Operator Action Predictions

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Short Introduction

- Common issues are errors in grid jobs, that may be due to missing/corrupt input files, high memory usage, etc.
- Currently all handled manually in Operations:
  - An operator must look at the error codes and decide on what appropriate actions to take on the workflow
- General Goal:
  - Deliver error handling predictions and mature towards moving manual operator intervention into automated actions

For more info look at Chrisians slides (slides 2-4):

https://github.com/chrisjcc/WorkflowWebTools/blob/ErrorHandlingAI/docs/Christian_Workflow_Handling_PR.pdf

Short Introduction

Having errors that happened and where happened (at which site) predict (total examples = 9522):

- Which *action* to choose
- Requested *memory*
- Job *splitting*
- Enabling *xrootd* or not

Inputs / X

- Each example consists of matrix w/ shape (errors,sites)
- On average 99.75% of all numbers in matrix will be 0
- 66% out of all combinations (error x site) are never used (are always 0) in dataset with 9522 examples

	site 1	site 2	site 3	site 4	. . .	site 140	site 141	site 142
error 1	1	1	1	1	1	1	1	1	1	1
error 2	4	0	0	0	0	0	0	0	0	0
error 3	8	1	0	0	0	0	0	0	0	0
. . .	0	2	0	0	0	0	0	0	2	0
error 52	0	0	0	0	0	0	0	0	0	5
error 53	0	0	0	0	0	0	0	0	0	1
error 54	1	0	0	0	0	0	0	0	0	0

single example shape = (54,142)

total examples = 9522

For more stats which errors are most common or examples look at Chrisians slides 5-7:

https://github.com/chrisjcc/WorkflowWebTools/blob/ErrorHandlingAI/docs/Christian_Workflow_Handling_PR.pdf

Outputs / Y Targets

Action

1. acdc (88%)
2. clone (10%)
3. special (2%)

Splitting

1. 98.5% default
2. 0.59% 10x
3. 0.31% 2x
4. 0.19% max
5. 0.12% 100x
6. 0.09% 20x
7. 0.05% 3x
8. 0.03% 50x

Memory

1. 92.6% default
2. 2.36% 20k
3. 1.55% 18k
4. 0.59% 12k
5. 0.54% 4k
6. 0.51% 9k
7. 0.40% 6k
8. 0.37% 10k
9. 0.25% 5k
10. 0.19% 8k
11. 0.17% 14k
12. 0.06% 7k
13. 0.05% 15k
14. 0.03% 2k
15. 0.03% 19k
16. 0.03% 16k
17. 0.02% 11k
18. 0.01% 40k
19. 0.01% 32k
20. 0.01% 30k
21. 0.01% 3k
22. 0.01% 28k
23. 0.01% 25k
24. 0.01% 20k
25. 0.01% 180k
26. 0.01% 15k

Xrootd

1. default (72%)
2. enabled (28%)
3. disabled (0.01%)

Outputs / Y Targets (merged)

Action

1. acdc (88%)
2. clone (10%)
3. special (2%)

Memory

1. default (92%)
2. 18k-20k (4%)
3. 2k-9k (2%)
4. 10k-16k (1.2%)

Splitting

1. default (98.5%)
2. 10x-100x (1%)
3. 2x-3x (0.4%)

Xrootd

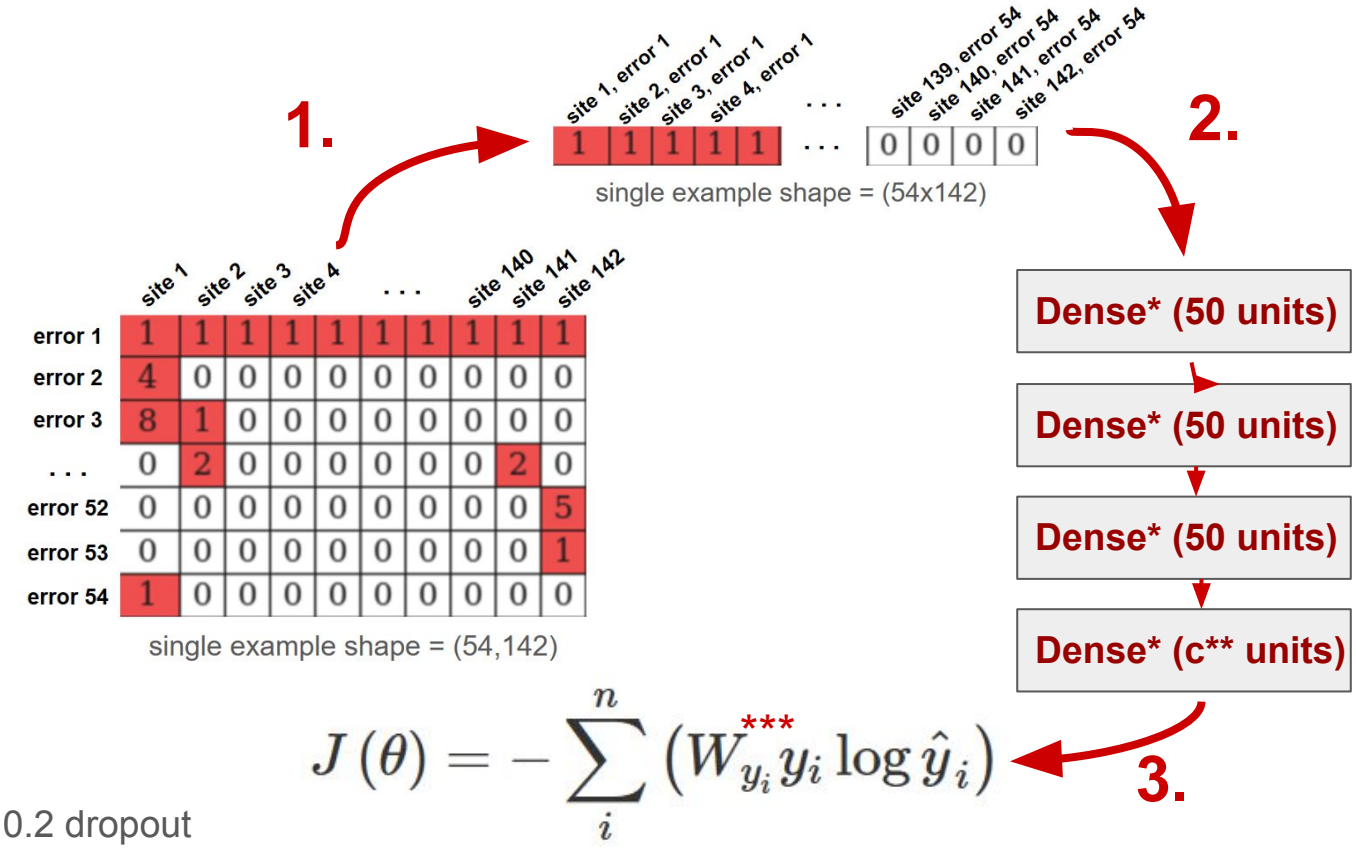
1. default (72%)
2. enabled (28%)
3. disabled (0.01%)

Models Ideas

- Because lack of examples, try to minimize model parameters (CNN Model)
- Change input so that model would generalize better (Create embeddings for each site and error)
- Try different ways of fighting class imbalance (SMOTE resampling, weighted cross entropy)
- Try to find a way to explain the output (by adding additional layers to network)
- Compare everything with simple feed forward network (Simple model)

Simple Model

1. inputs are flatten
2. fed to feed forward neural network
3. everything is optimized with weighted cross entropy (wCE)



