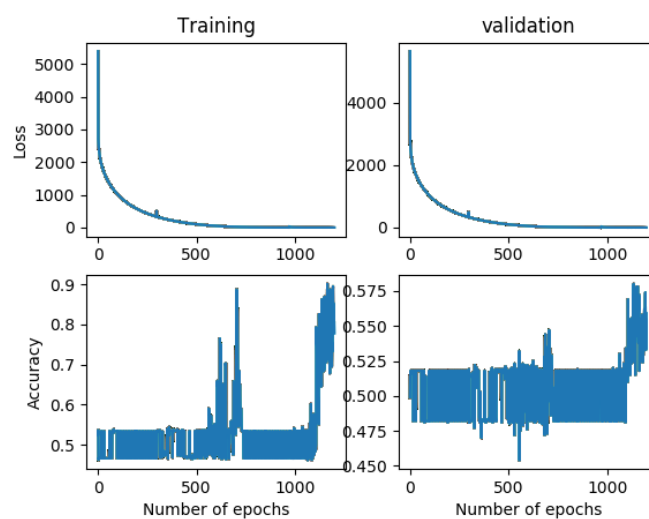FIGURE 25. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5
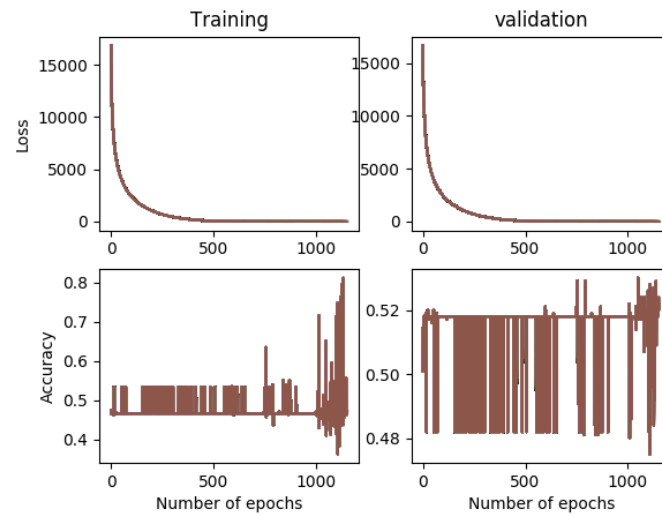
FIGURE 26. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.3
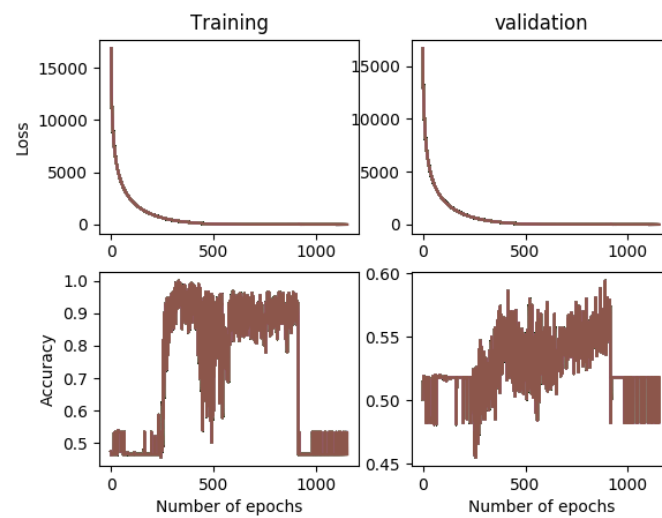
FIGURE 27. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4
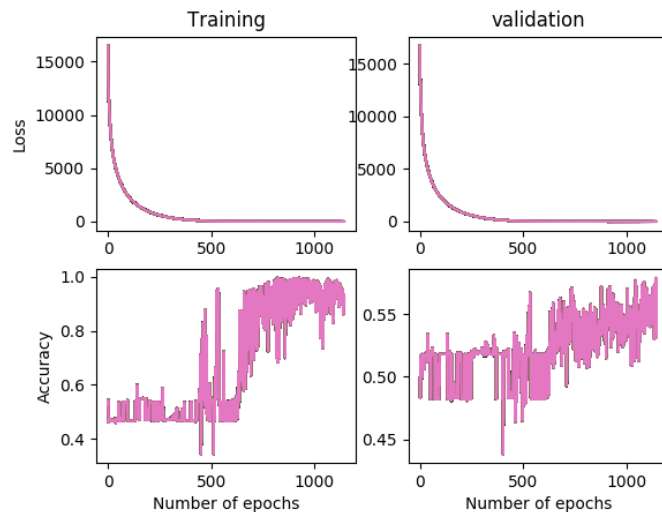
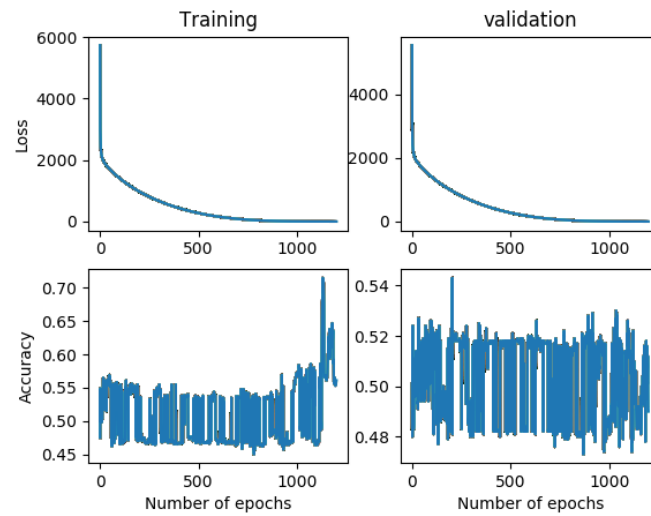FIGURE 28. Batch Size = 200, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.4
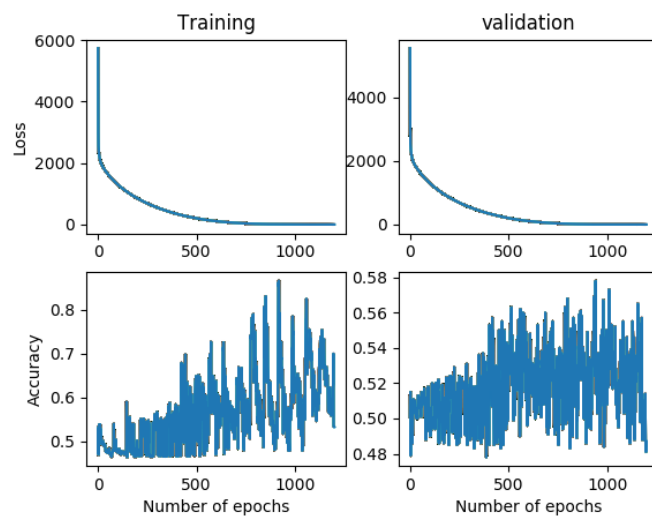
FIGURE 29. Batch Size = 20, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5
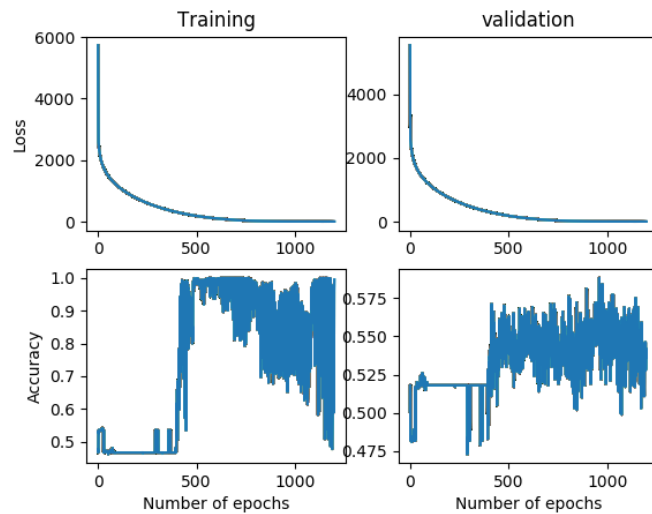
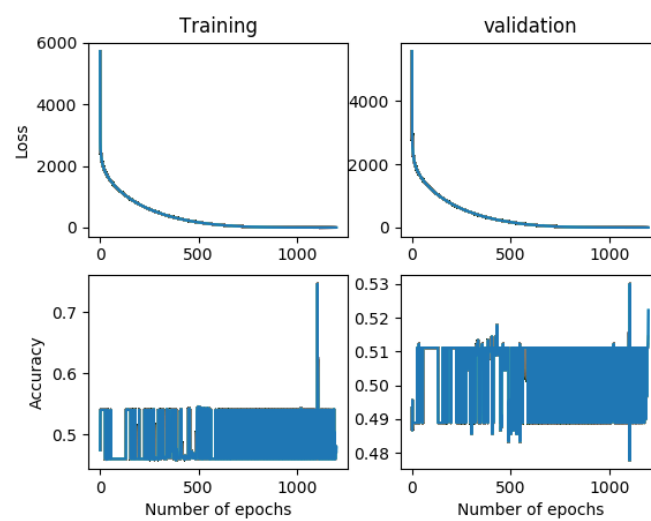FIGURE 30. Batch Size = 250, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5
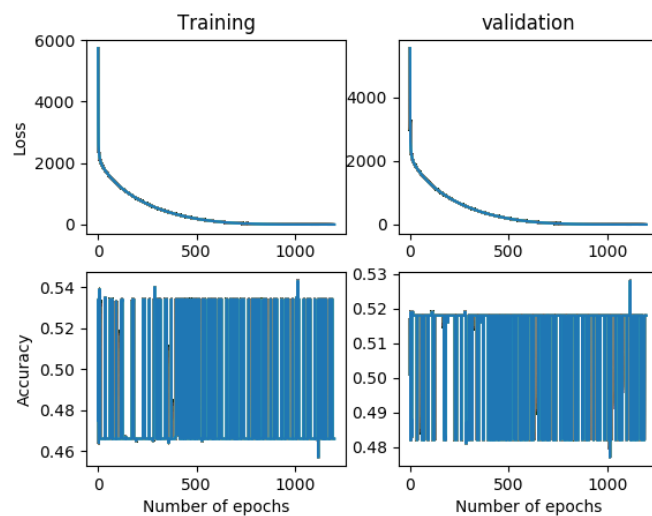
FIGURE 31. Batch Size = 25, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5
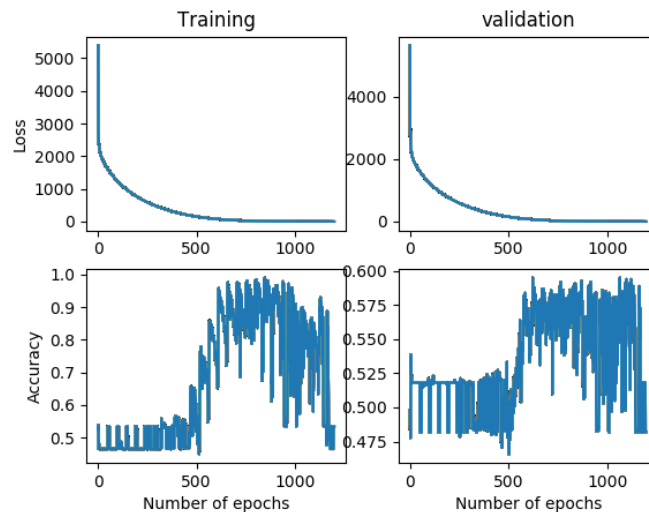
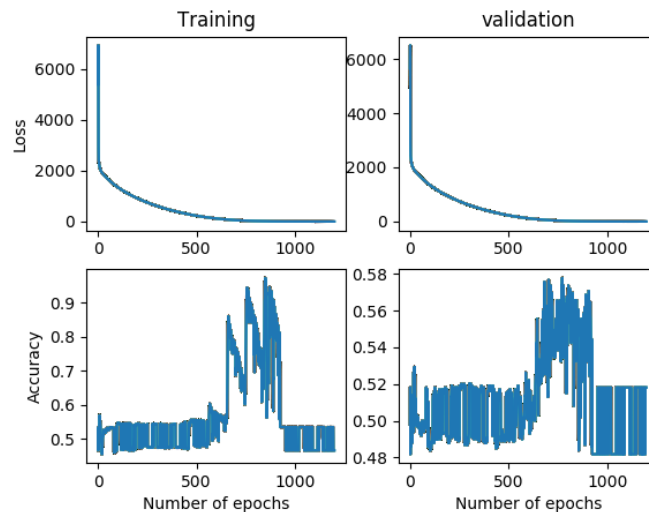FIGURE 32. Batch Size = 30, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5
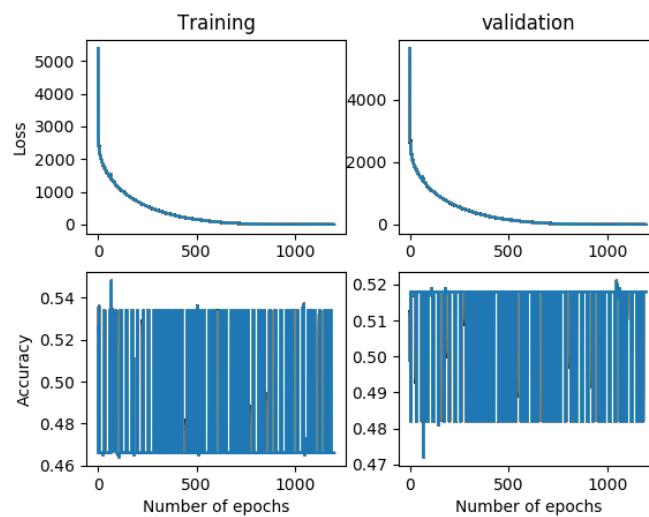
FIGURE 33. Batch Size = 50, Learning Rate = 1e-3, Beta = 0.01, Dropout = 0.5

