

Experiments

All our experiments are developed in the notebooks in the ./experiments folder.

We did the following experiments:

Modify the improved and dropout parameters in GCNConv: after trying all the possible combinations, we obtained the best result setting improved=False and dropout = 0, differently from the Paper instructions.

· Changing the learning rate:

trying to stabilize the shapes, we tried to modify the starting learning rate in Adam, having worse results in increasing and decreasing the number.

· Changing the convolutional method:

we tried to apply other two different libraries for convolution: *GraphConv* and *GeneralConv*.

We had the best result applying the *GeneralConv* method.

• Trying different parameters within GeneralConv:

we tried different configurations of parameters applying I2 normalization, attention, both types of attention (dot_product and additive), and multi-head attention.

We had the best result with *attention=True*, *attention_type='dot_product'*, without multi-head attention or normalization.

Trying adding residual connections:

we had really bad results.

• Trying using a different type of activation function:

we tried using both ReLU and LeakyReLU, having worse results.

• Changing the batch size = 32:

Changing the batch size, we had test loss and accuracy a little bit worse than our best case but we had smoother shapes. Nevertheless, we have bad shapes in validation tests, which seem to tend toward overfitting.

Removing the decoder:

We did three versions:

- 1. Paper implementation without decoder
- 2. Best results we had in the past without decoder
- 3. Paper implementation without decoder with residual connections (the best result we ever had)

Improved and dropout experiments

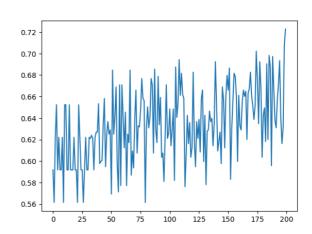
Improved=True, con dropout

Test loss epoch 199: 0.6707518696784973 Test accuracy epoch 199: 0.5892857142857143

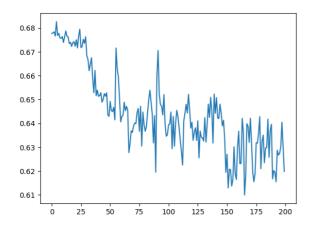
Train Losses

0.72 -0.70 -0.66 -0.64 -0.62 -0.60 -0 25 50 75 100 125 150 175 200

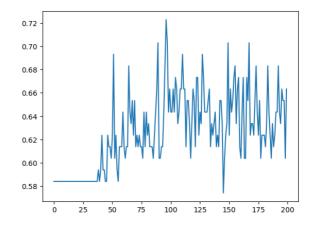
Train Accuracies



Validation Losses



Validation Accuracies

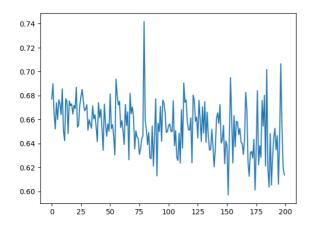


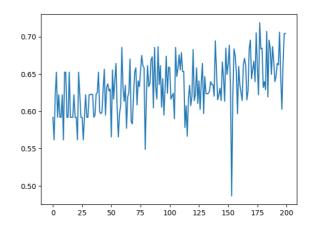
Improved=True, senza dropout

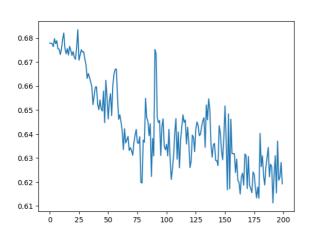
Test loss epoch 199: 0.6591243147850037 Test accuracy epoch 199: 0.6428571428571429

Train Losses

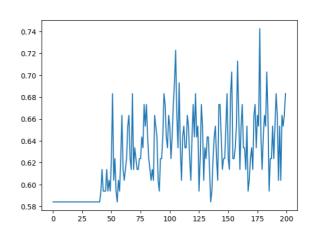
Train Accuracies







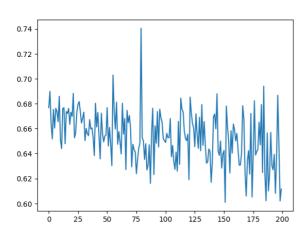
Validation Accuracies



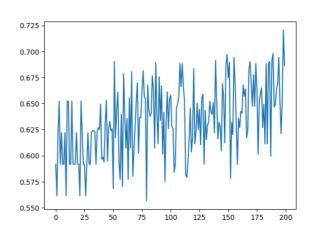
Improved=False, senza dropout

Test loss epoch 199: 0.631967306137085 Test accuracy epoch 199: 0.6696428571428571