$$J(\theta) = -\sum_{i}^{n} \left(W_{y_i}^{***} y_i \log \hat{y}_i \right)$$

* - All Dense layers are with 0.2 dropout

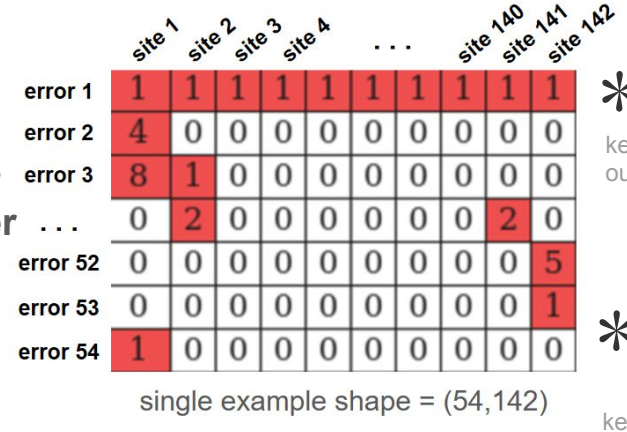
** - number of classes

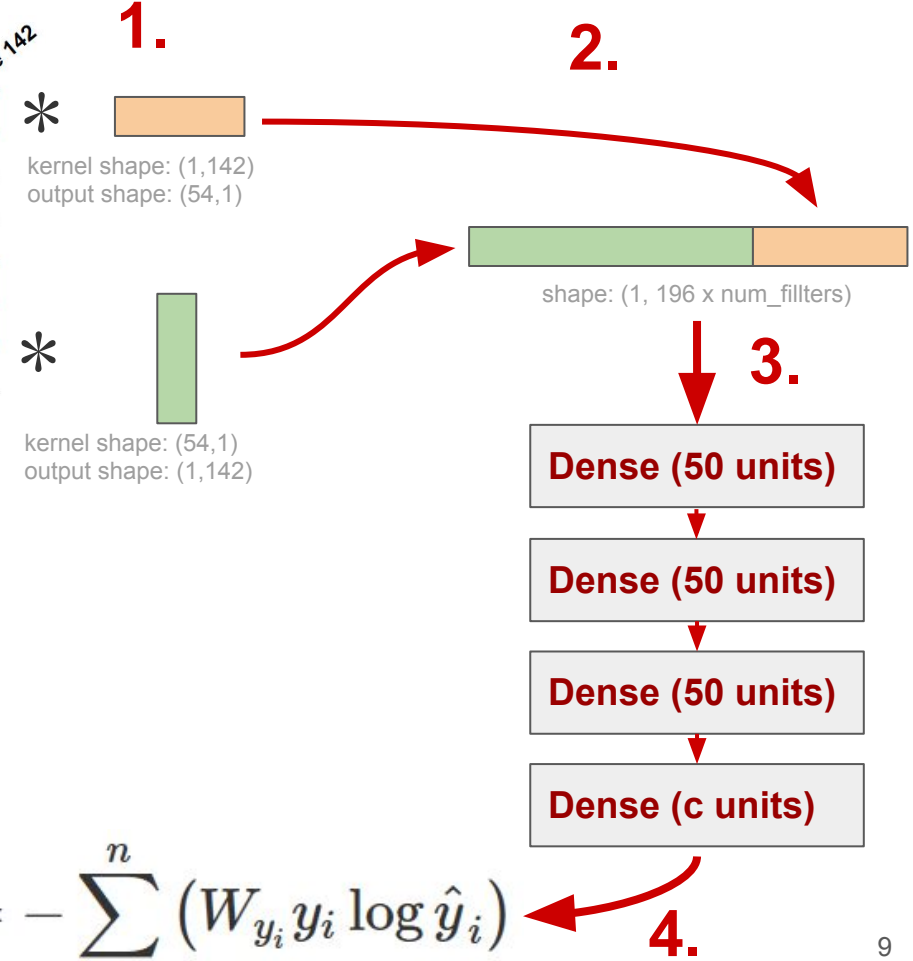
*** - $W_{y_i} = \frac{total\ examples}{\#\ classes} \times \frac{1}{\#\ y_i\ examples}$

*** when resampling (using SMOTE) all classes become same size, which results in W = 1 and loss = cross entropy*

CNN Model

1. input matrix is convolved * across both axis
2. convolution layer outputs are concatenated
3. concat vector is fed to feed forward layers
4. everything is optimized with weighted cross entropy (wCE)



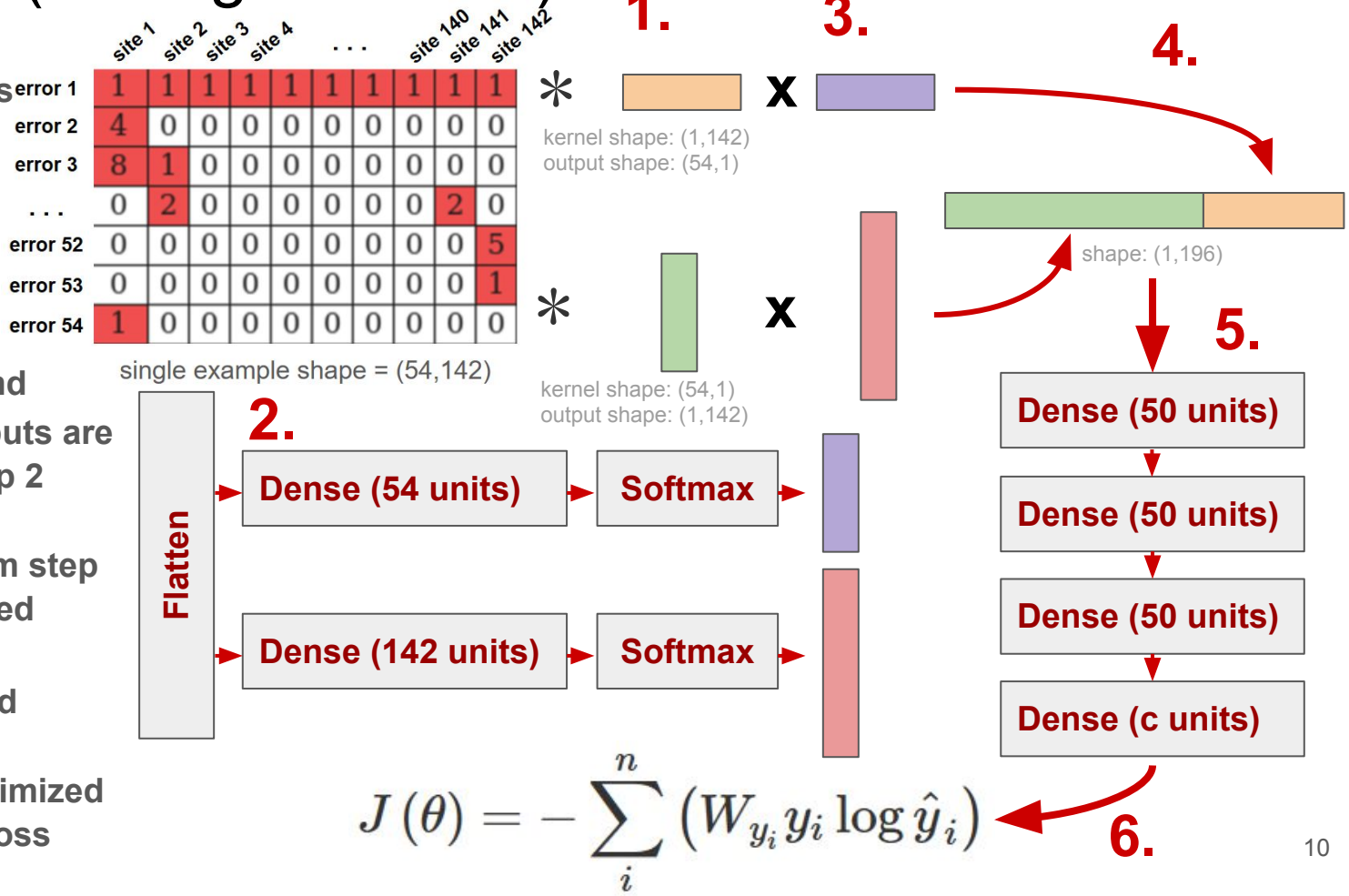


$$J(\theta) = -\sum_{i}^{n} \left(W_{y_i} y_i \log \hat{y}_i \right)$$

* - number of filters = 5

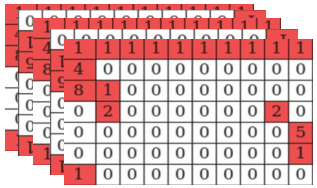
CNN Model (adding Attention)

1. input matrix is convolved across both axis
2. input matrix is flatten and connected to 2 feed forward layers with softmax at the end
3. convolution outputs are multiplied by step 2 outputs
4. both outputs from step 3 are concatenated
5. concat vector is connected to feed forward layers
6. everything is optimized with weighted cross entropy (wCE)



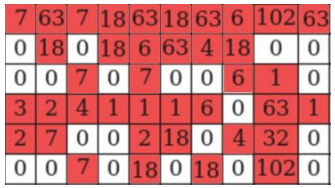
Error and Site embeddings

1. all examples are summed across axis 0
2. all numbers that are greater than 0 are replaced by 1
3. by doing dot product* of error embedding matrix times sites embedding matrix try to recreate matrix from step 2
4. everything is optimized with mse



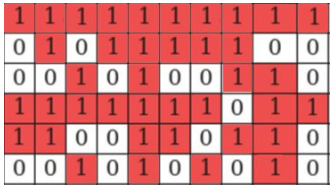
shape = (9522,54,142)

1.



shape = (54,142)

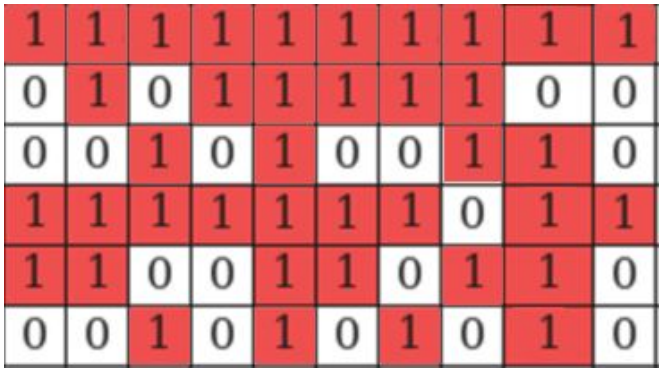
2.