(10) Visualizations.
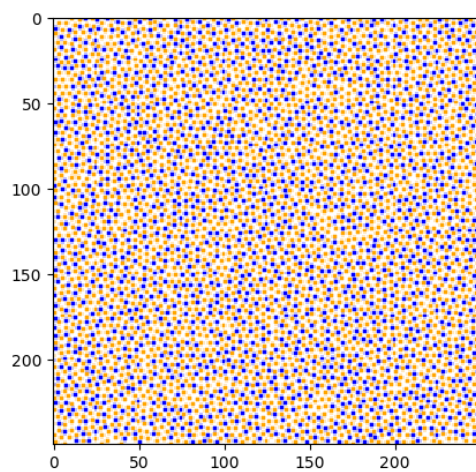
FIGURE 34. Glass original
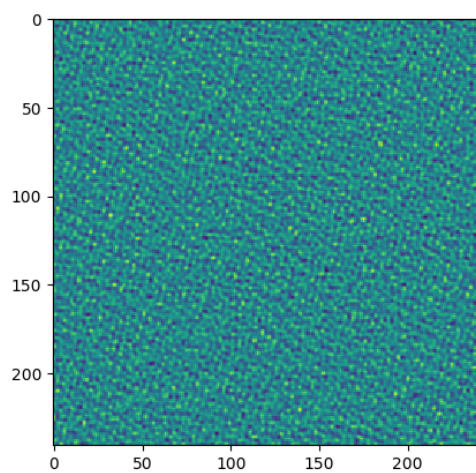
FIGURE 35. Glass channel 1
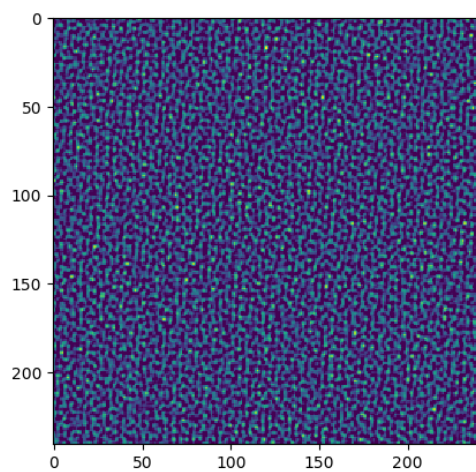
FIGURE 36. Glass channel 2
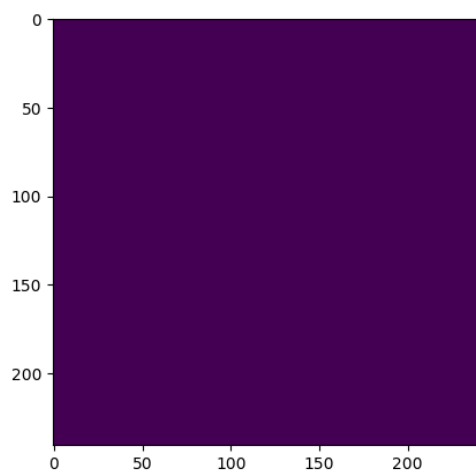
FIGURE 37. Glass channel 3
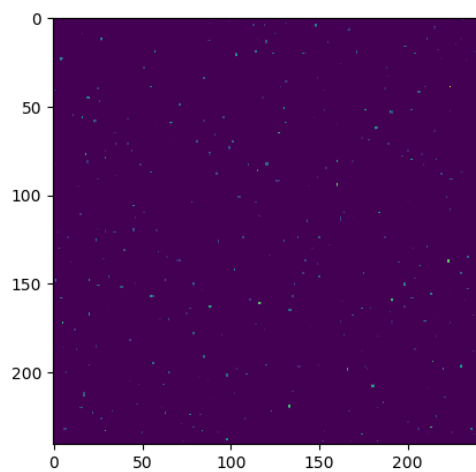
FIGURE 38. Glass channel 4
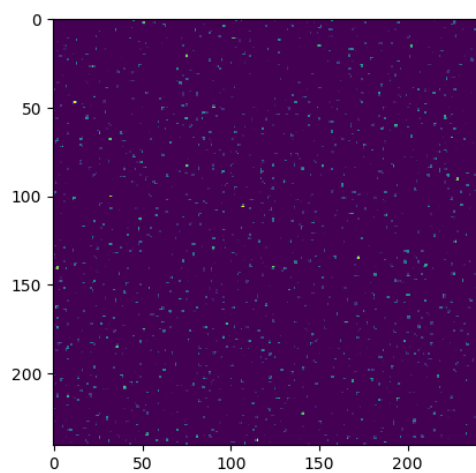
FIGURE 39. Glass channel 5
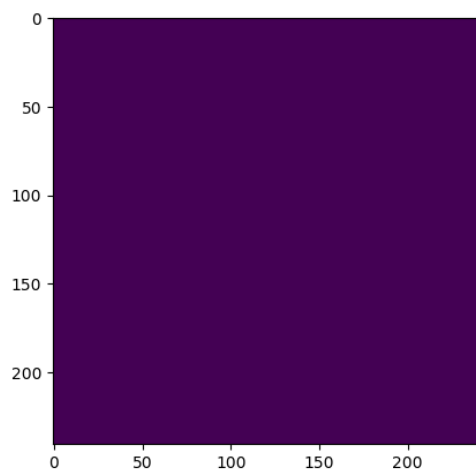
FIGURE 40. Glass channel 6
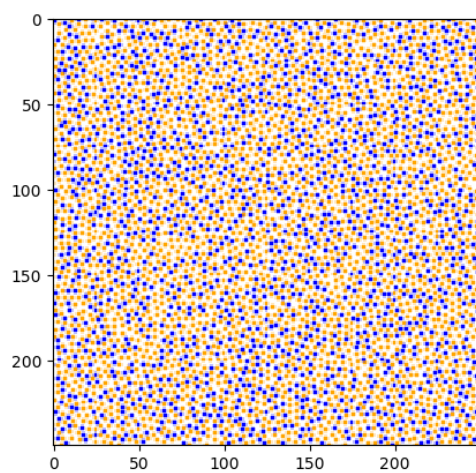
FIGURE 41. Liquid original
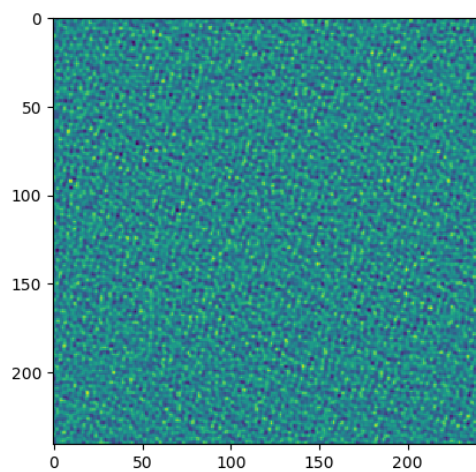
FIGURE 42. Liquid channel 1
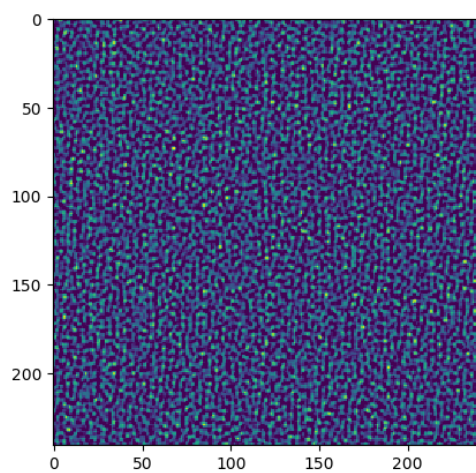
FIGURE 43. Liquid channel 2
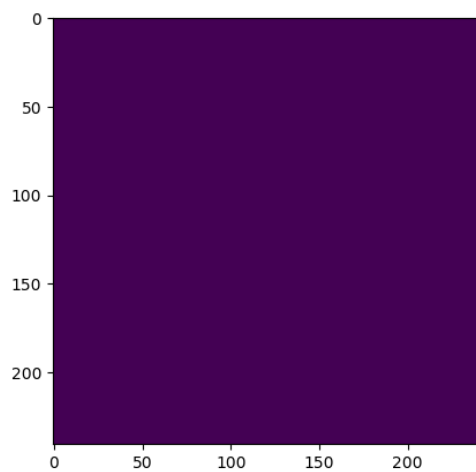
FIGURE 44. Liquid channel 3
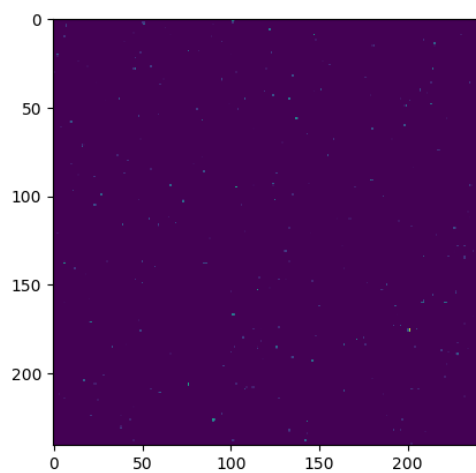
FIGURE 45. Liquid channel 4
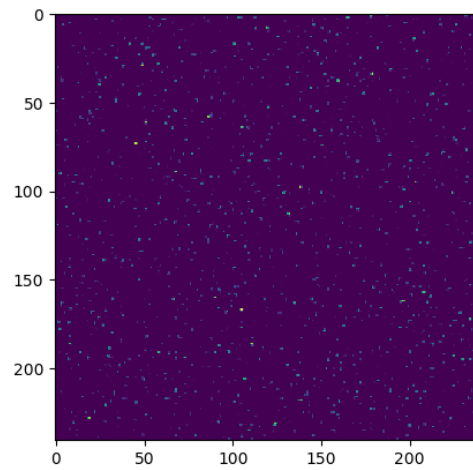
FIGURE 46. Liquid channel 5
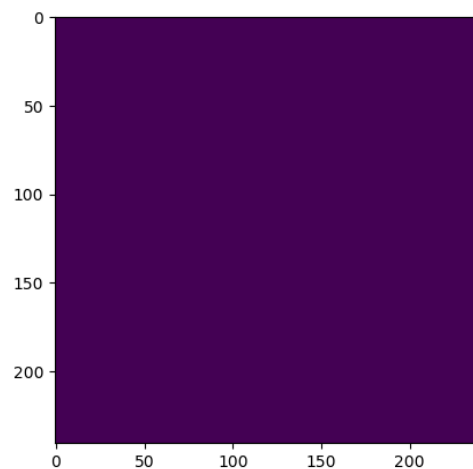
FIGURE 47. Liquid channel 6

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,
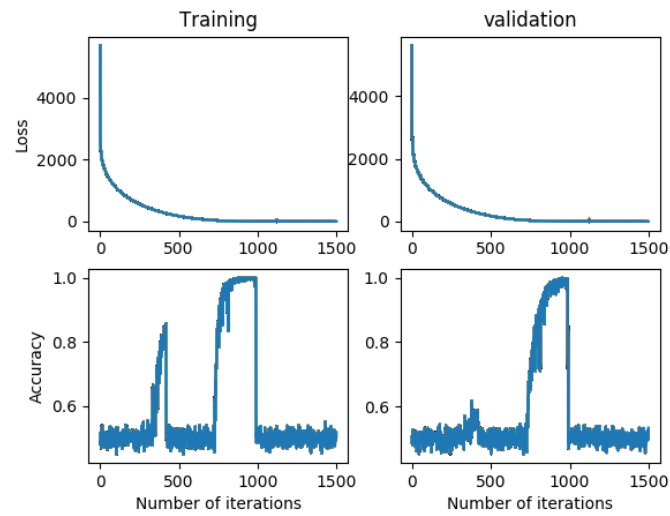Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

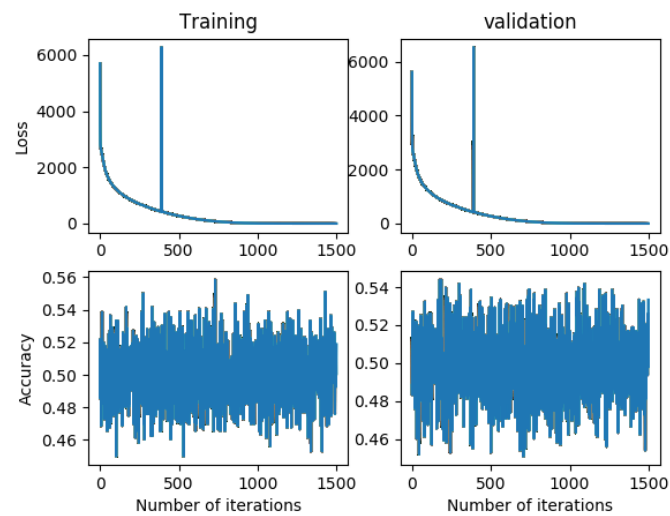FIGURE 57. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4,
Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5
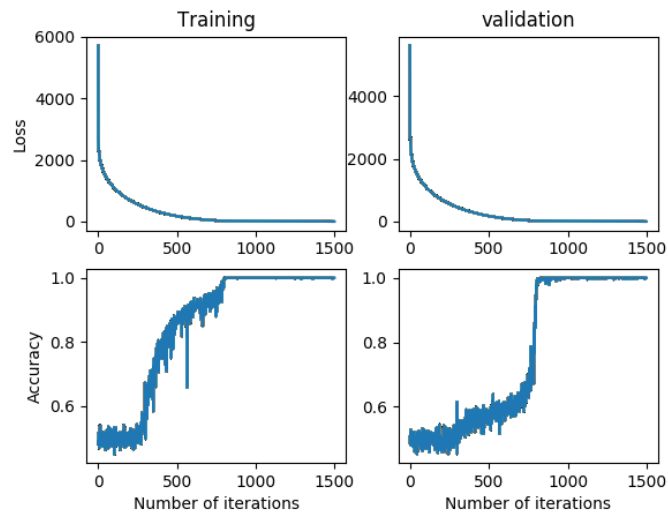
FIGURE 58. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5
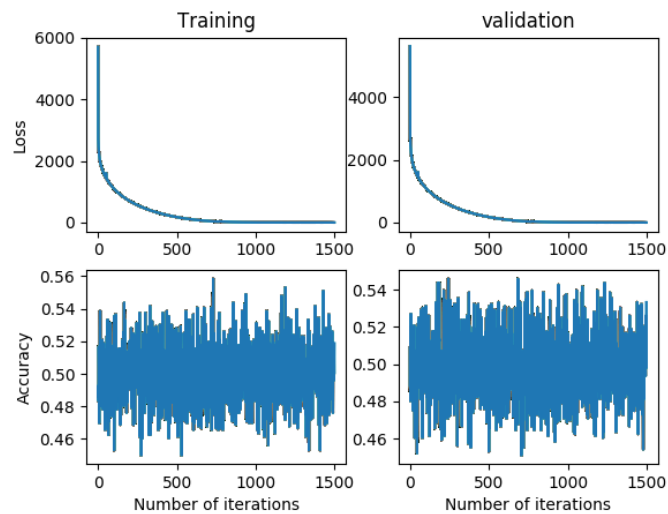
FIGURE 59. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5
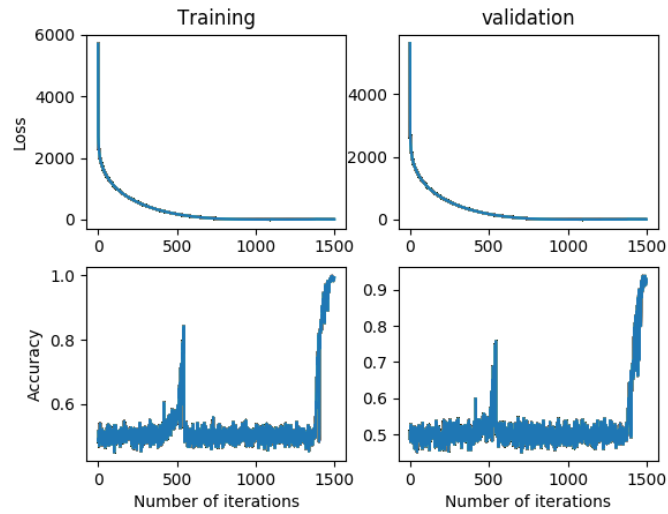
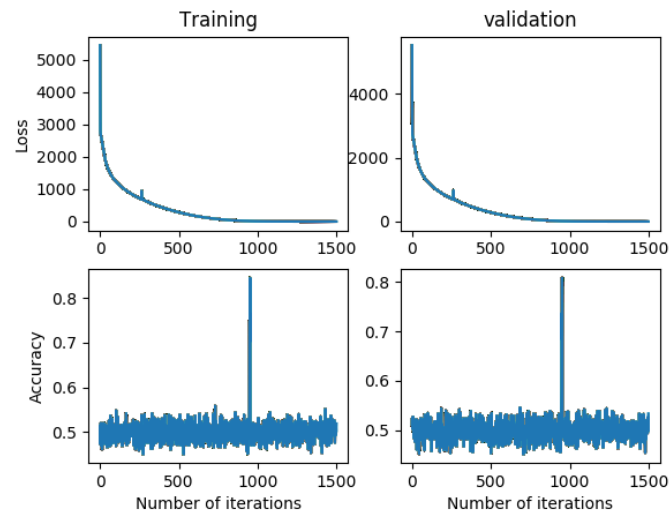FIGURE 60. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4,
Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5
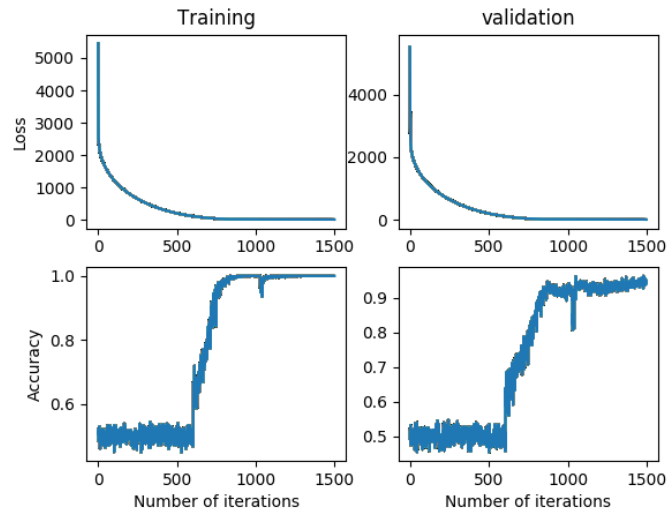
FIGURE 61. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4,
Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