Train Losses

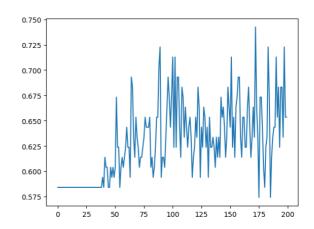


Train Accuracies



0.68 - 0.66 - 0.62 - 0.60 - 0.60 - 0.5 50 75 100 125 150 175 200

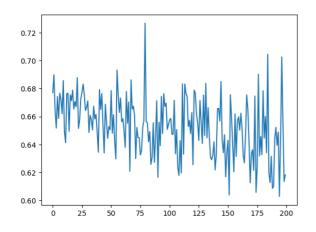
Validation Accuracies



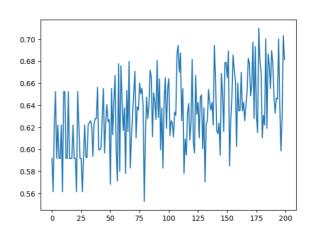
Improved=False, con dropout (Paper)

Test loss epoch 199: 0.6583368182182312 Test accuracy epoch 199: 0.6517857142857143

Train Losses

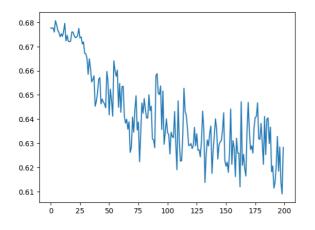


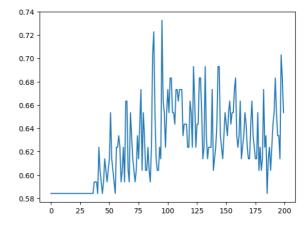
Train Accuracies



Validation Losses

Validation Accuracies





Learning rate experiments

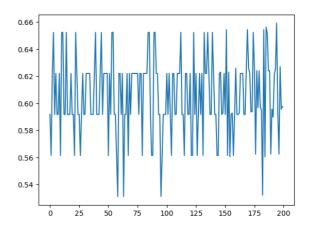
Adam starting at 0,0001

Test loss epoch 199: 0.6822512745857239 Test accuracy epoch 199: 0.5446428571428571

Train Losses

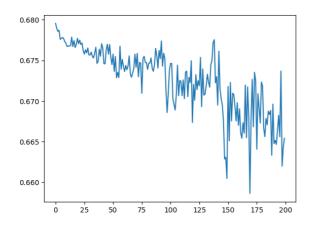
0.70 -0.69 -0.68 -0.67 -0.66 -0.65 -0.64 -0 25 50 75 100 125 150 175 200

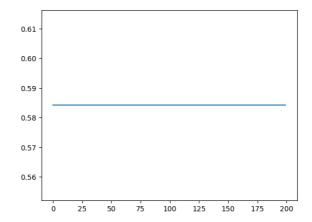
Train Accuracies



Validation Losses

Validation Accuracies

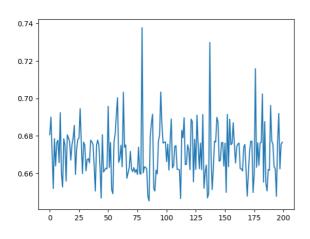




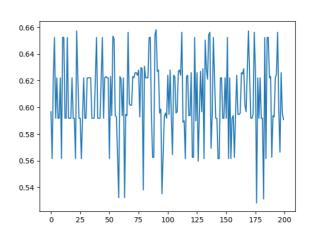
Adam starting at 0,01

Test loss epoch 199: 0.6921302676200867 Test accuracy epoch 199: 0.5446428571428571