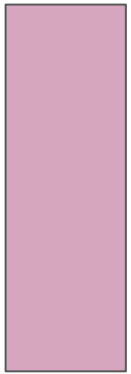


shape = (54,142)

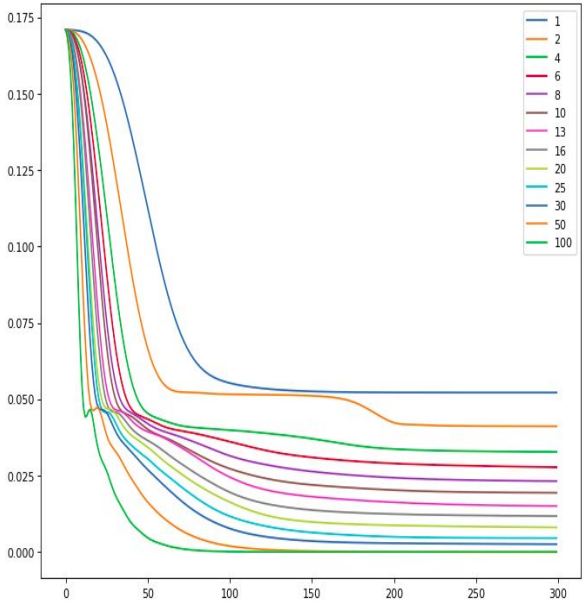
3.

sites embedding matrix with shape (e,142) **





error embedding matrix with shape (54,e) **

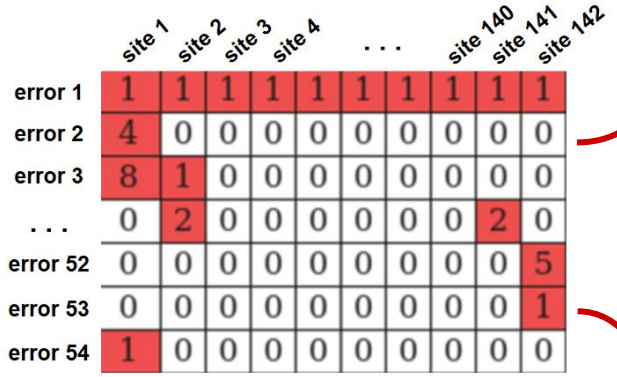


mse error with different embedding sizes

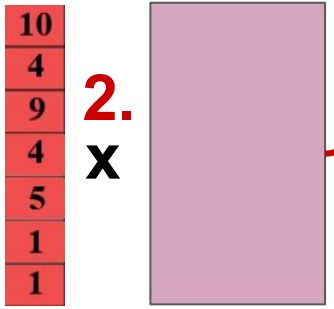
* - (54,e) . (e,142) = (54,142)

** - e = 20

Pseudo-Embedding Model

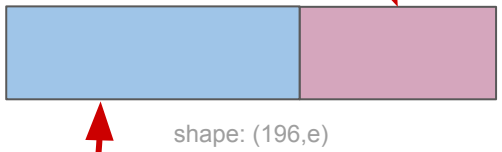


1.1.



2. x

3.



4.

Dense (50 units)

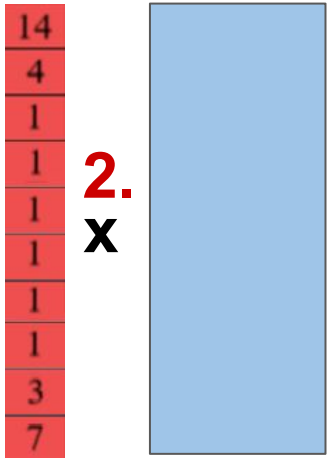
Dense (50 units)

Dense (50 units)

Dense (c units)

5.

1.2.



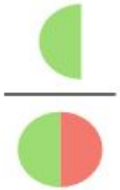
2. x

1. 1. count number of errors
   2. count errors in each site
2. each count is multiplied by its embedding
3. site embeddings and error embeddings are concatenated
4. concat vector is fed to feed forward layers
5. everything is optimized with weighted cross entropy (wCE)

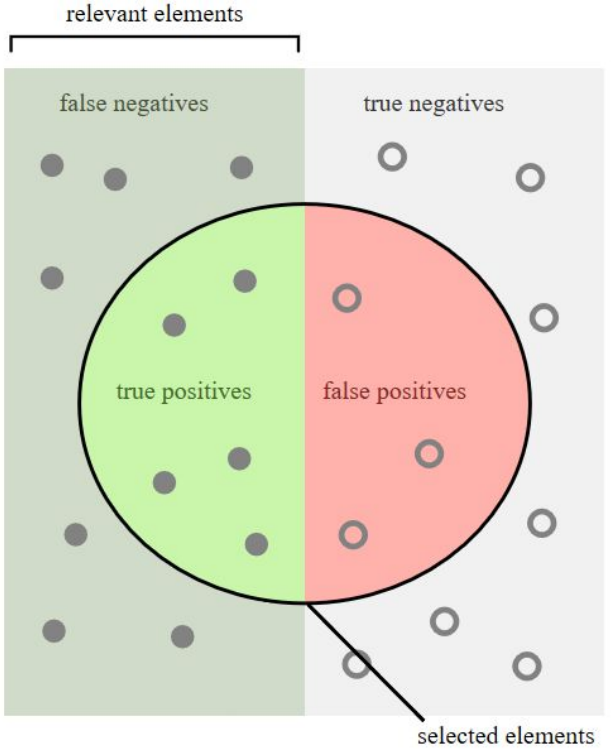
$$J(\theta) = -\sum_{i}^{n} \left(W_{y_i} y_i \log \hat{y}_i \right)$$

Evaluation Metrics

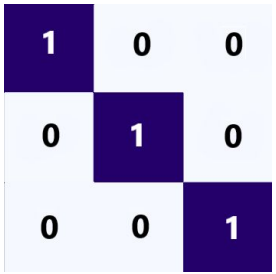
- Precision (for each class) *
  how many selected items are relevant?
- Recall (for each class) **
  How many relevant items are selected?
- Confusion MSE (main) ***
  Mean squared error of normalized confusion matrix and identity matrix

* - precision = 

** - recall = 



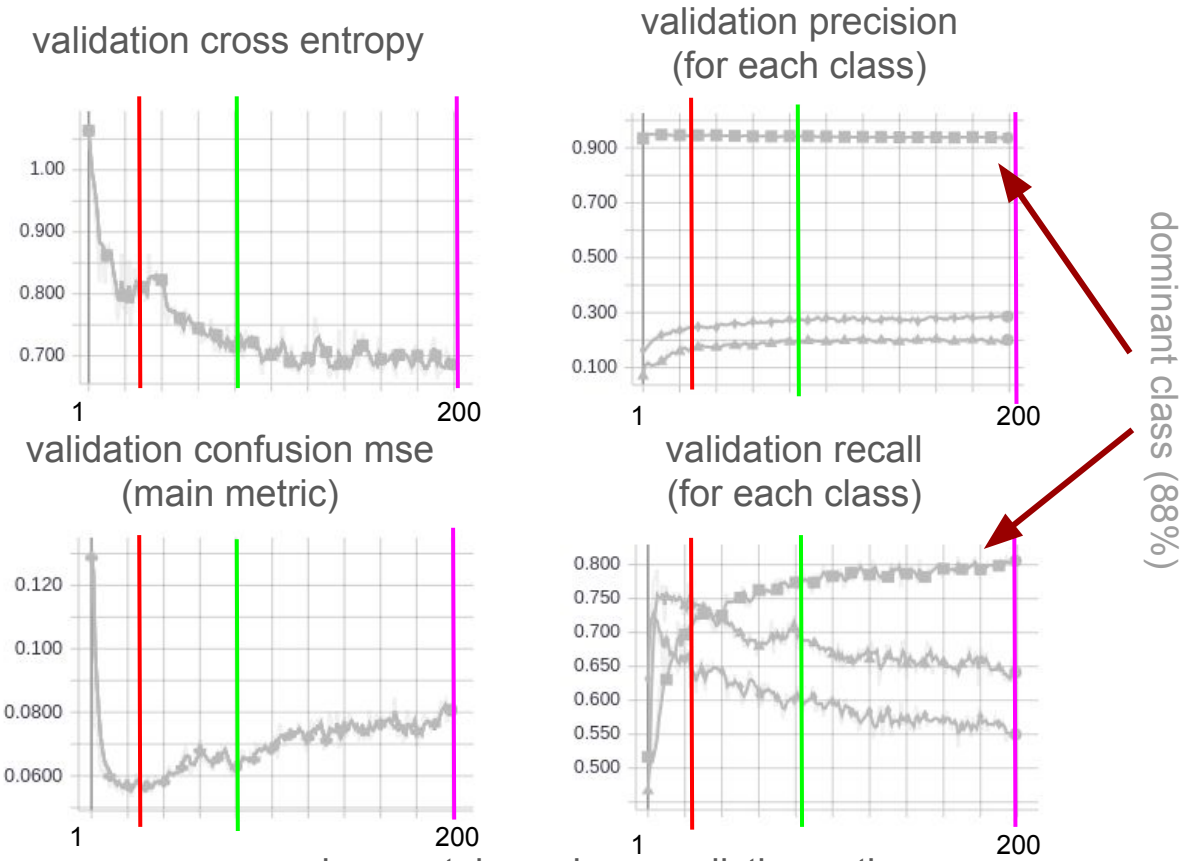
Macro average is calculated for Recall and Precision !