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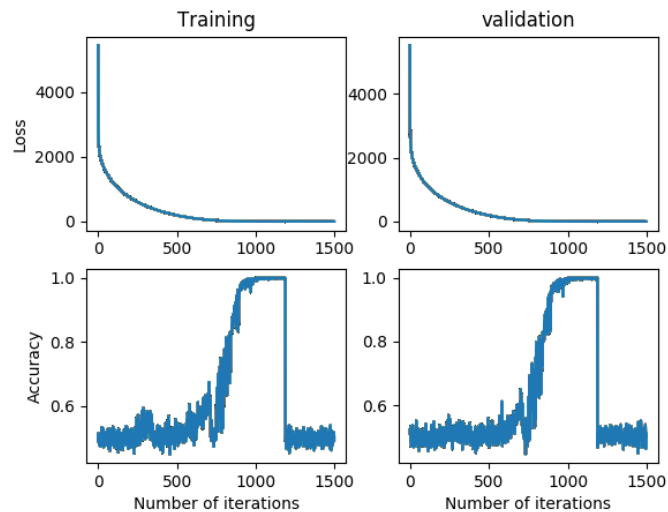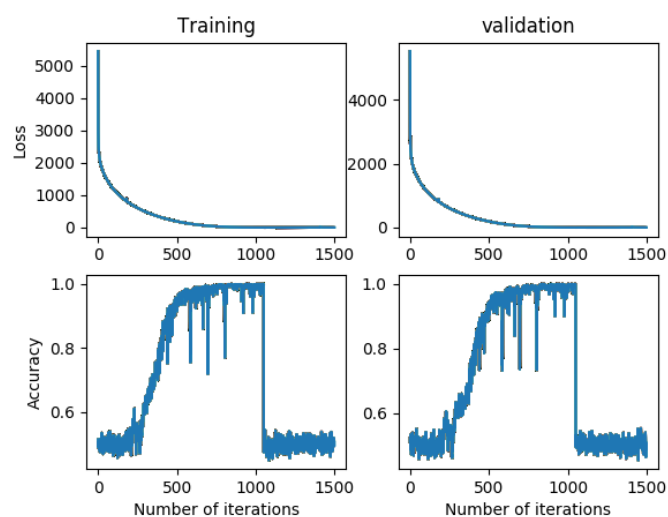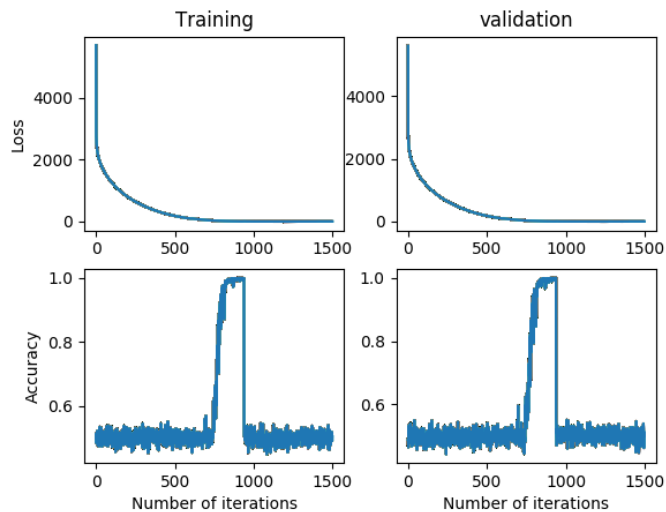
FIGURE 64. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4,
Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

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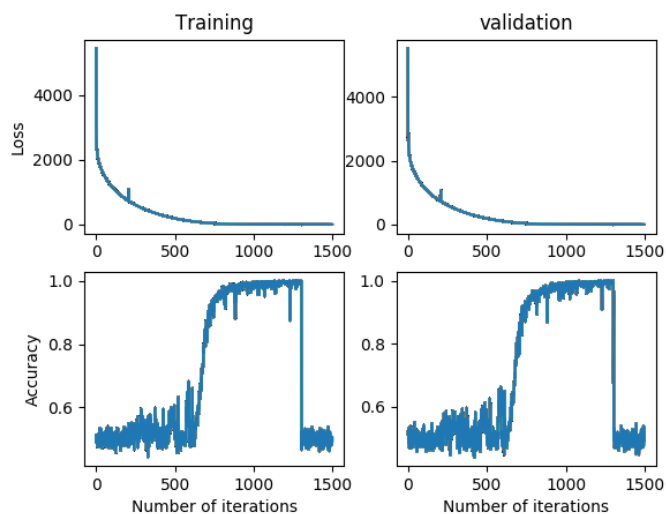Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

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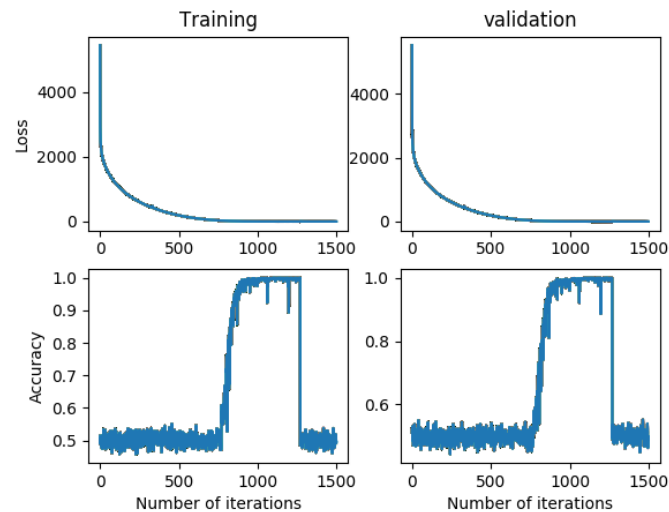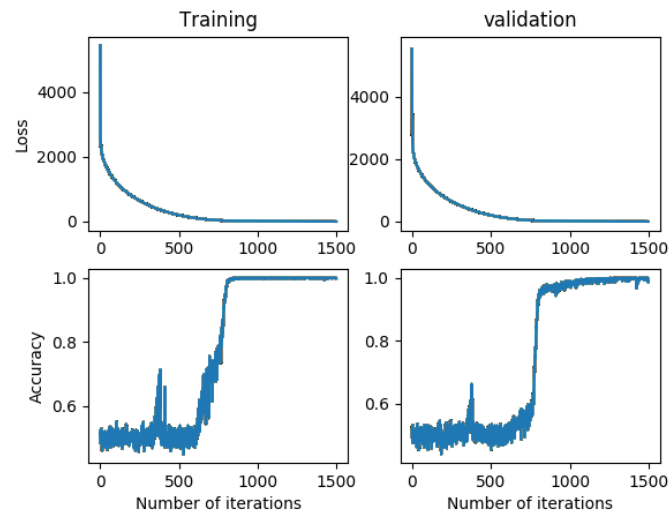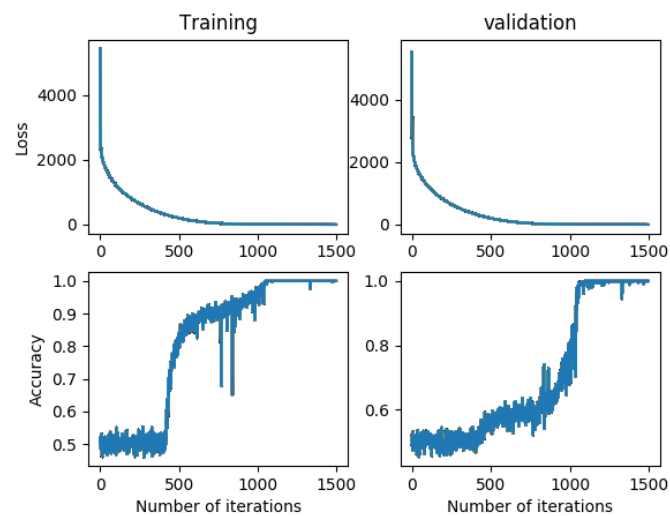
FIGURE 68. Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5