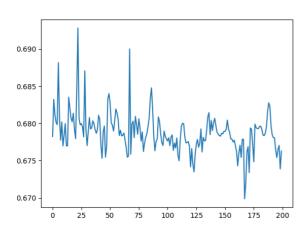
Train Losses



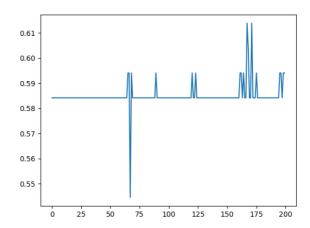
Train Accuracies



Validation Losses



Validation Accuracies

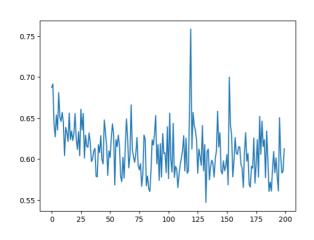


6

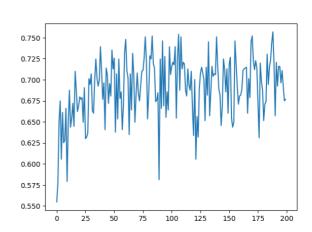
Try GraphConv

Test loss epoch 199: 0.6018216013908386 Test accuracy epoch 199: 0.6964285714285714

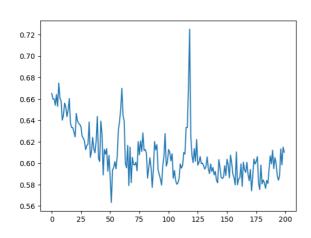
Train Losses



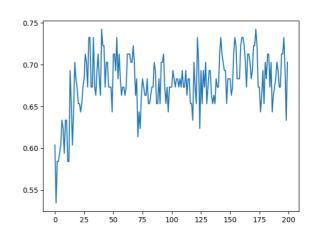
Train Accuracies



Validation Losses



Validation Accuracies



Try GeneralConv

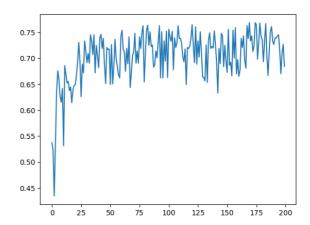
GeneralConv(dataset.num_features, 16, directed_msg = False, attention_type= 'dot_product')

Test loss epoch 199: 0.5975242853164673 Test accuracy epoch 199: 0.6696428571428571

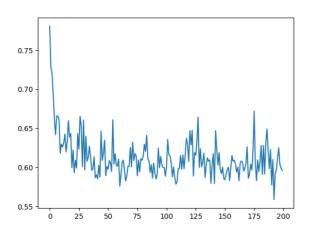
Train Losses

2.25 -2.00 -1.75 -1.50 -1.25 -1.00 -0.75 -0.50 -0 25 50 75 100 125 150 175 200

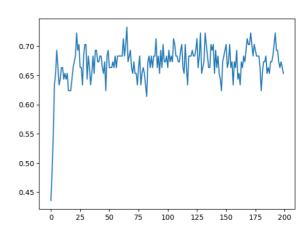
Train Accuracies



Validation Losses



Validation Accuracies



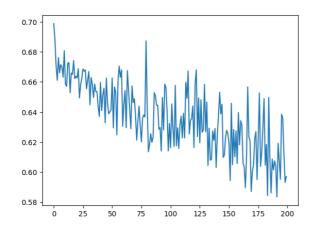
8

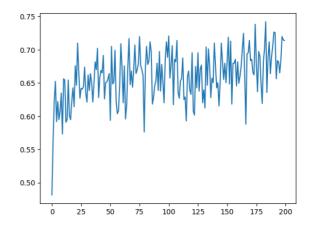
GeneralConv(dataset.num_features, 16, directed_msg = False,l2_normalize=True, attention_type= 'dot_product')

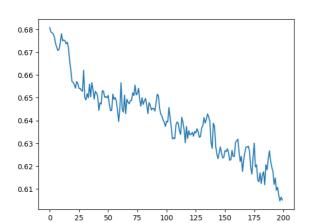
Test loss epoch 199: 0.6247297525405884 Test accuracy epoch 199: 0.6875