*** - confusion mse = mse( , )

Optimal Stopping when Training

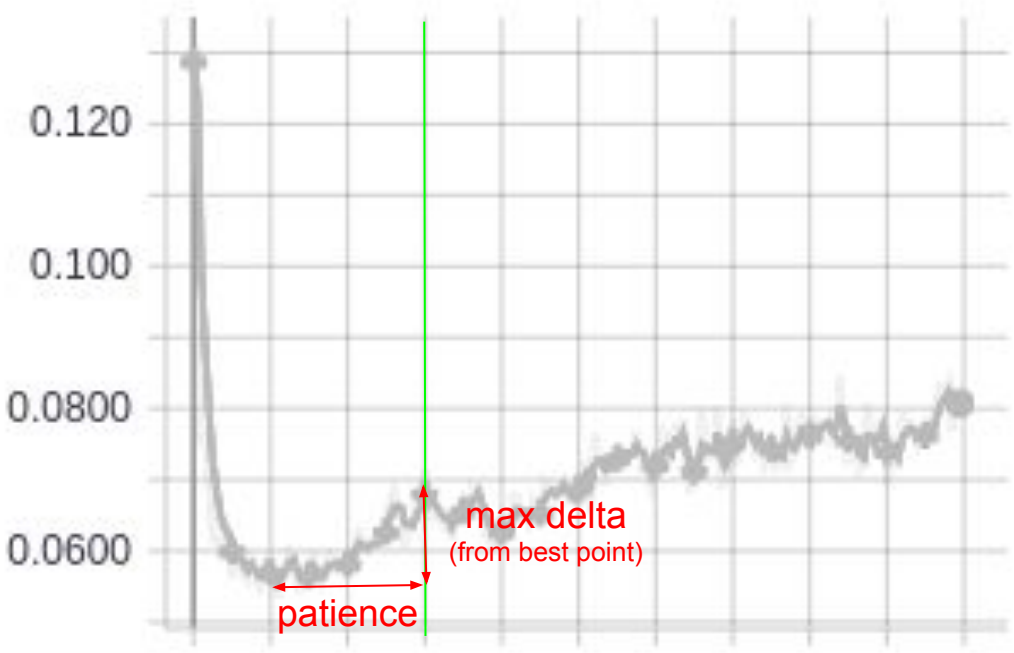
- Early stopping with single metric can lead training to stop too fast
- Looking at multiple metrics as equal can lead to stopping too late
- Optimal stopping point should be somewhere in between, that main metric doesn't deviate from best score and other metrics get better

- too early stopping
- optimal stopping
- too late stopping



Multiple Metric Early Stopping

1. At each epoch set best scores from all picked metrics
2. If none of the metrics gets better in n* epoch then stop
3. If main score is worse compared to best score by T** then stop

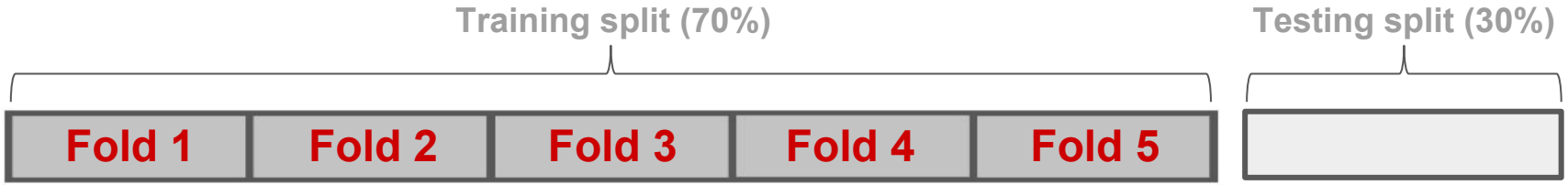


| - stopping point

* - n - patience

** - T - max delta, maximum allowed decrease of score from best score (in %)

Picking Single Best Model



- Splitting* dataset into testing and training datasets
- For each model**:
  - Split training dataset into 5 equal size folds
  - Train on 4 Folds and test on 1 Fold (do this for each fold)
- Average each fold results into mean and std of each metric
- Model that results with best confusion mse on most outputs is considered best

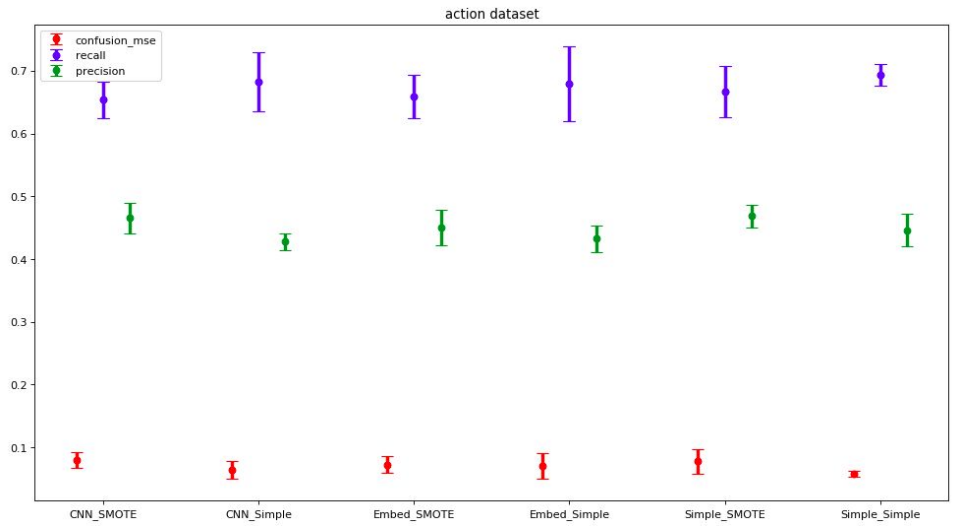
* - numpy seed = 42

** - Modals that were looked at were: Total of 3 x 4 = 12 Models

- Simple, CNN, Embedding with different methods:
  - trained using SMOTE resampling
  - trained with Attention
  - trained using both
  - trained with no SMOTE resampling and no Attention

Used Early Stopping Parameters:

- patience = 7
- maximum percentage delta = 30%
- moving average length = 2


action dataset
confusion_mse
recall
precision
0.7
0.6
0.5
0.4
0.3
0.2
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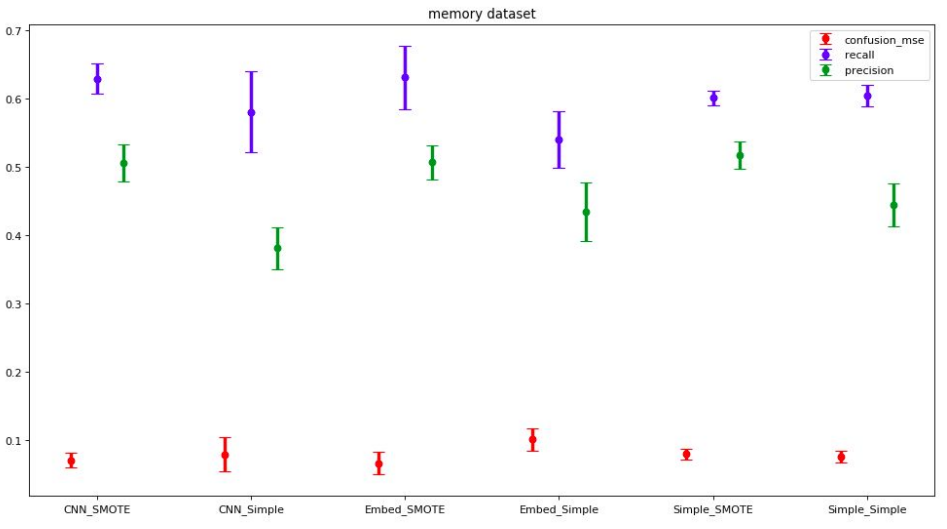
CNN_SMOTE
CNN_Simple
Embed_SMOTE
Embed_Simple
Simple_SMOTE
Simple_Simple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confusion_mse
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precision
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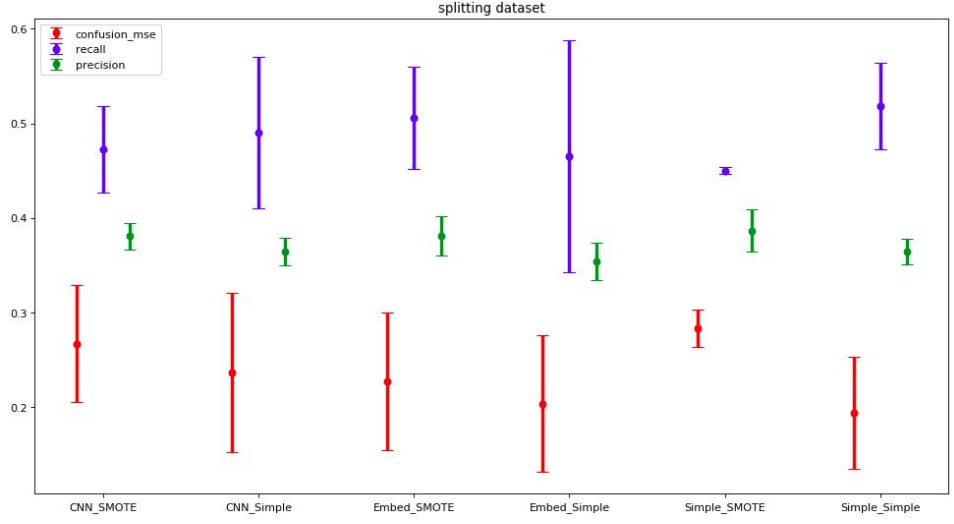
CNN_SMOTE
CNN_Simple
Embed_SMOTE
Embed_Simple
Simple_SMOTE
Simple_Simple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confusion_mse
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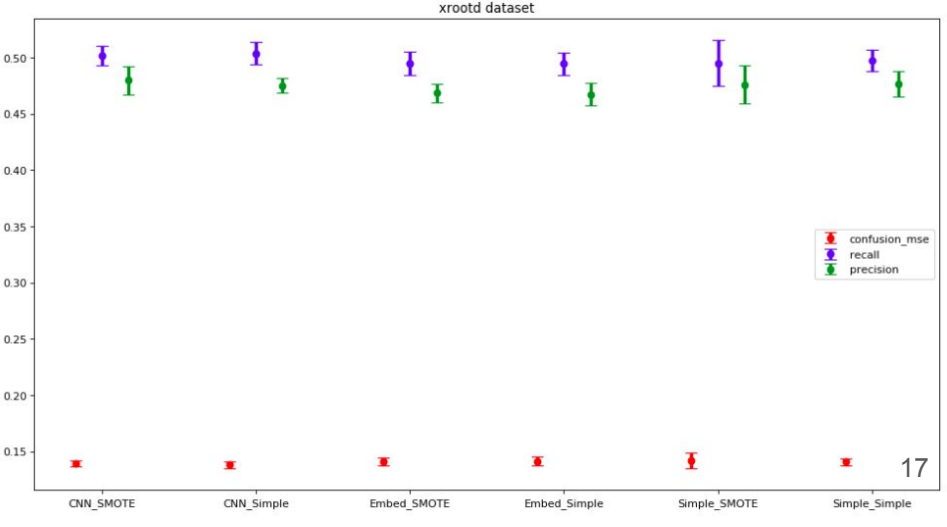
Simple_Simple