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
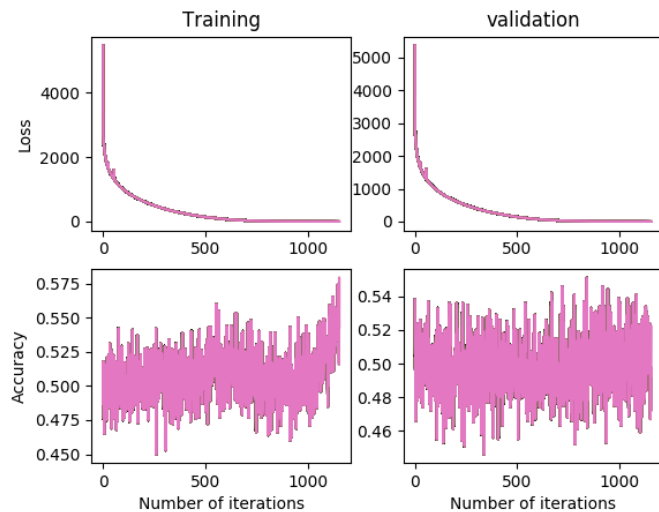
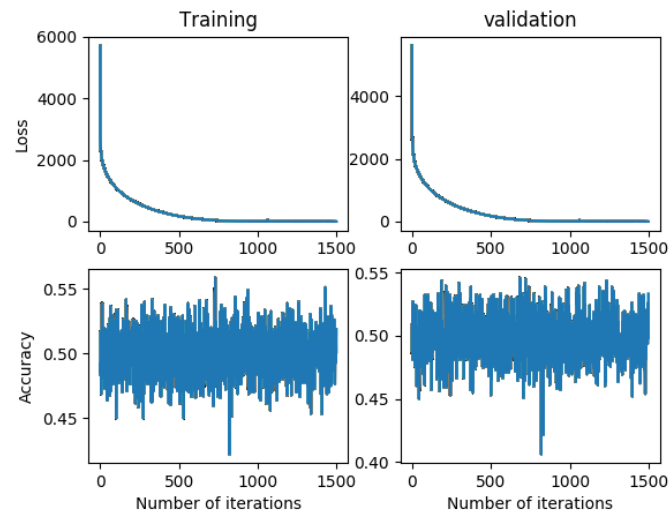FIGURE 71. Version 3: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
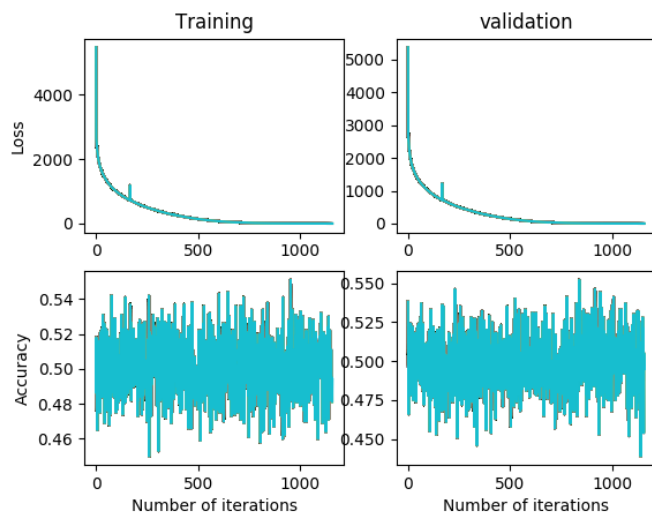
FIGURE 72. Version 4: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
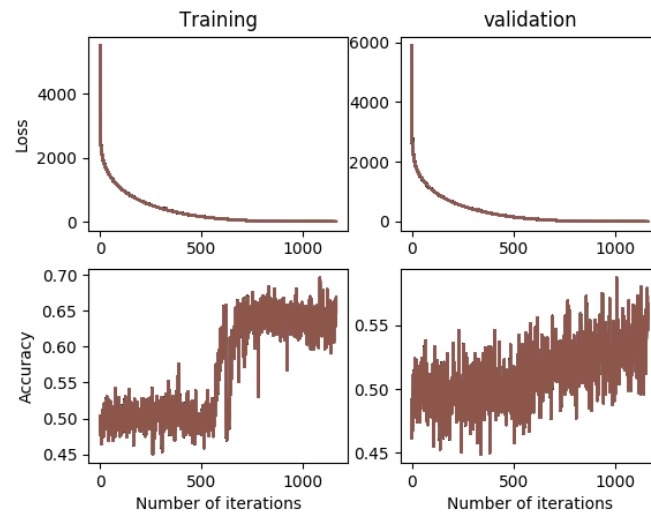
FIGURE 73. Version 5: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
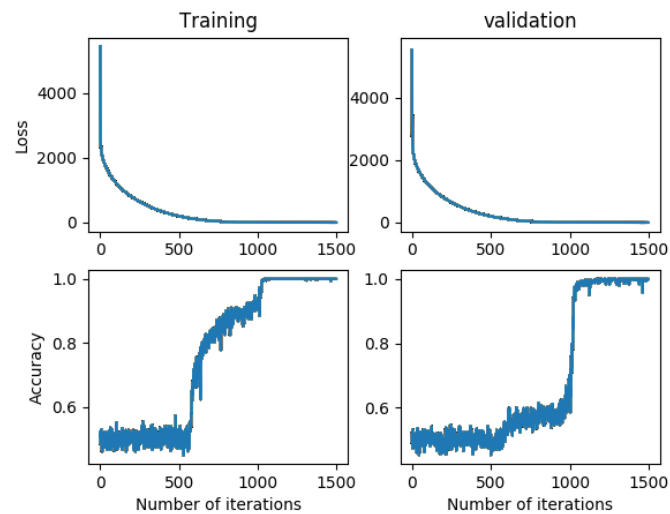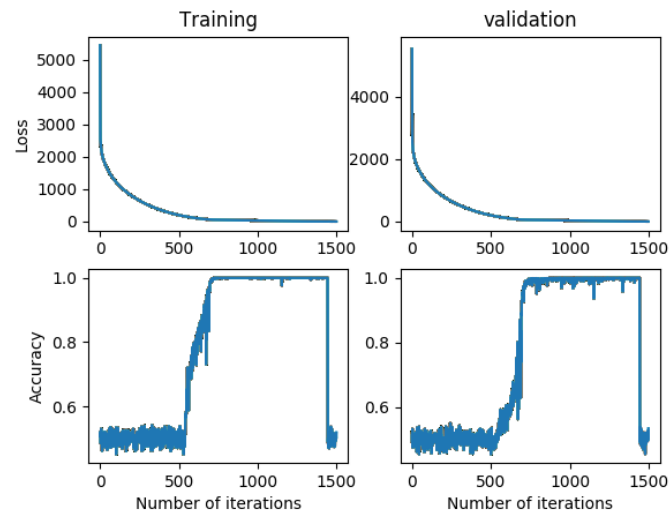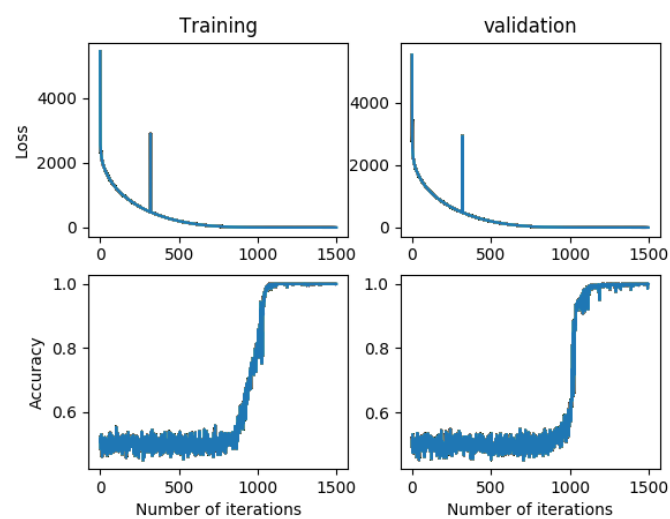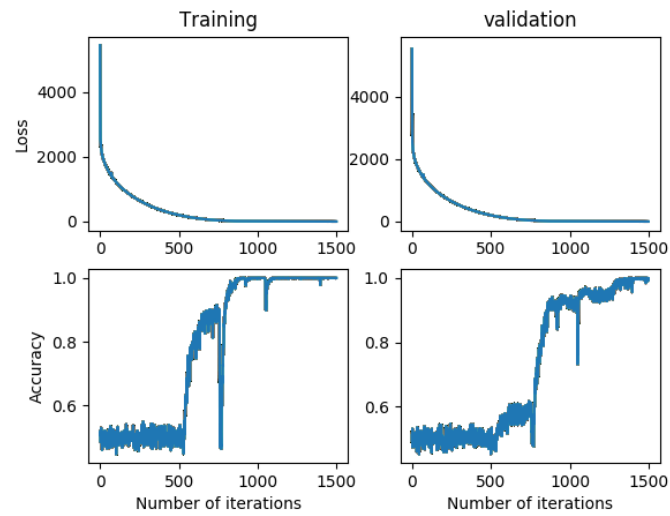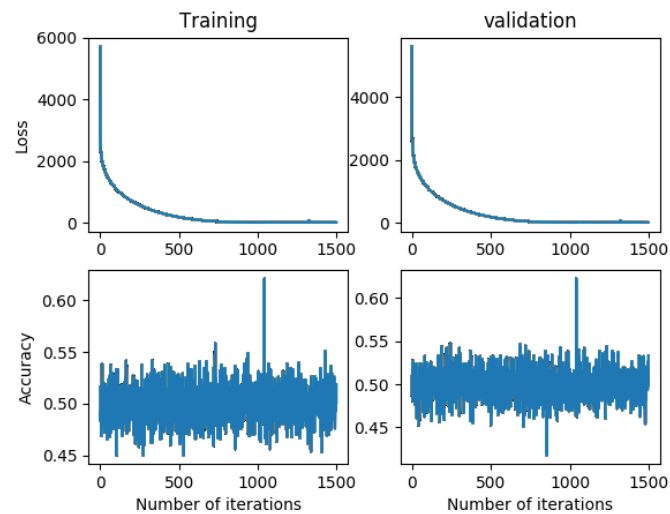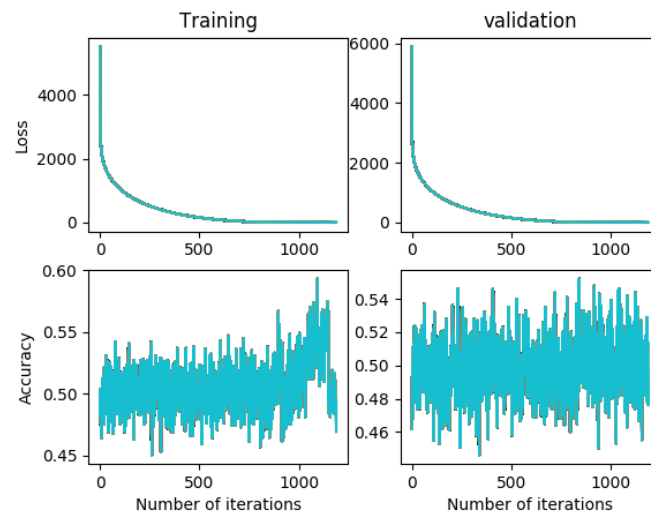

FIGURE 74. Version 6: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

(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.
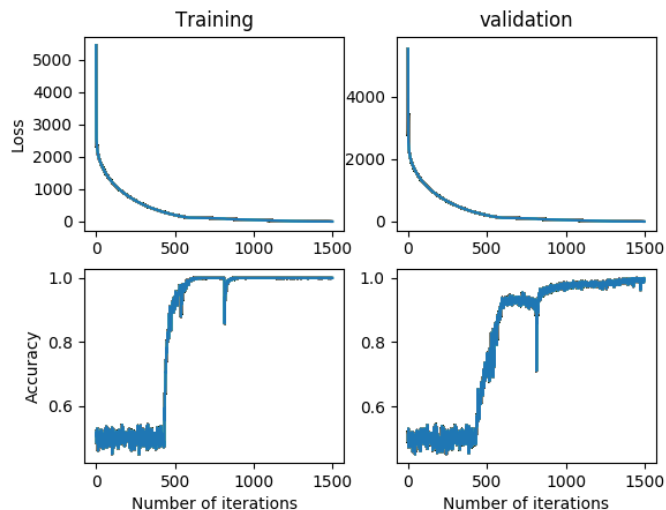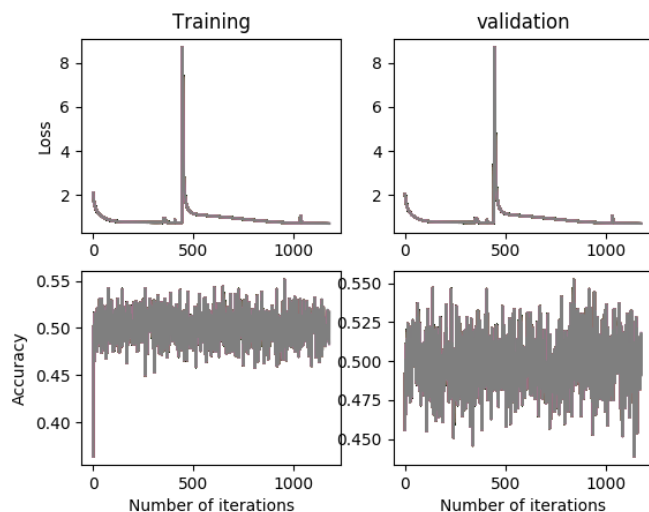

FIGURE 75. Version 5 step 1 trial 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
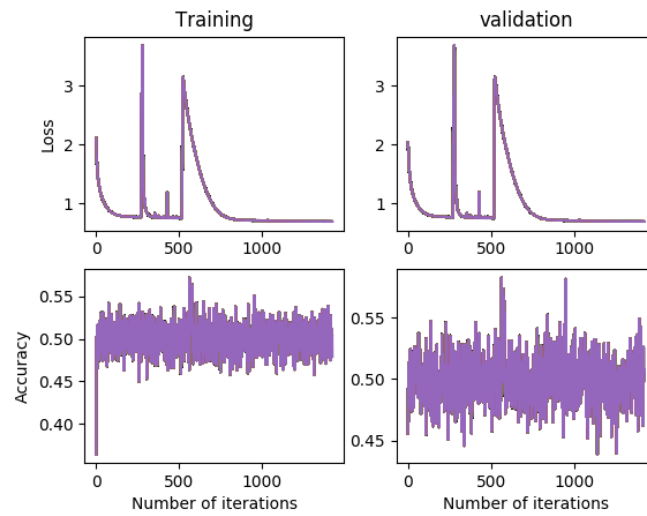
FIGURE 76. Version 5 step 1 trial 2: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
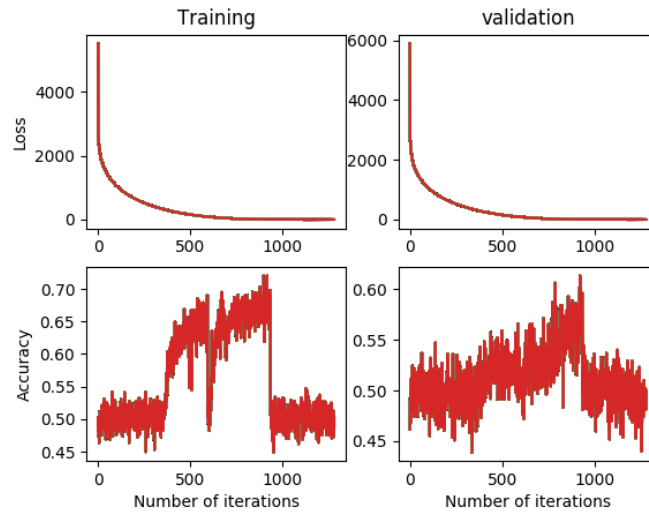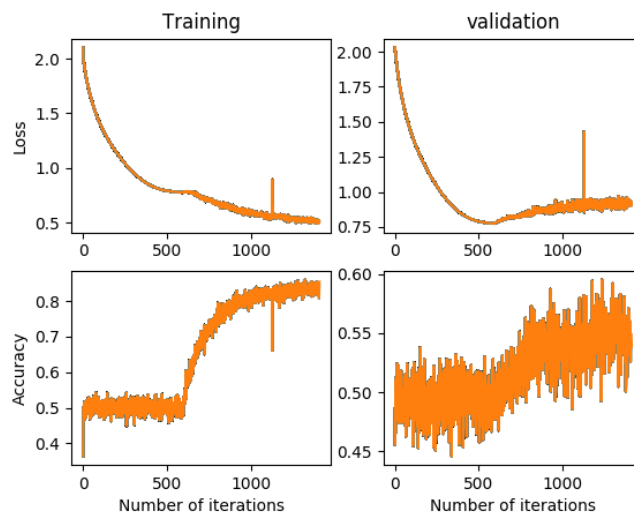