Train Losses

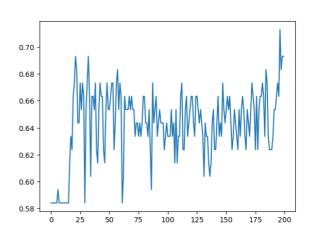
Train Accuracies







Validation Accuracies

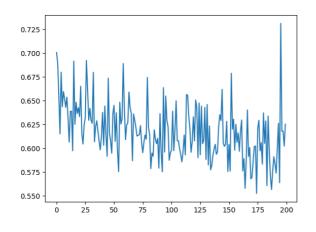


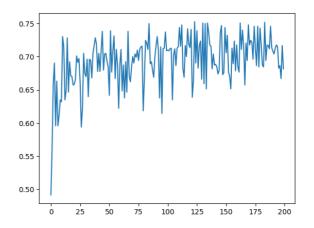
GeneralConv(dataset.num_features, 16, directed_msg = False,attention= True, attention_type= 'dot_product') (best result)

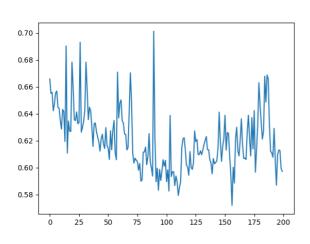
Test loss epoch 199: 0.6134846806526184
Test accuracy epoch 199: 0.7232142857142857

Train Losses

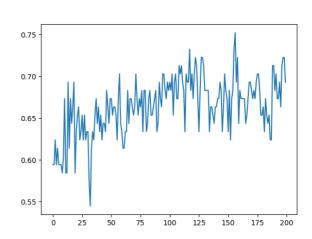
Train Accuracies







Validation Accuracies

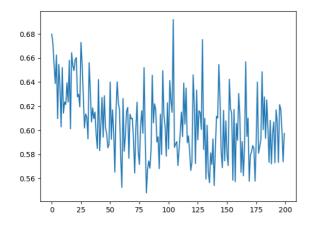


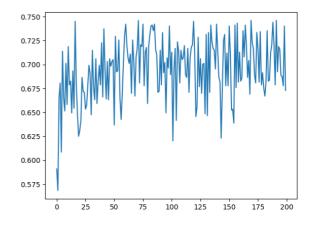
GeneralConv(dataset.num_features, 16, directed_msg = False,attention= True, attention_type= 'additive')

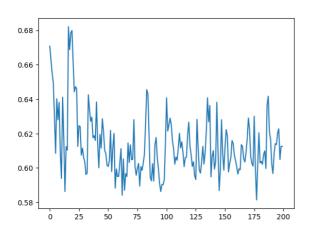
Test loss epoch 199: 0.6249549984931946 Test accuracy epoch 199: 0.6875

Train Losses

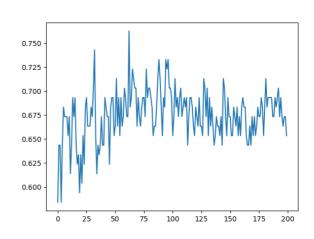
Train Accuracies







Validation Accuracies

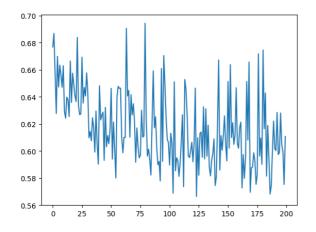


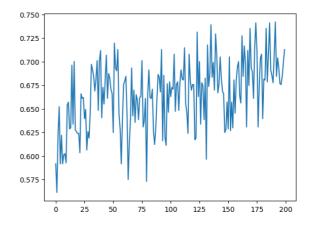
GeneralConv(dataset.num_features, 16, directed_msg = False,heads = 4,attention= True, attention_type= 'additive')

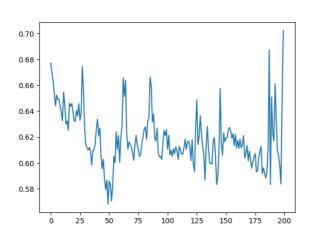
Test loss epoch 199: 0.7227734327316284 Test accuracy epoch 199: 0.6339285714285714