xrootd dataset
confusion_mse
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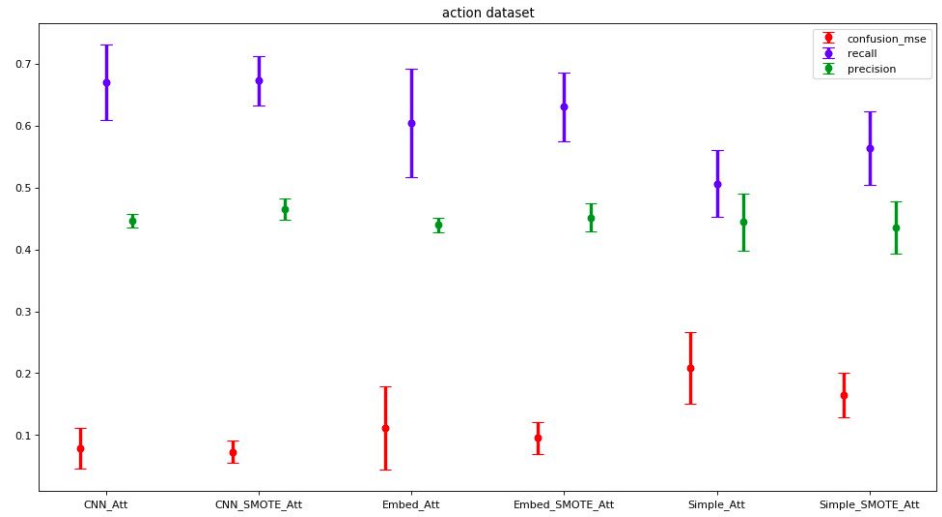
CNN_SMOTE
CNN_Simple
Embed_SMOTE
Embed_Simple
Simple_SMOTE
Simple_Simple


action dataset
confusion_mse
recall
precision
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0.4
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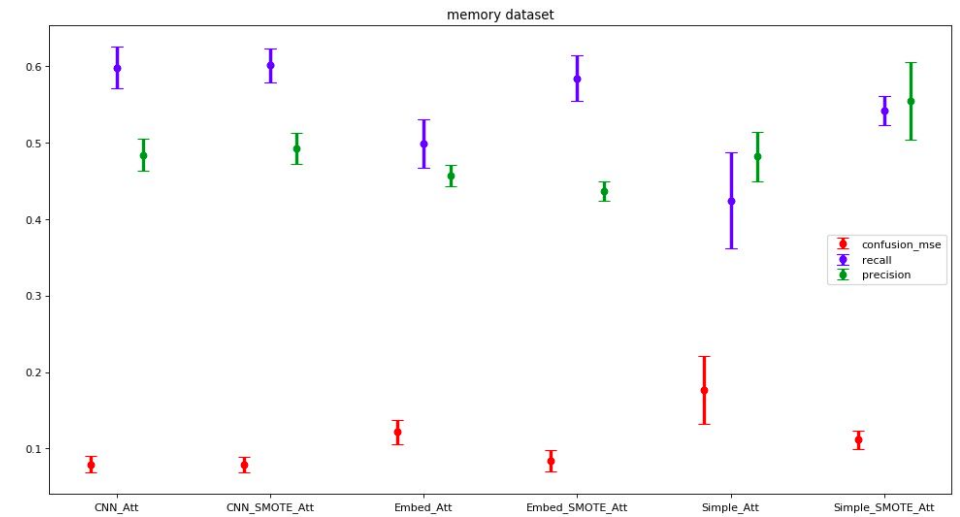
0.2
0.1
CNN_Att
CNN_SMOTE_Att
Embed_Att
Embed_SMOTE_Att
Simple_Att
Simple_SMOTE_Att


memory dataset
confusion_mse
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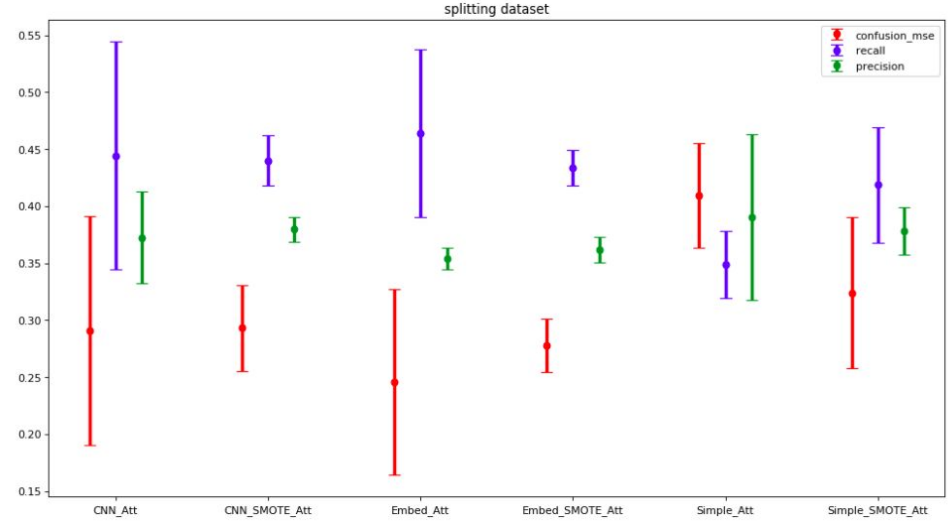
CNN_Att
CNN_SMOTE_Att
Embed_Att
Embed_SMOTE_Att
Simple_Att
Simple_SMOTE_Att


splitting dataset
confusion_mse
recall
precision
0.55
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0.45
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0.35
0.30
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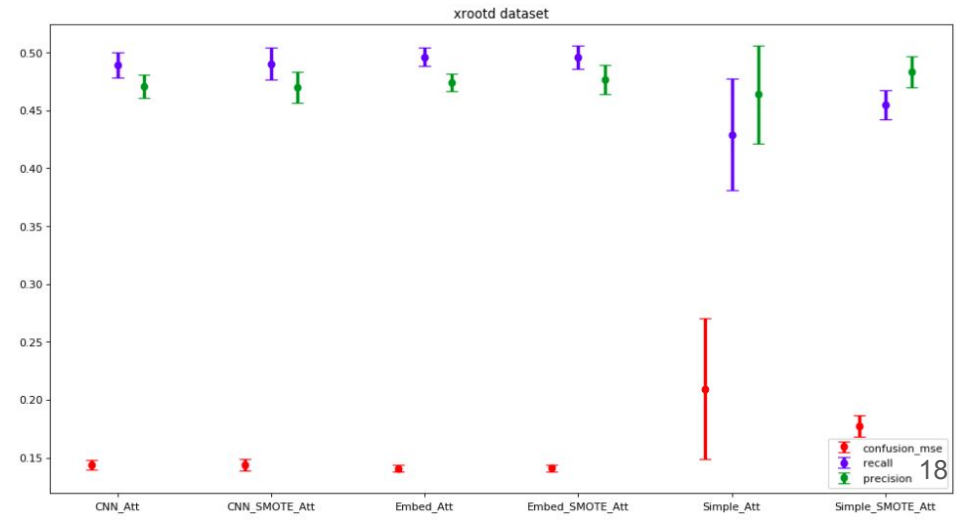
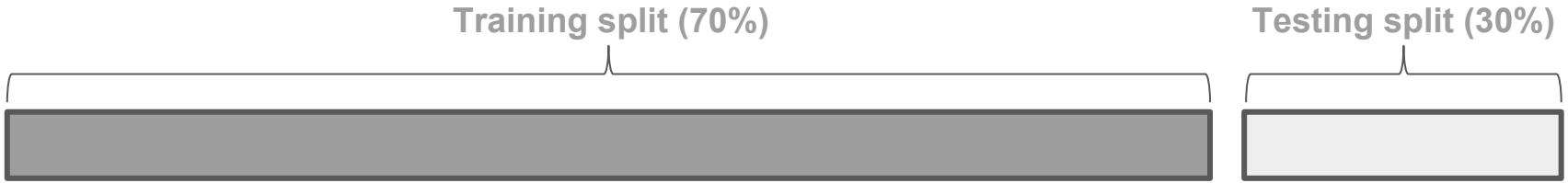
0.20
0.15
CNN_Att
CNN_SMOTE_Att
Embed_Att
Embed_SMOTE_Att
Simple_Att
Simple_SMOTE_Att


xrootd dataset
confusion_mse
recall
precision
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
CNN_Att
CNN_SMOTE_Att
Embed_Att
Embed_SMOTE_Att
Simple_Att
Simple_SMOTE_Att

Testing Models



- Splitting* dataset into testing and training datasets
- For 5 times:
  - Train chosen model on training dataset
  - Get all metrics results with this model on testing dataset
- Average each results into mean and std of each metric