FIGURE 77. Version 5 step 1 trial 3: Initial Learning Rate = 1e-4, Final Learning Rate = 1e-5, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
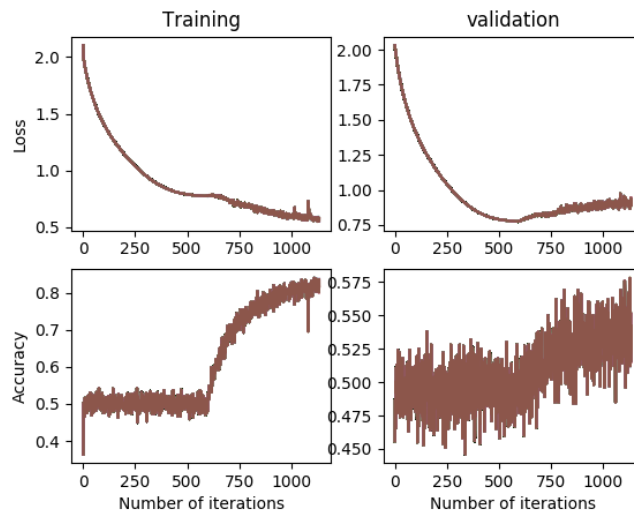
FIGURE 78. Version 5 step 1 trial 4: Initial Learning Rate = 1e-4, Final Learning Rate = 1e-5, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
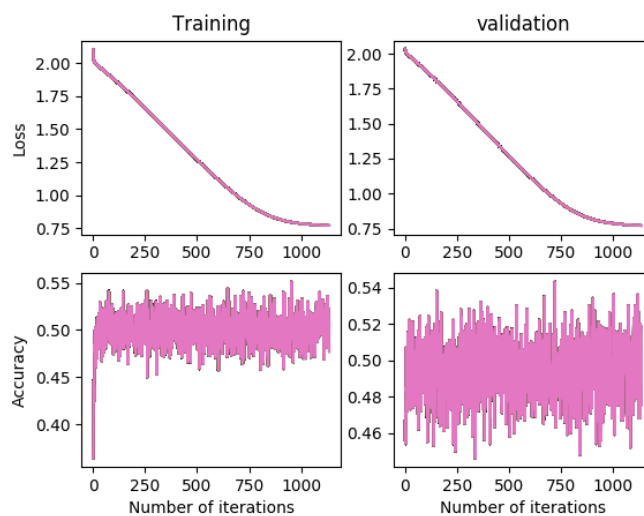
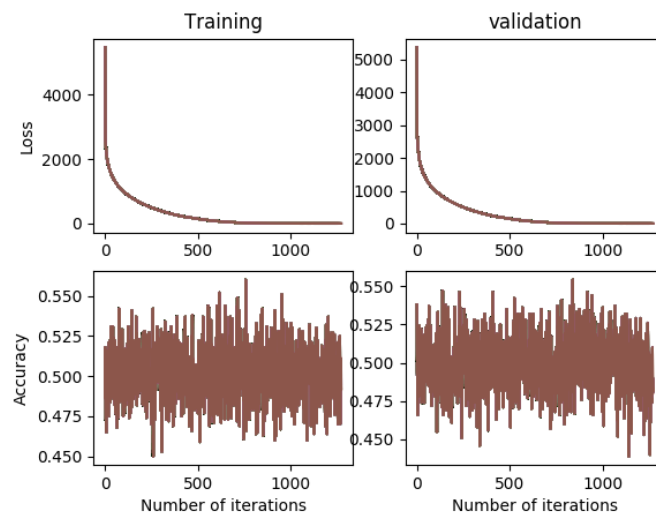FIGURE 79. Version 5 step 1 trial 5: Initial Learning Rate = 1e-5, Final Learning Rate = 1e-6, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true
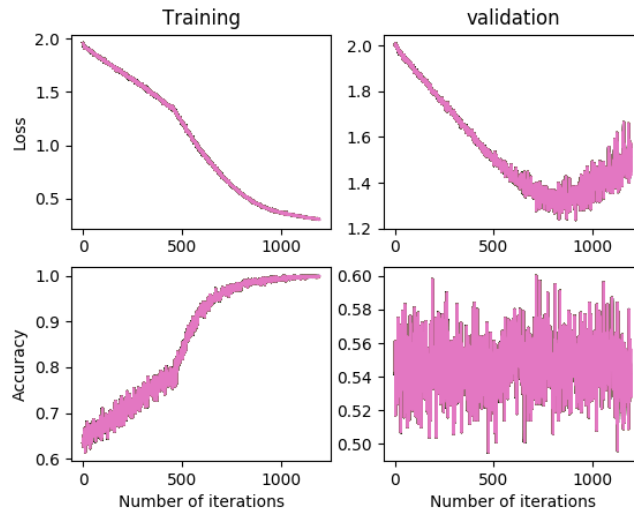
FIGURE 80. Version 5 step 1 trial 6: Initial Learning Rate = 1e-5, Final Learning Rate = 1e-6, Schedule Length = NA, Batch Size = 80, L2 beta = 0.01, Dropout = 0.4, data aug = true

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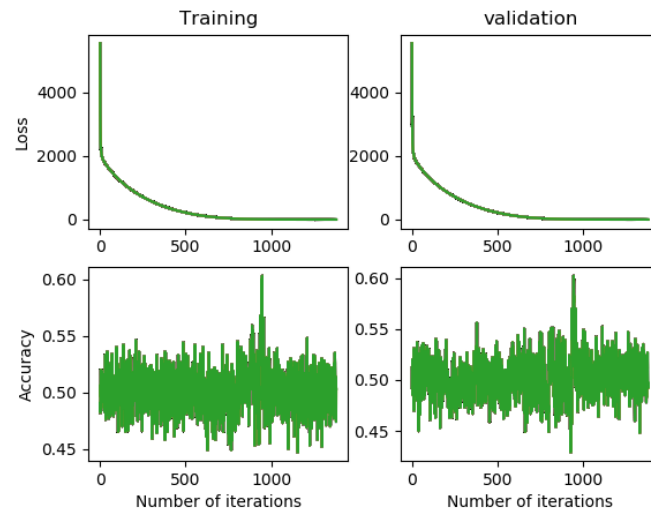
FIGURE 82. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

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 Learn-
ing 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 Learn-
ing 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 Learn-
ing Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01,
Dropout = 0.5, data aug = true
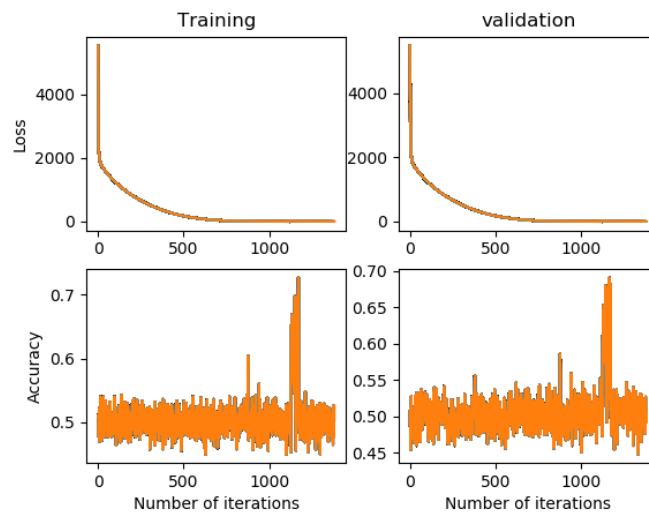

FIGURE 89. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learn-
ing Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01,
Dropout = 0.5, data aug = true

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.
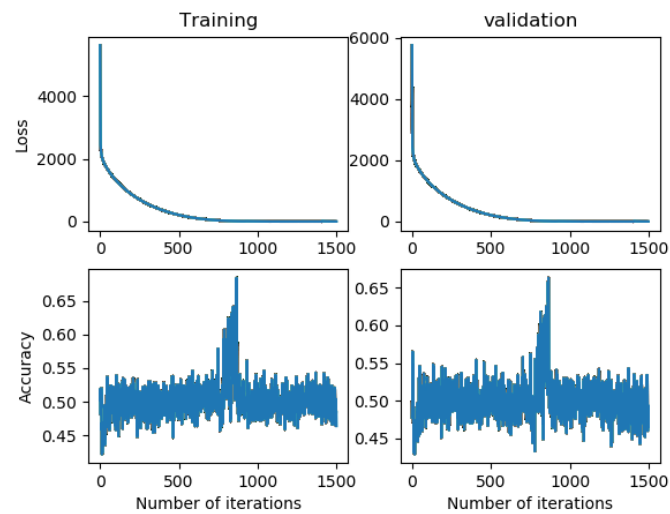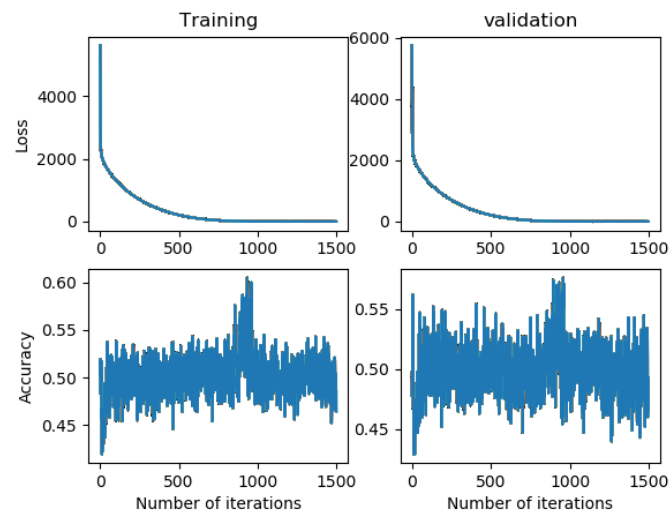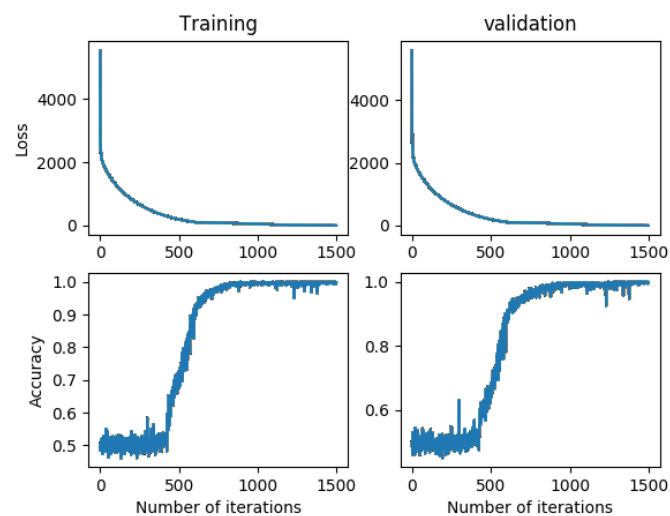(3) V2-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
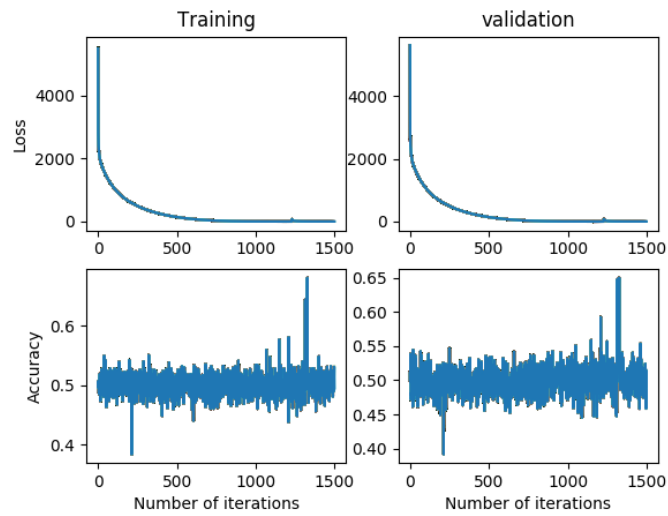(4) V3-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.
(5) V4-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, 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.
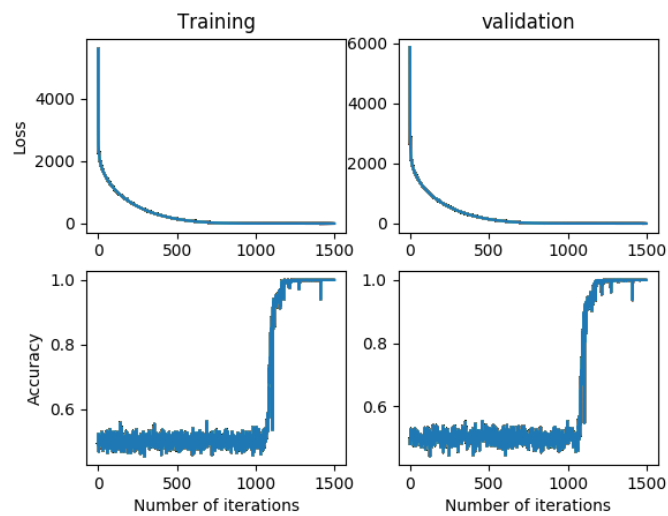
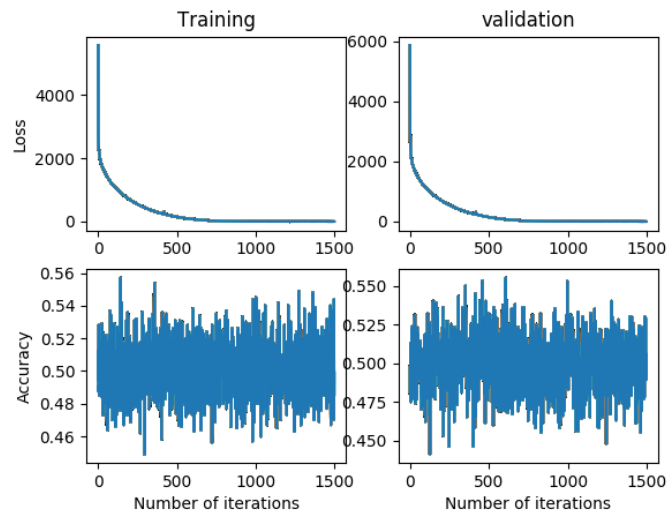(7) V6-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(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.
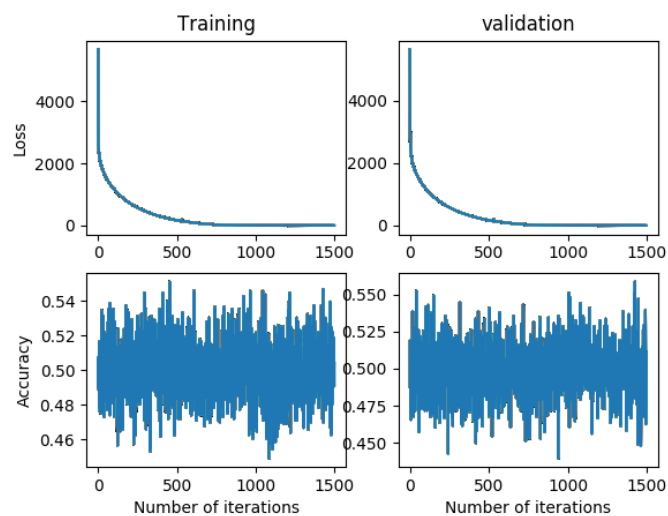
(10) V9-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.
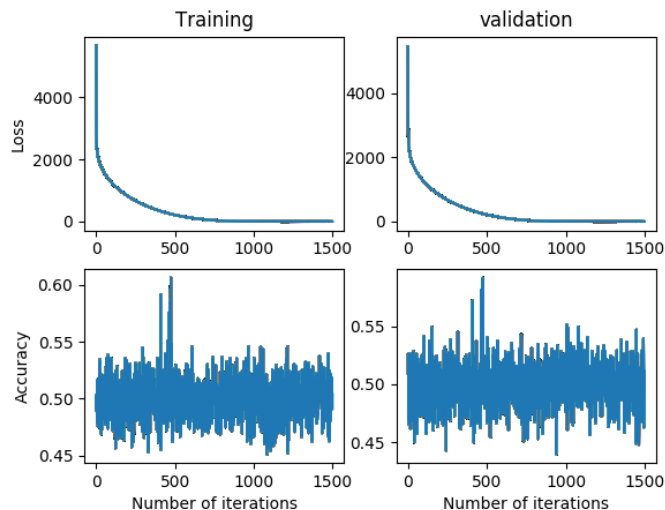
(11) V10-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(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
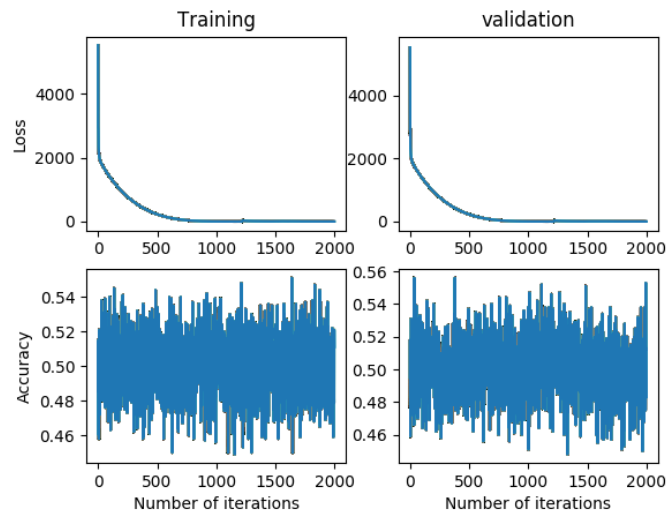