Train Losses

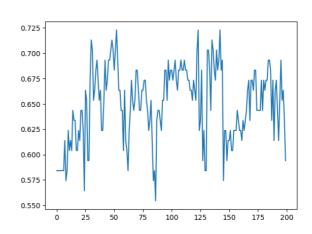
Train Accuracies







Validation Accuracies

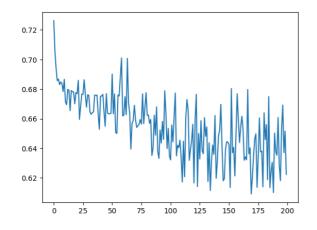


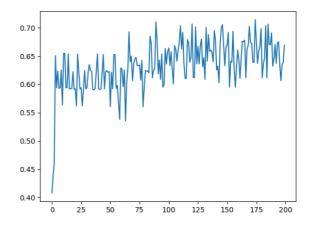
GeneralConv(dataset.num_features, 16, directed_msg = False,heads = 8,attention= True, attention_type= 'additive')

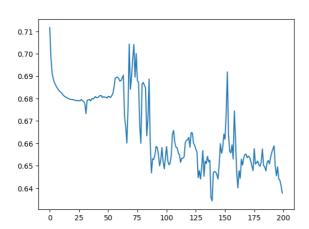
Test loss epoch 199: 0.7227734327316284 Test accuracy epoch 199: 0.6339285714285714

Train Losses

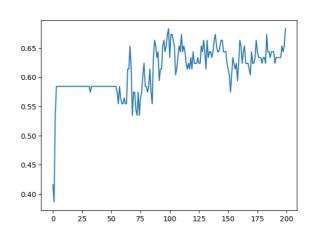
Train Accuracies







Validation Accuracies

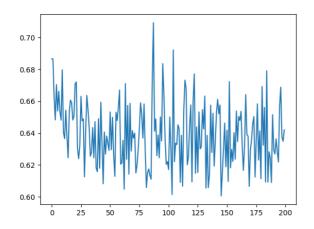


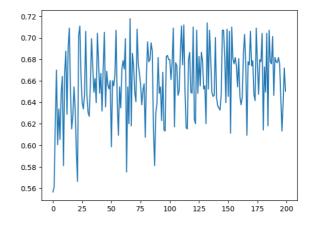
GeneralConv(dataset.num_features, 16, directed_msg = False,heads = 4,attention= True, attention_type= 'dot_product')

Test loss epoch 199: 0.6792422533035278
Test accuracy epoch 199: 0.6071428571428571

Train Losses

Train Accuracies



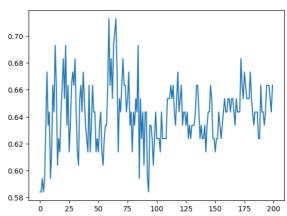


0.64

0.62



Validation Accuracies



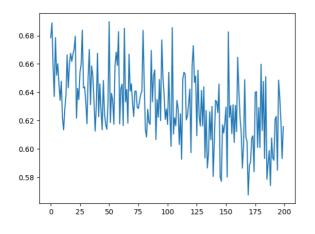
GeneralConv(dataset.num_features, 16, directed_msg =

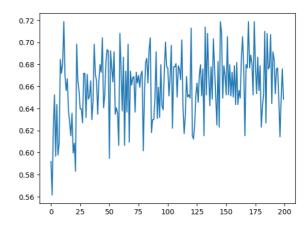
False,heads = 8,attention= True, attention_type= 'dot_product')

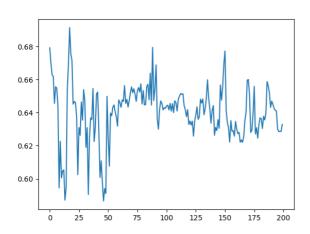
Test loss epoch 199: 0.6555837392807007 Test accuracy epoch 199: 0.5714285714285714