* - numpy seed = 42

Best Model Results on Test Set

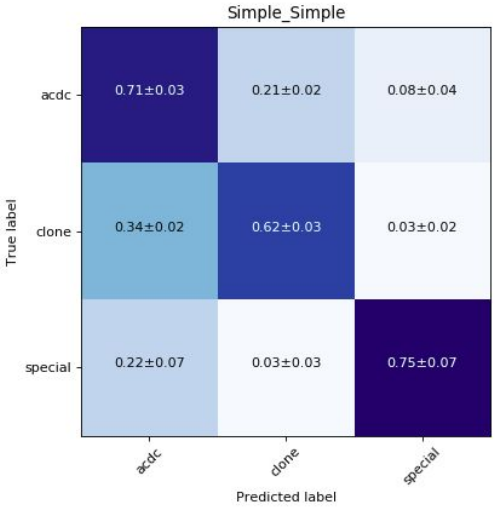
Best model - Simple_Simple

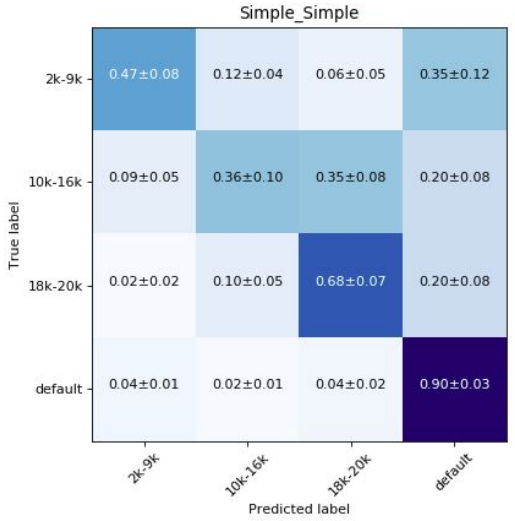
Dataset	Model	SMOTE	Attention	conf mse	recall	precision
action	simple	-	-	.0576 ± .0068	.691 ± .017	.447 ± .005
memory	simple	-	-	.0873 ± .0160	.582 ± .028	.450 ± .022
splitting	simple	-	-	.2112 ± .0321	.482 ± .028	.366 ± .008
xrootd	simple	-	-	.1456 ± .0027	.497 ± .009	.476 ± .011

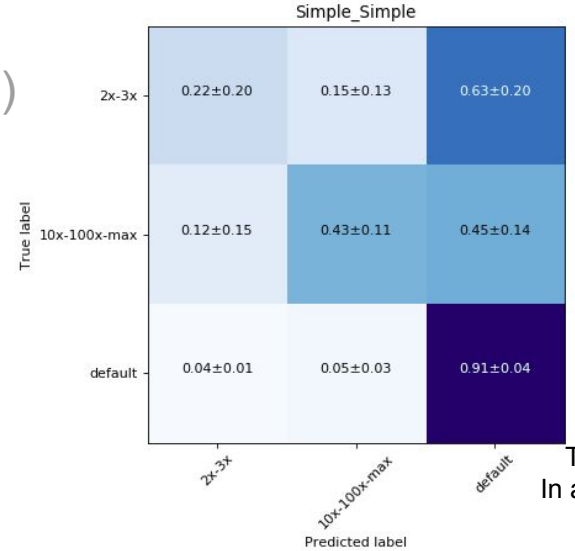
Best Model Results on Test Set

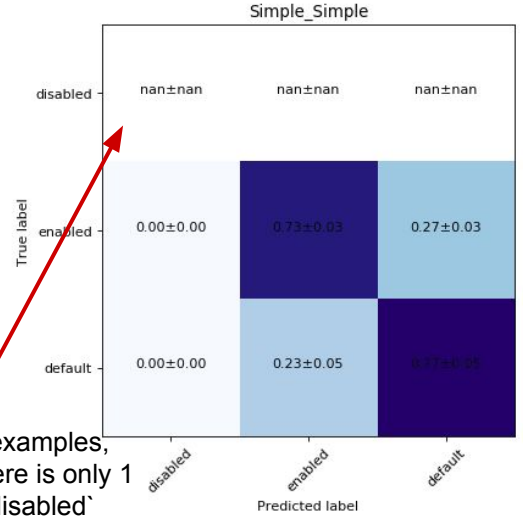
Note: model always prioritizes on bigger classes except in `action` target: it is easier to predict special (138 examples) then clone (934 examples)

Y targets:
action - top left
memory - top right
splitting - bottom left
xrootd - bottom right









There was 0 examples,
In all dataset there is only 1 sample on `disabled`

Bonus Slides

- Other Results (Best of SMOTE, Attention, XGBoost)
- SMOTE vs weighted cross entropy (Metric evolution plots)
- Best of Attention and no Attention (confusion matrices)

Other Results

Following slides show:

- Results using SMOTE resampling (results and confusion matrices)
- Results using Attention (results and confusion matrices)
- XGBoost model results (results)

SMOTE Results

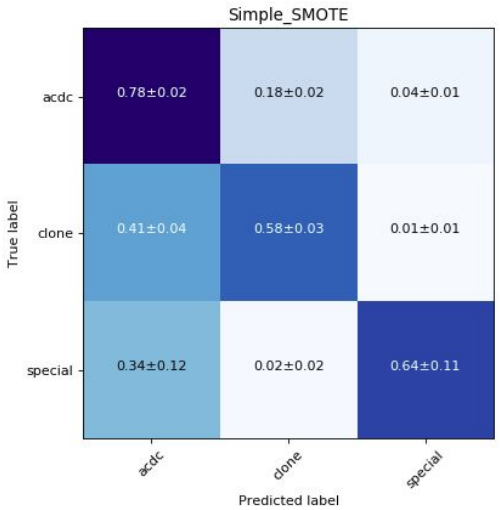
Best model - Simple_SMOTE

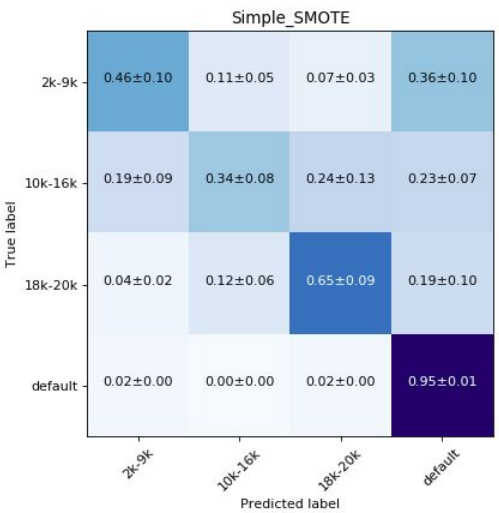
Gets higher precision then without SMOTE, but recall and conf mse are worse

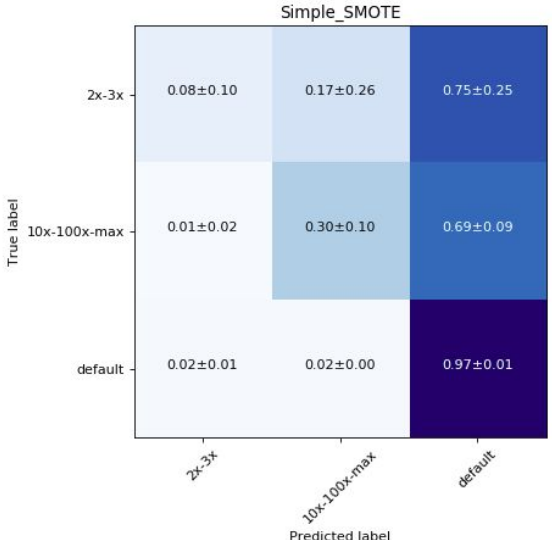
Dataset	Model	SMOTE	Attention	conf mse	recall	precision
action	simple	+	-	.0780 ± .0195	.666 ± 040	.468 ± .018
memory	simple	+	-	.0759 ± .0073	.611 ± .011	.515 ± .019
splitting	simple	+	-	.2834 ± .0200	.449 ± .003	.386 ± .022
xrootd	simple	+	-	.1417 ± .0070	.495 ± .020	.475 ± .017

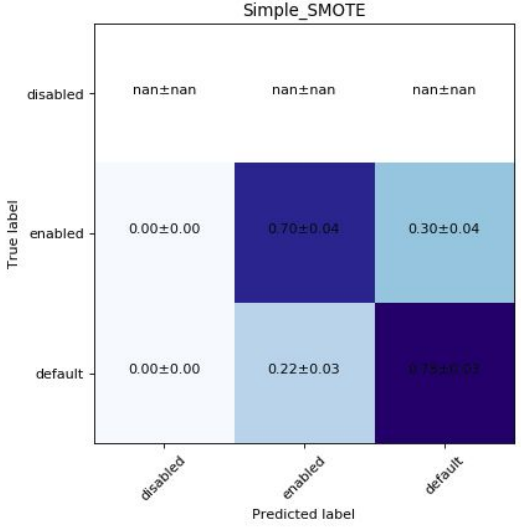
everything is trained with early stopping on confusion mse
with patience = 10, maximum percentage delta = 30%, moving average length = 2

SMOTE Results









Y targets:
action - top left
memory - top right
splitting - bottom left
xrootd - bottom right