FIGURE 96. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true
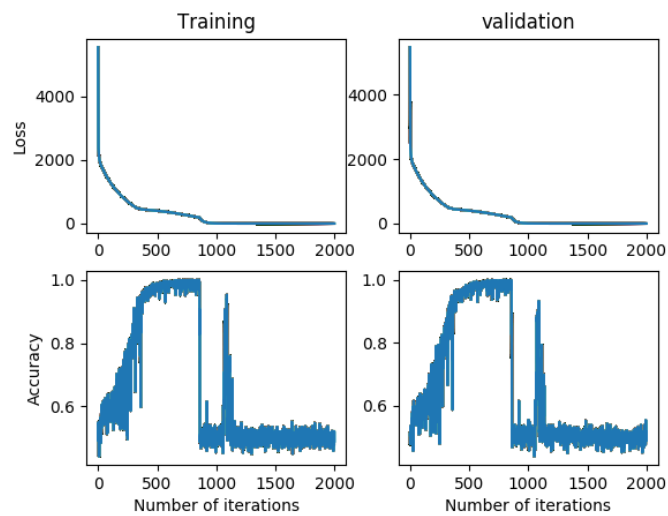
FIGURE 97. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

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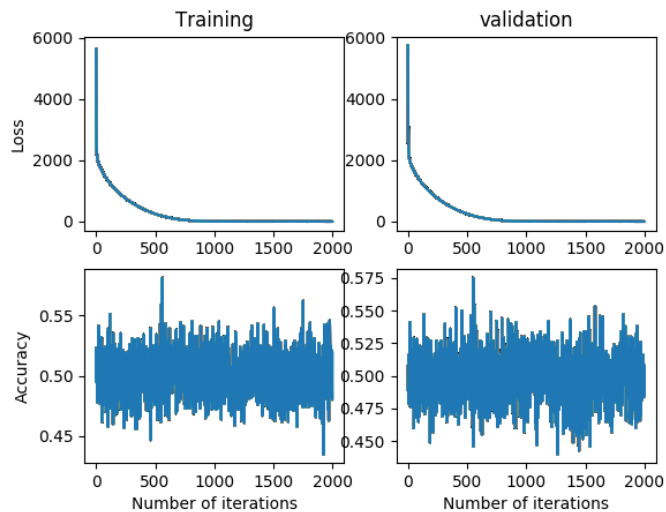
FIGURE 99. Version 9 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true

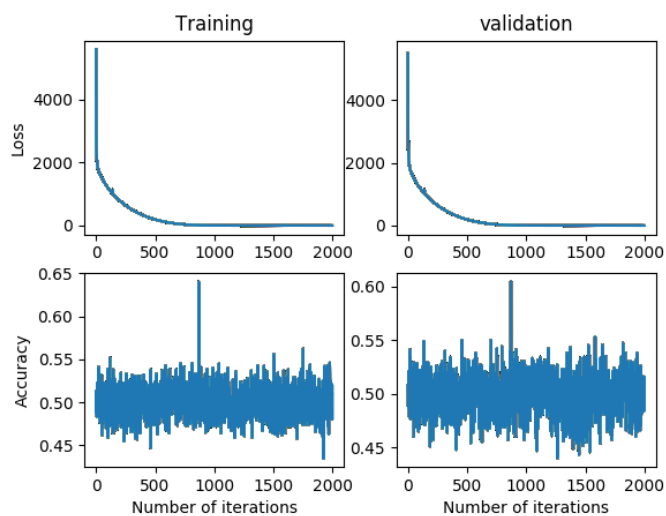FIGURE 100. Version 10 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta = 0.01, Dropout = 0.5, data aug = true
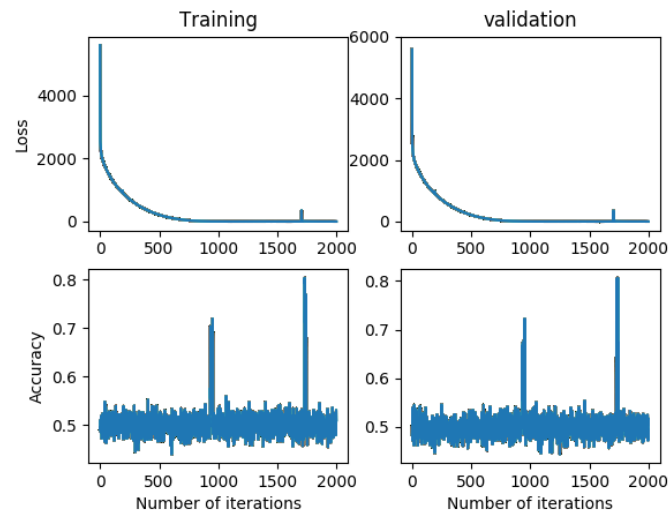
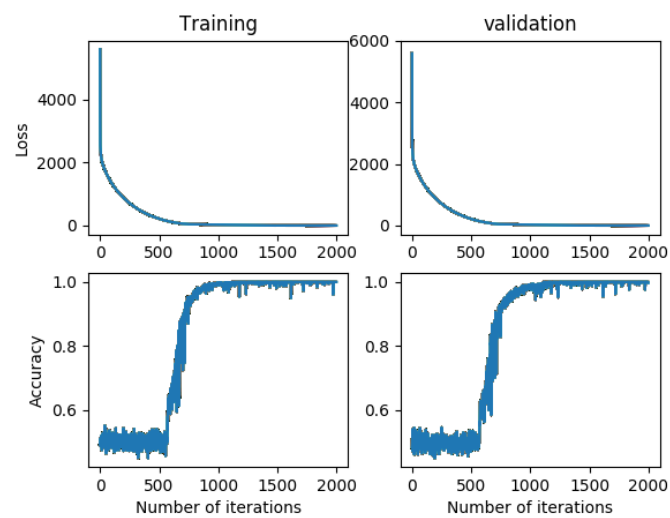FIGURE 101. Version 11 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

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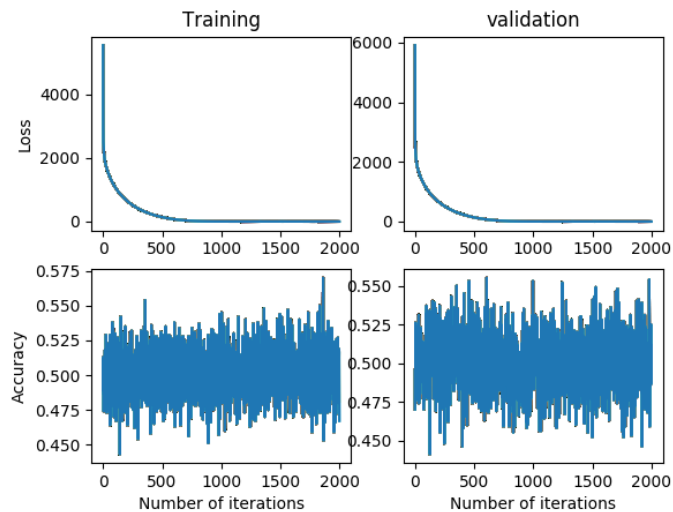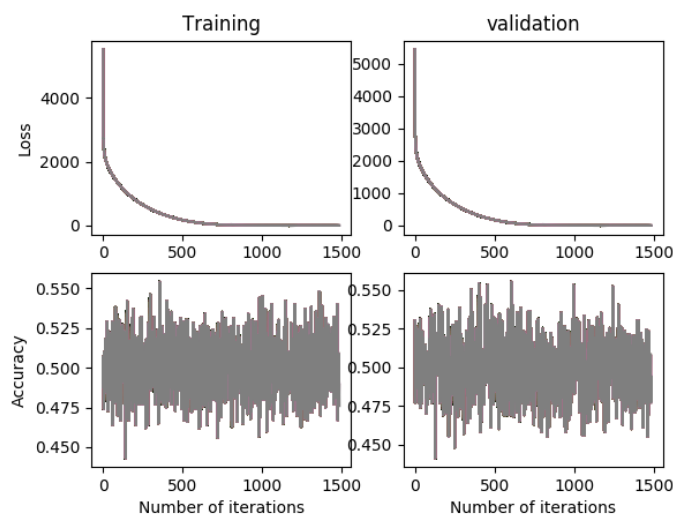
FIGURE 105. Version 15 step 1: Initial Learning Rate = 1e-3, Final
Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 150, L2 beta =
0.01, Dropout = 0.5, data aug = true

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 =
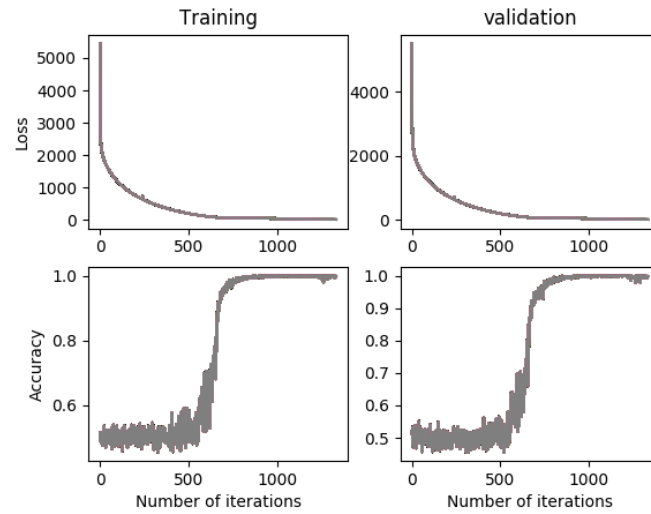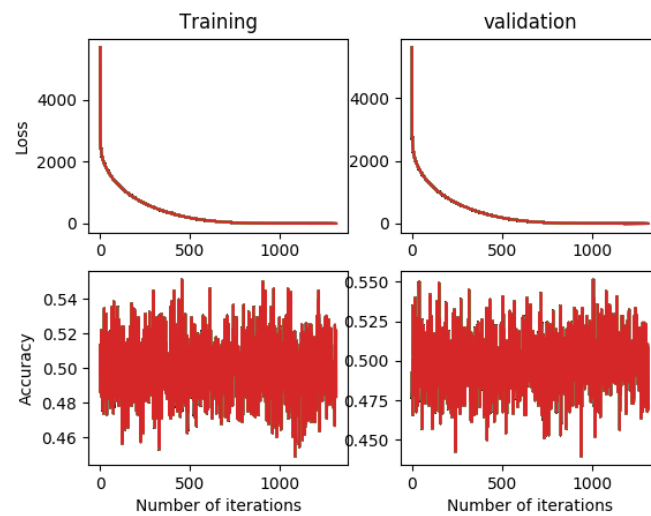0.01, Dropout = 0.5, data aug = true