Train Losses

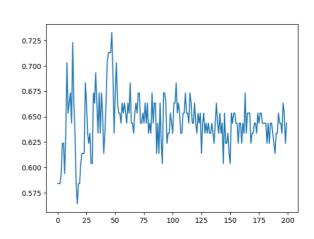
Train Accuracies







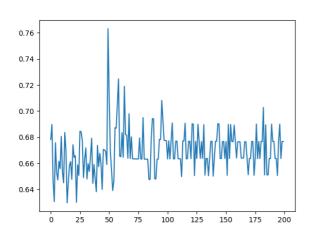
Validation Accuracies



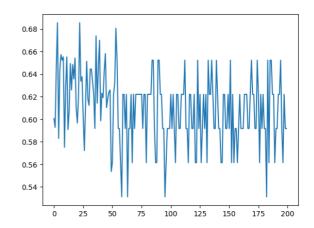
Add residual connections

Test loss epoch 199: 0.7007536292076111
Test accuracy epoch 199: 0.5357142857142857

Train Losses

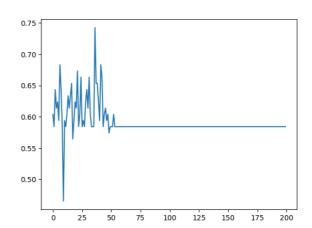


Train Accuracies



0.72 -0.70 -0.68 -0.64 -0.62 -0 25 50 75 100 125 150 175 200

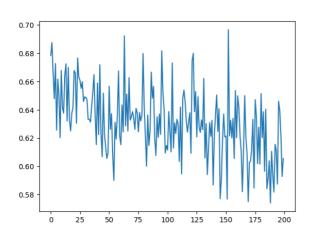
Validation Accuracies



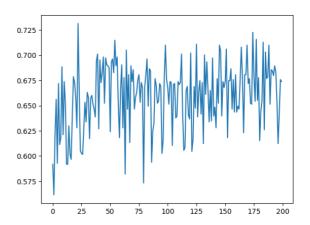
Use ReLU

Test loss epoch 199: 0.6443879008293152 Test accuracy epoch 199: 0.6339285714285714

Train Losses

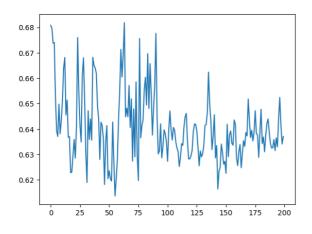


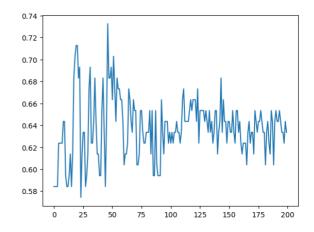
Train Accuracies



Validation Losses

Validation Accuracies





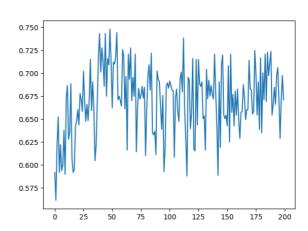
Use LeakyReLU

Test loss epoch 199: 0.6375139355659485 Test accuracy epoch 199: 0.6517857142857143