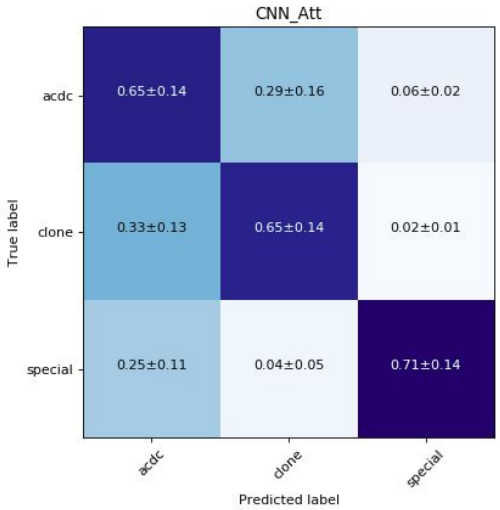
Attention Results

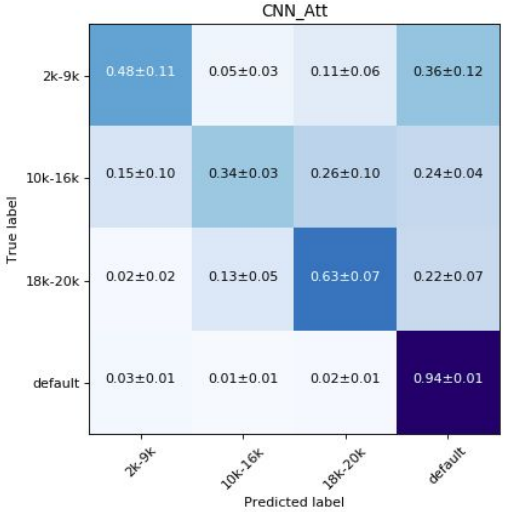
Best model - CNN_Att

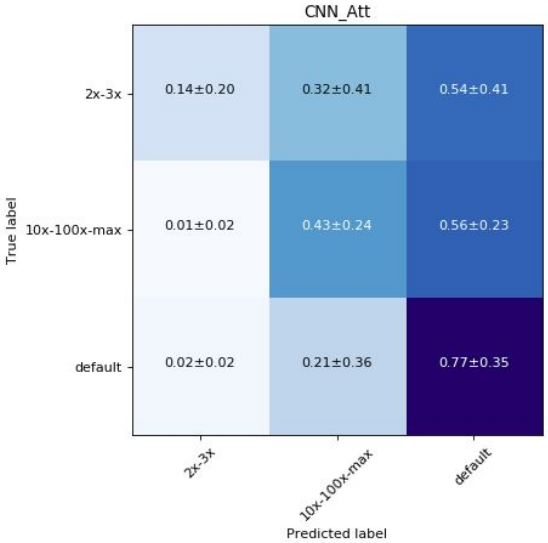
Still most metrics are worse in comparison with models without Attention

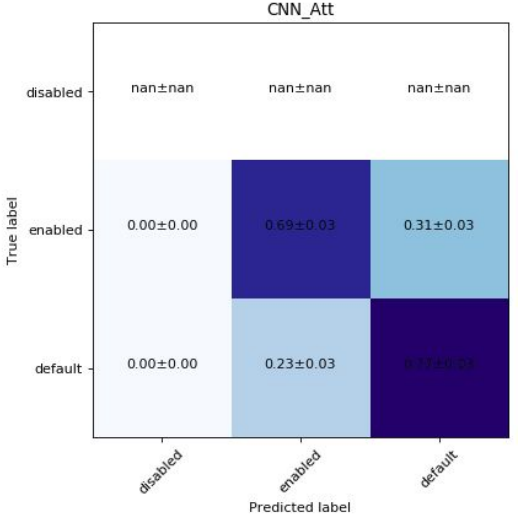
Dataset	Model	SMOTE	Attention	conf mse	recall	precision
action	cnn	-	+	.0690 ± .0159	.684 ± .016	.445 ± .022
memory	cnn	-	+	.0985 ± .074	.567 ± .027	.474 ± .021
splitting	cnn	-	+	.2907 ± .1007	.395 ± .100	.321 ± .040
xrootd	cnn	-	+	.1437 ± .0039	.489 ± .010	.470 ± .010

Best model with Attention (confusion matrices)









Y targets:
action - top left
memory - top right
splitting - bottom left
xrootd - bottom right

XGBoost Results

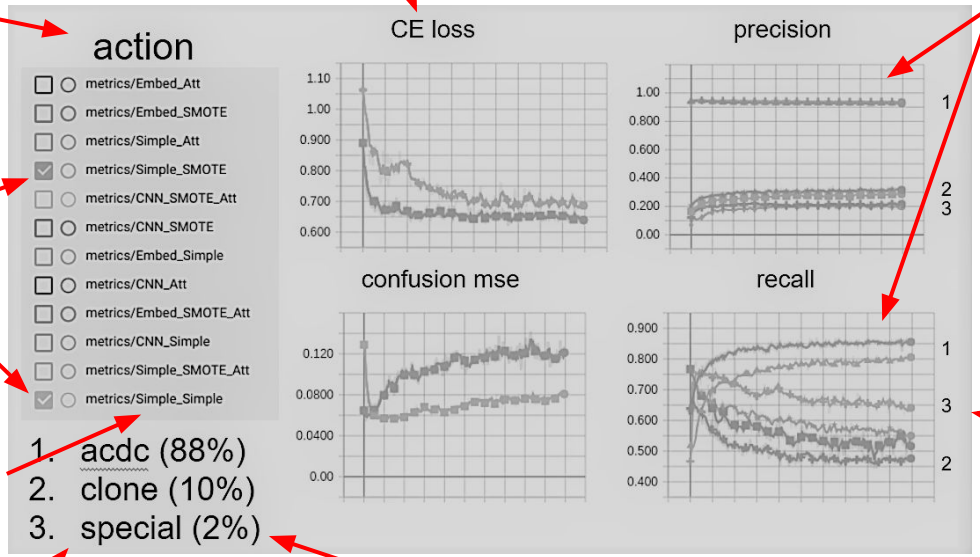
When training with max depth 4 all metrics are worse

Dataset	SMOTE	conf mse	recall	precision
action	-	.308	.443	.754
action	+	.095	.633	.456
memory	-	.129	.536	.751
memory	+	.090	.593	.594
splitting	-	.395	.362	.528
splitting	+	.384	.368	.371
xrootd	-	.291	.459	.508
xrootd	+	.252	.507	.507

everything is trained with early stopping on confusion mse with patience = 10

SMOTE vs weighted cross entropy

Following slides show: Metrics evolution on different Models over 200 epochs
Each dataset has 3 slides for models: (Simple, CNN, Embedding)
Single slide has evolution of metrics for model using and not using SMOTE resampling



Y (target)

cross entropy

recall and precision for each class

shown models

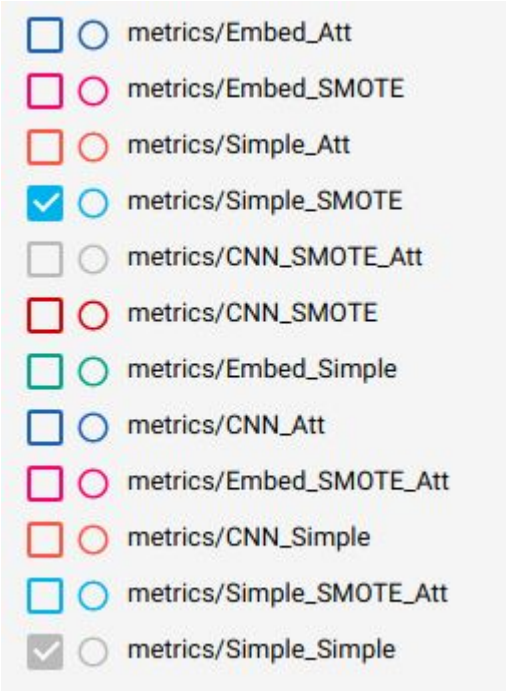
{model name}_{info}
where info can be:
SMOTE - uses SMOTE resampling
Att - uses Attention
Simple - doesn't use any of the above

class number for that single curve

each class with its number

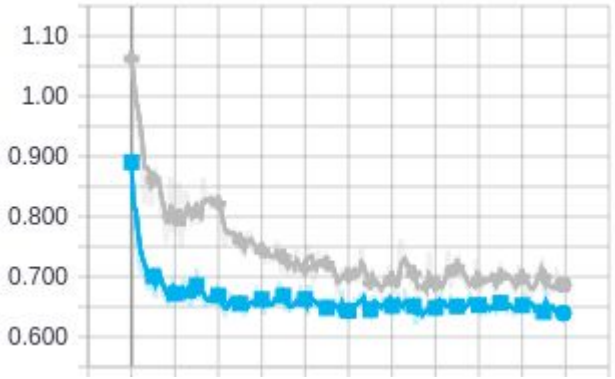
% of all elements

action

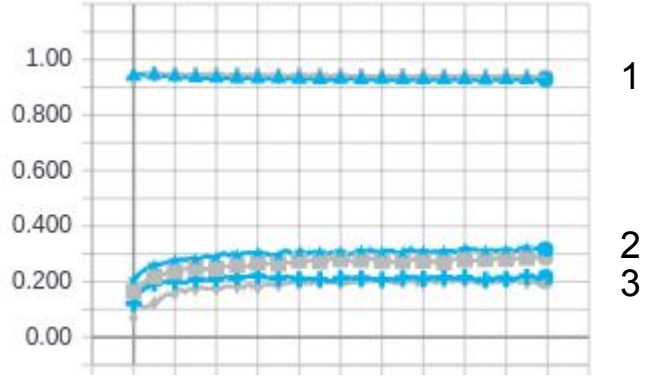


1. acdc (88%)
2. clone (10%)
3. special (2%)