(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.
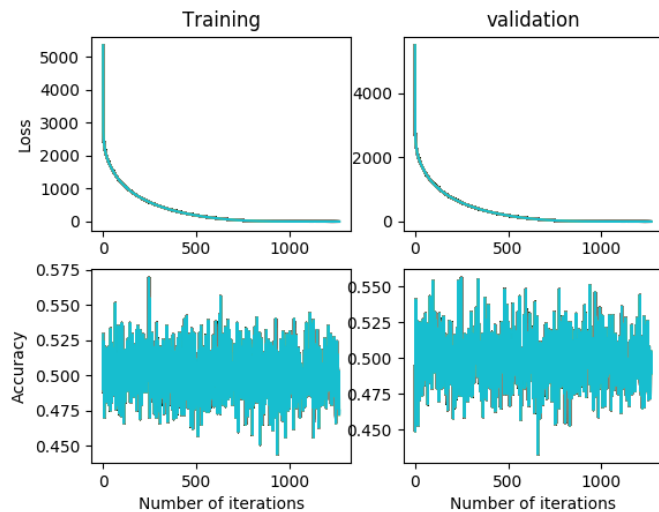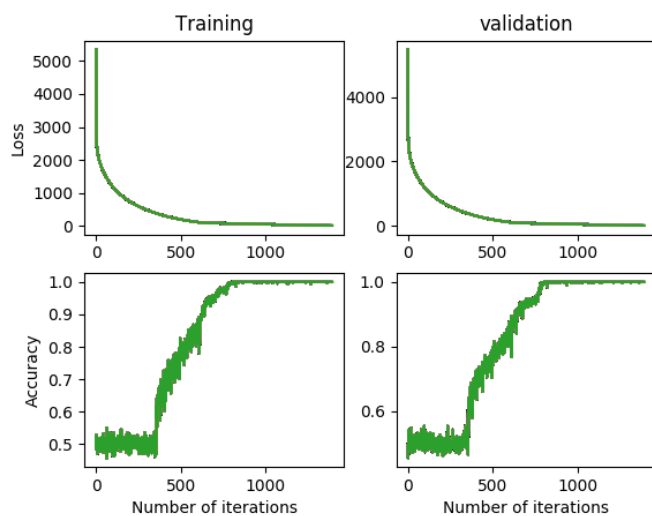
(6) V2-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true.
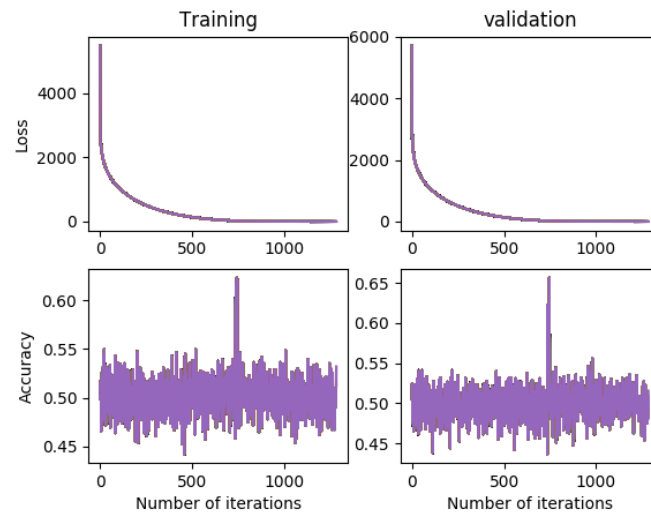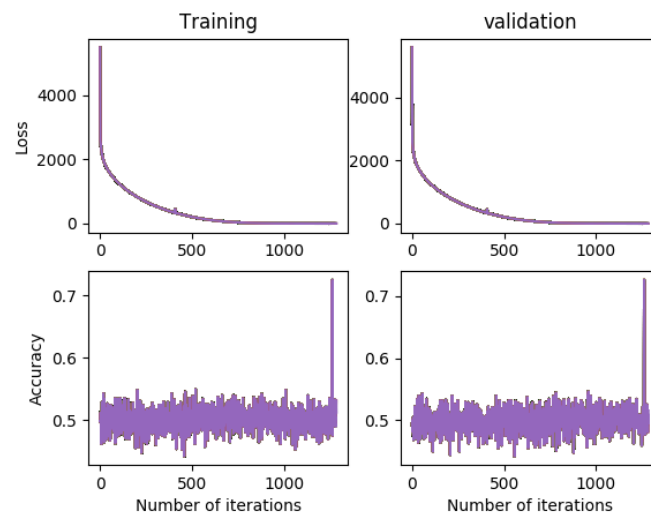
(7) V3-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(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.

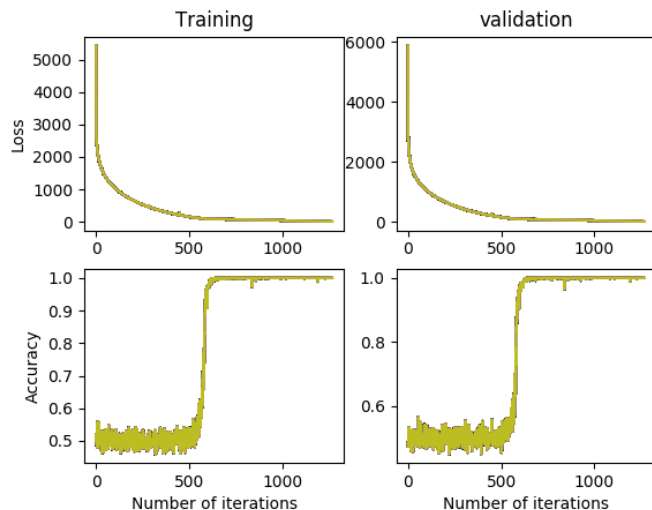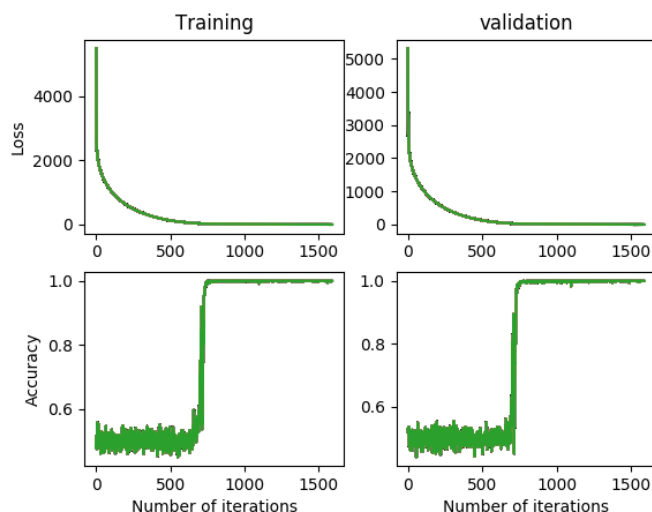(10) V6-S1 has hyperparameters: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true.

(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
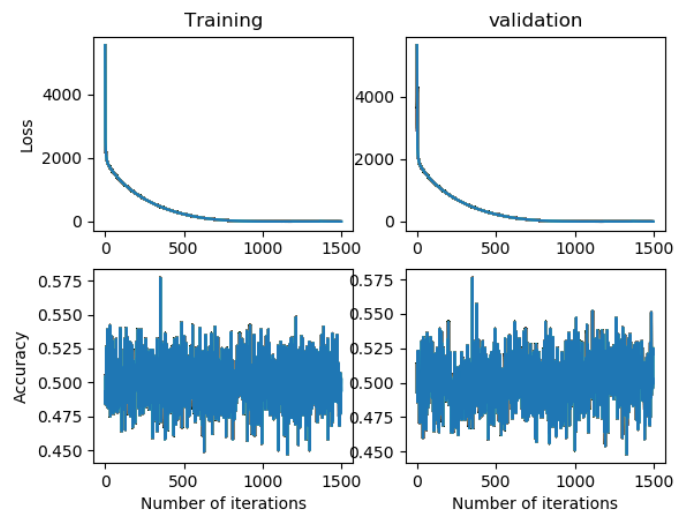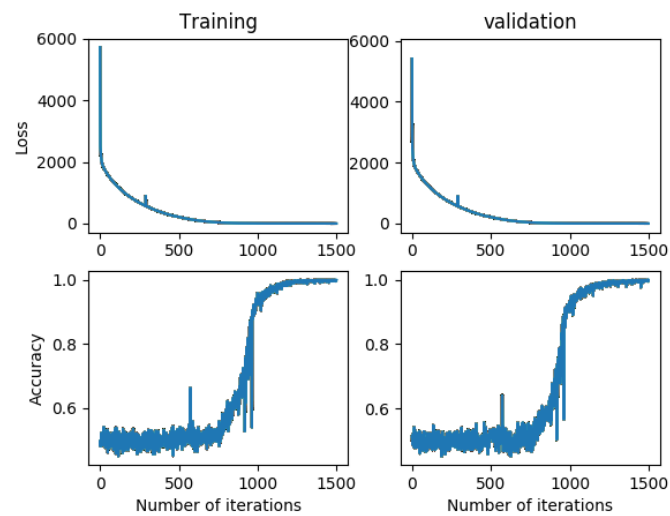

FIGURE 110. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true
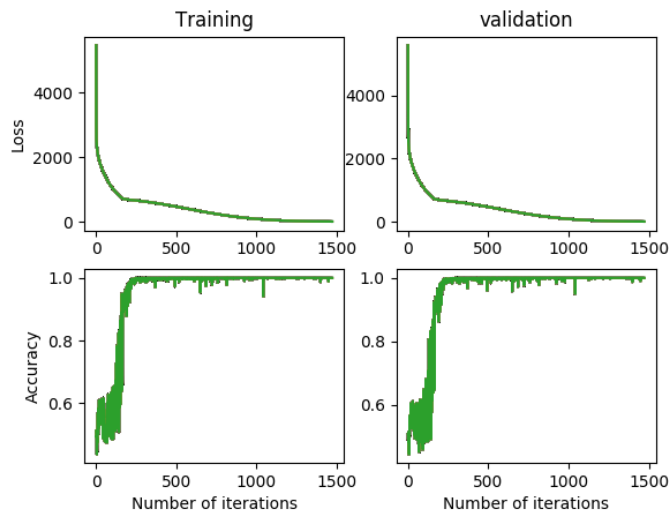
FIGURE 111. Version 5 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true

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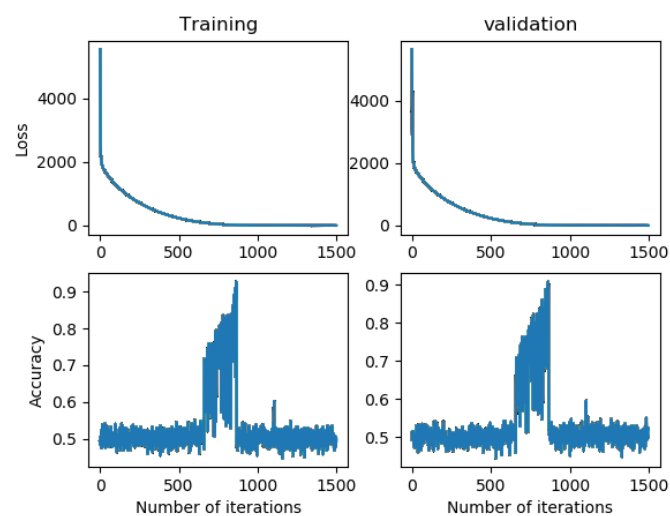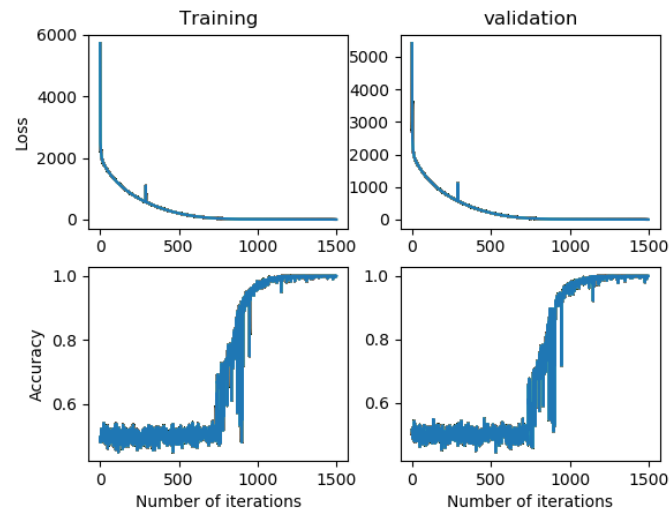
FIGURE 113. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true

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

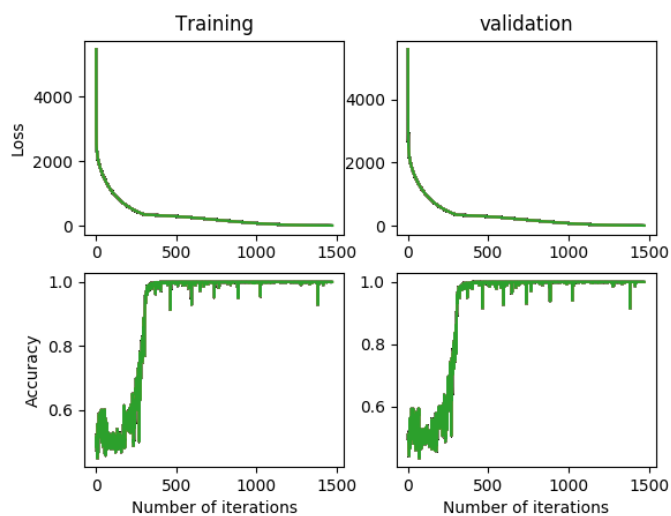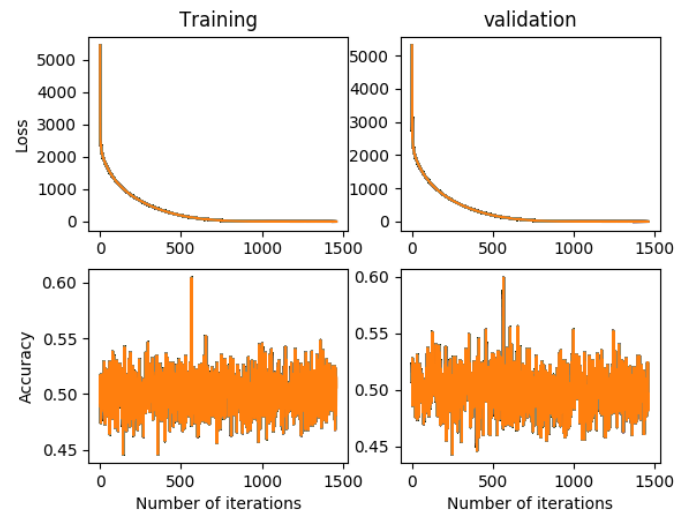FIGURE 116. Version 2 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 10, L2 beta = 0.01, Dropout = 0.5, data aug = true

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
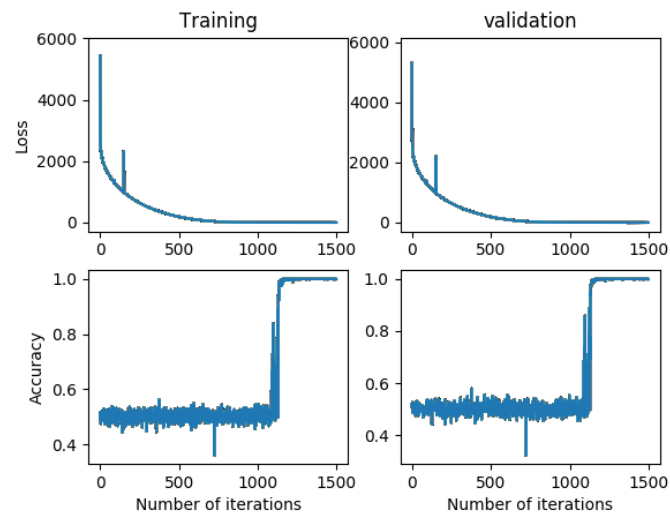