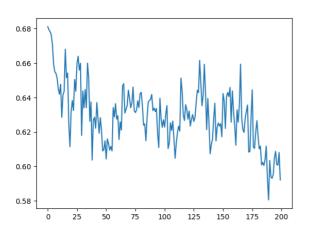
Train Losses

0.68 -0.66 -0.64 -0.62 -0.60 -0.58 -0.56 -0 25 50 75 100 125 150 175 200

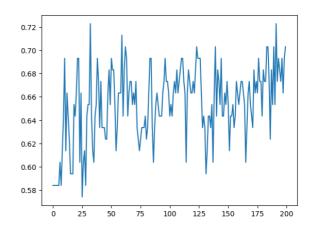
Train Accuracies



Validation Losses



Validation Accuracies



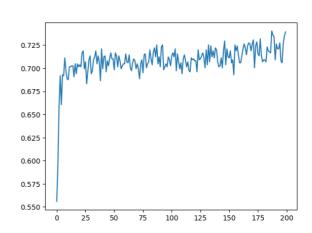
Change the batch size = 32

Test loss epoch 199: 0.6346642673015594 Test accuracy epoch 199: 0.7109375

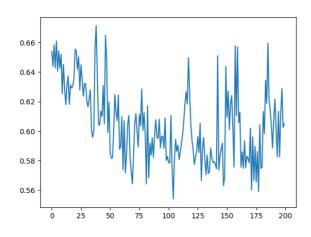
Train Losses

0.68 -0.66 -0.64 -0.60 -0.58 -0.56 -0 25 50 75 100 125 150 175 200

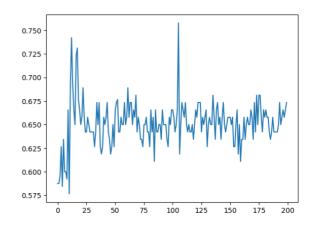
Train Accuracies



Validation Losses



Validation Accuracies



Remove the decoder

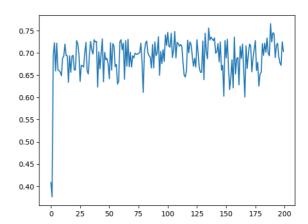
On paper implementation

Test loss epoch 199: 0.6045722961425781 Test accuracy epoch 199: 0.7142857142857143

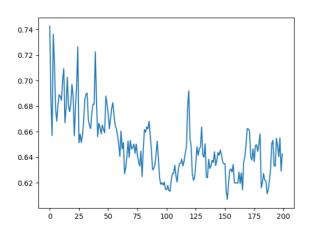
Train Losses

0.75 -0.70 -0.65 -0.60 -0.55 -0 25 50 75 100 125 150 175 200

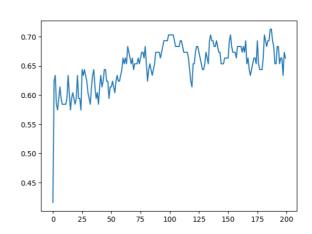
Train Accuracies



Validation Losses



Validation Accuracies

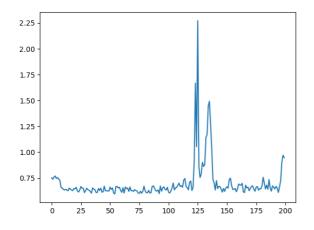


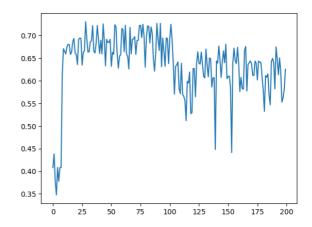
On best case

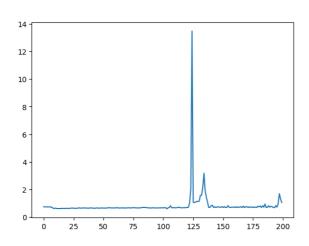
Test loss epoch 199: 0.948885440826416 Test accuracy epoch 199: 0.5982142857142857

Train Losses

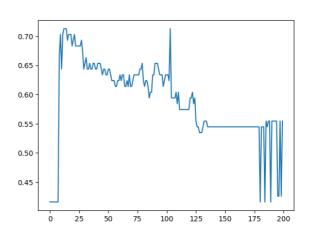
Train Accuracies







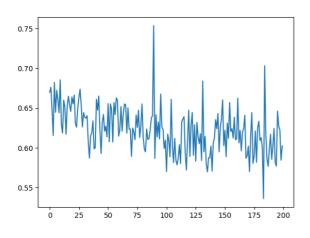
Validation Accuracies



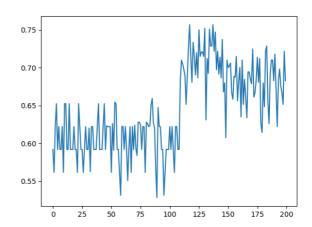
With residual

Test loss epoch 199: 0.597978949546814 Test accuracy epoch 199: 0.7410714285714286

Train Losses



Train Accuracies



0.70 0.68 0.66 0.64 0.62 0.60 0.58 0.56 0 25 50 75 100 125 150 175 200

Validation Accuracies