FIGURE 118. Version 4 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 20, L2 beta = 0.01, Dropout = 0.5, data aug = true

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
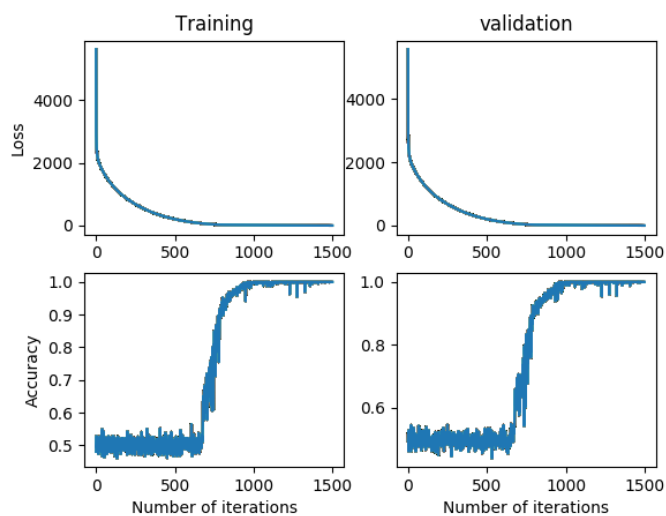
FIGURE 120. Version 6 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 30, L2 beta = 0.01, Dropout = 0.5, data aug = true
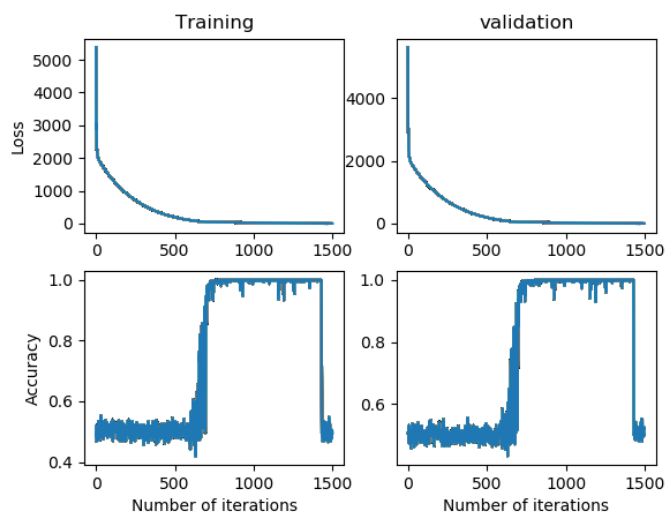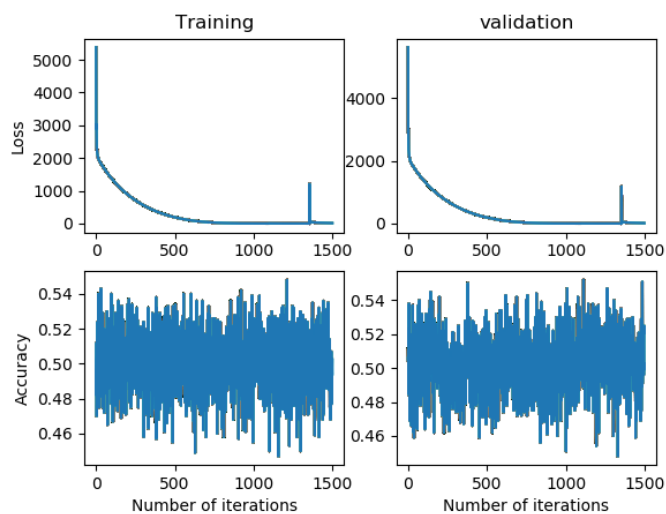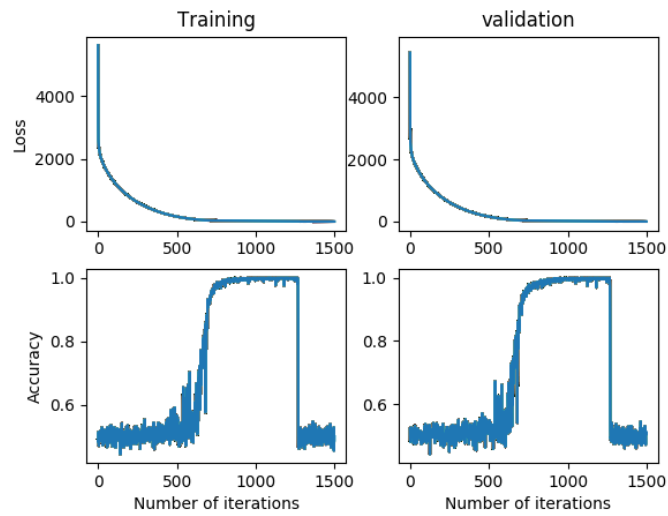
FIGURE 121. Version 7 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true
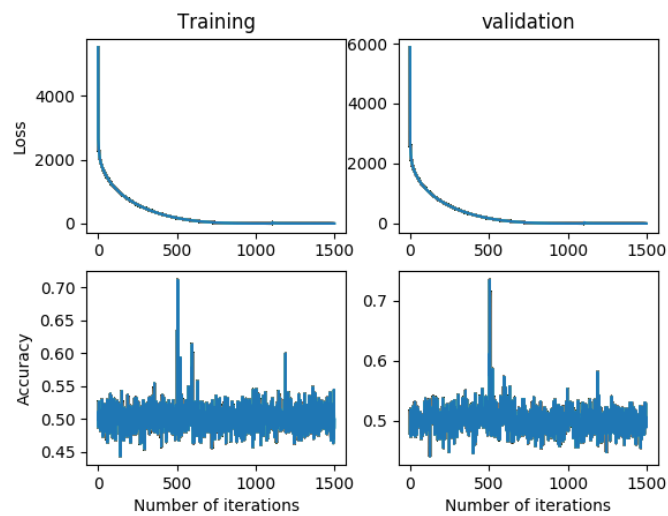
FIGURE 122. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 50, L2 beta = 0.01, Dropout = 0.5, data aug = true
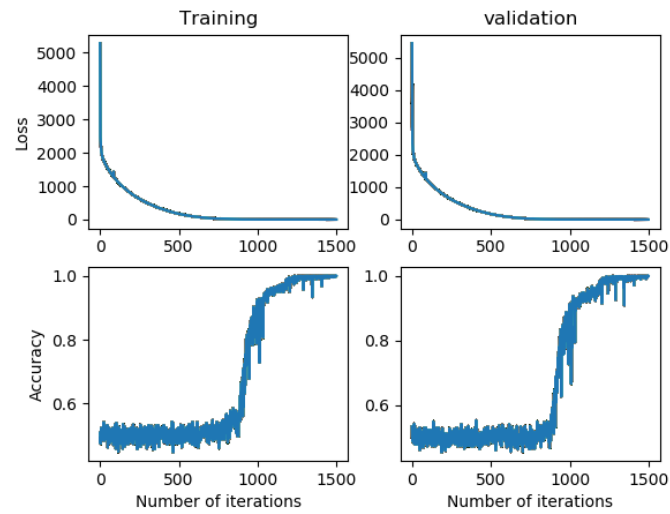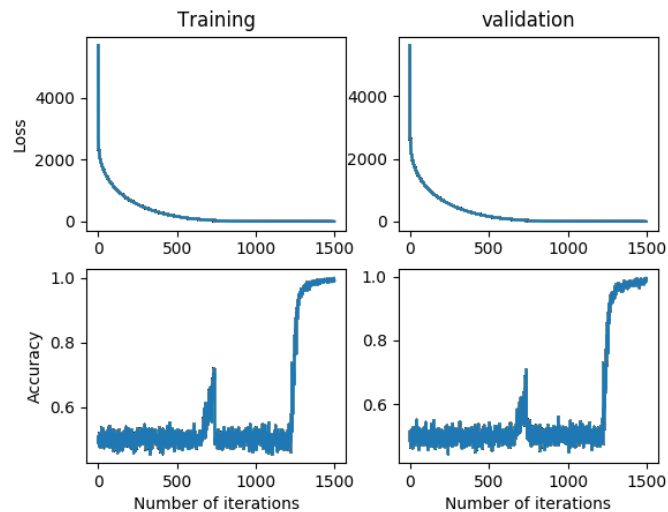
FIGURE 123. Version 8 step 1: Initial Learning Rate = 1e-3, Final
Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta
= 0.01, Dropout = 0.5, data aug = true
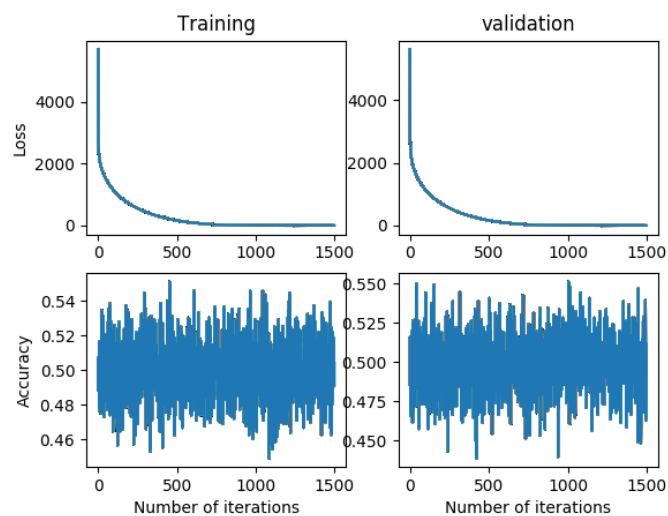
FIGURE 124. Version 8 step 1: Initial Learning Rate = 1e-3, Final
Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 80, L2 beta
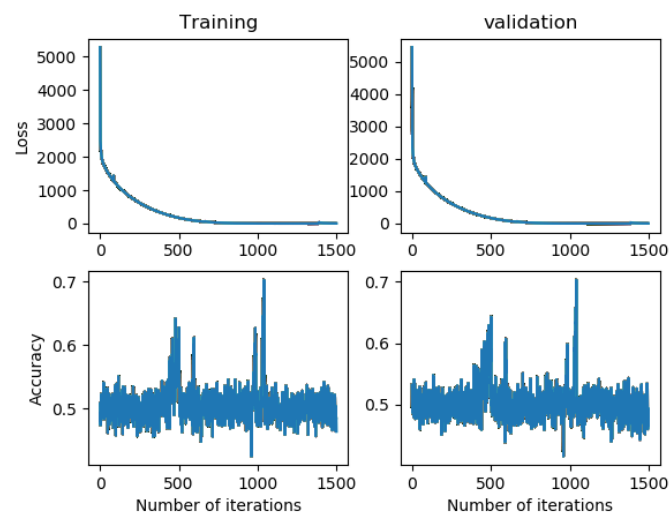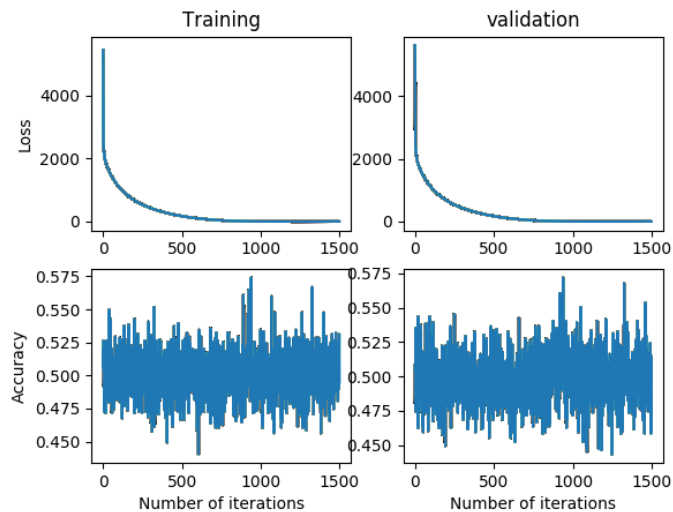= 0.01, Dropout = 0.5, data aug = true
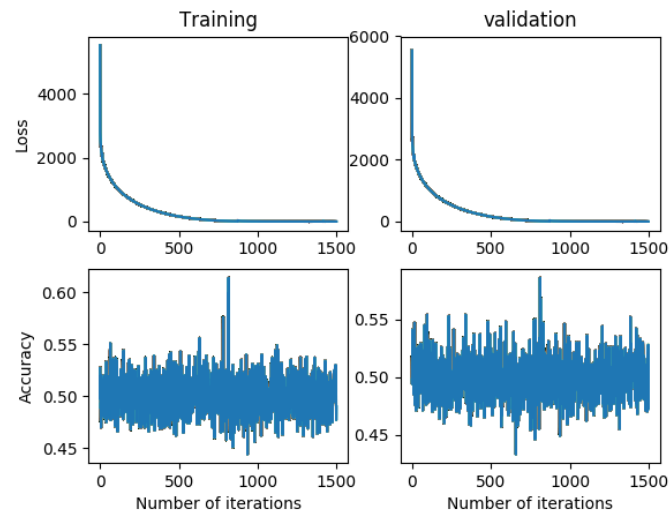
FIGURE 125. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true
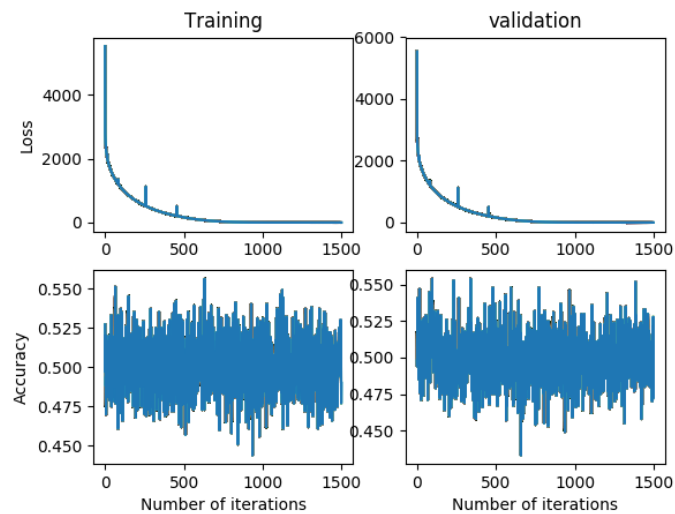
FIGURE 126. Version 8 step 1: Initial Learning Rate = 1e-3, Final Learning Rate = 1e-4, Eta threshold = 0.90, Batch Size = 100, L2 beta = 0.01, Dropout = 0.5, data aug = true

(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 metadata 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.

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