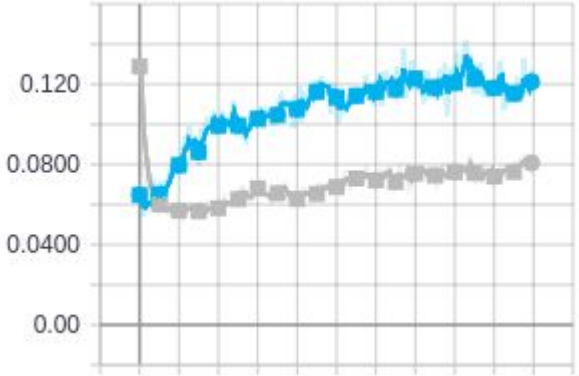
CE loss



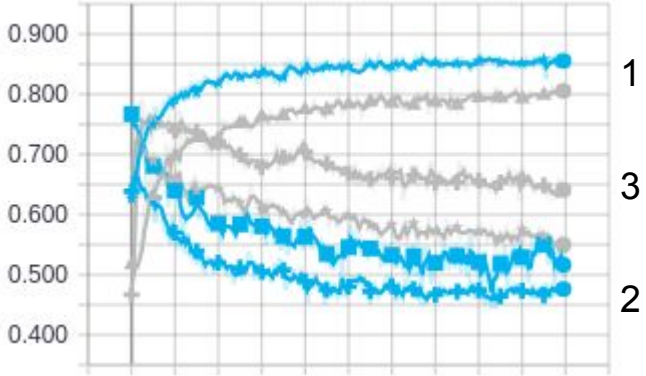
precision



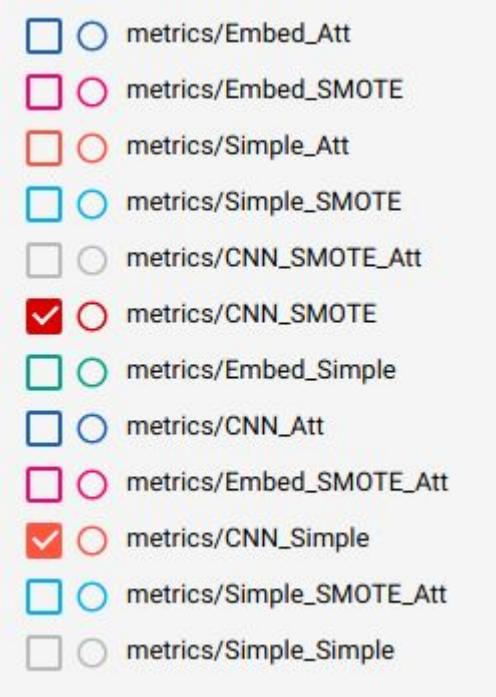
confusion mse



recall



action



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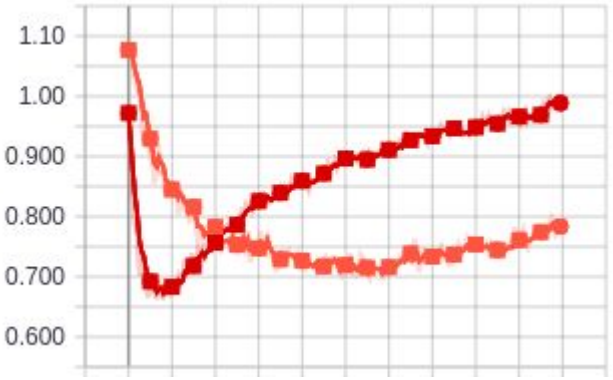
CE loss



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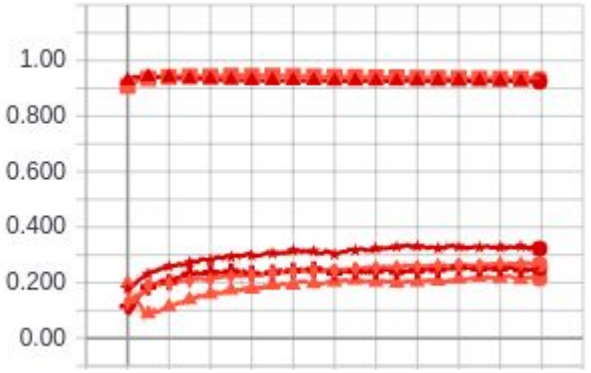
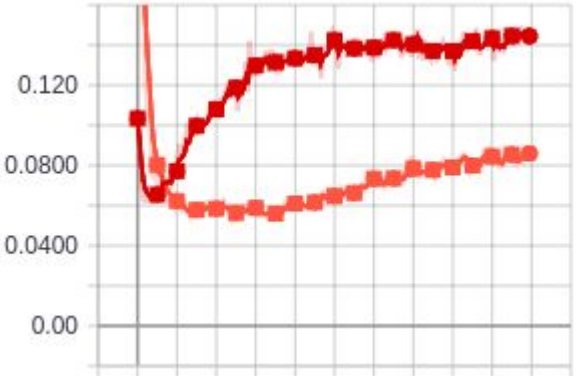
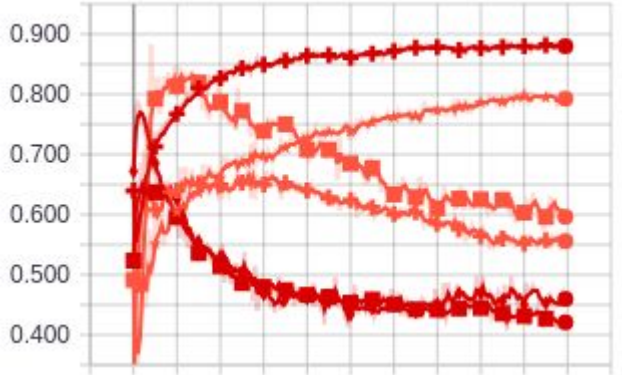


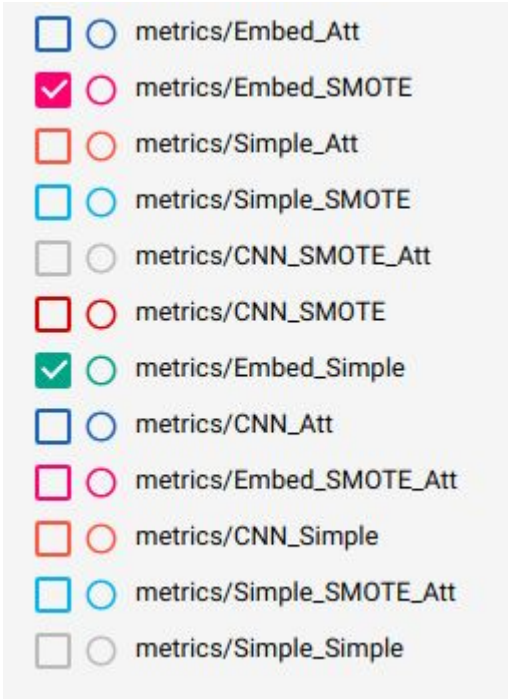
confusion mse



recall



action



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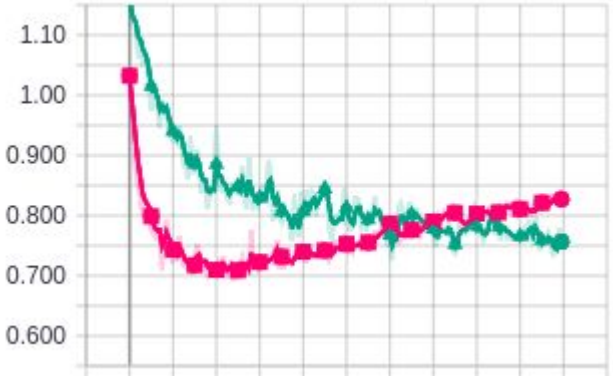
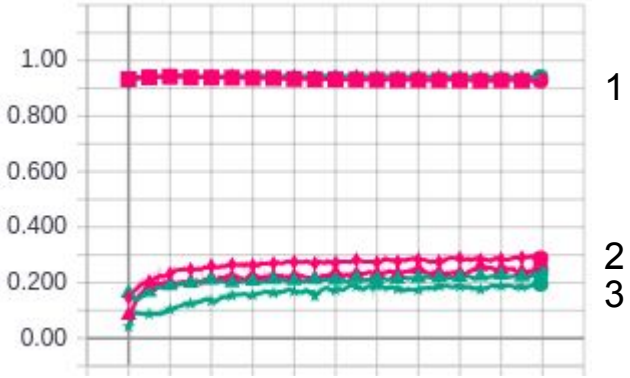
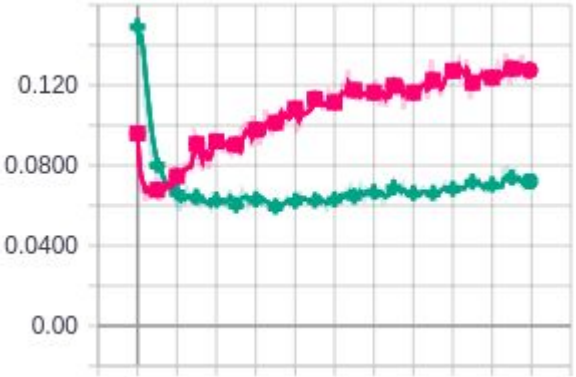
CE loss



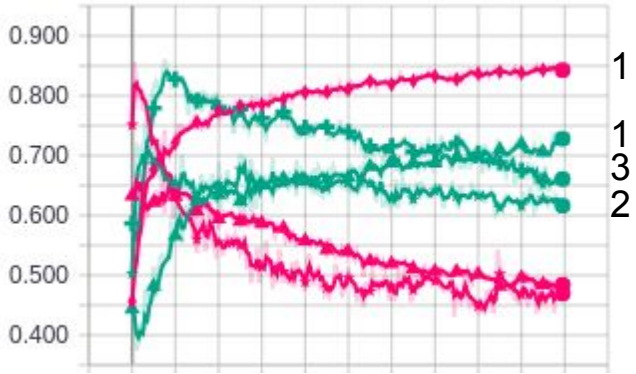
precision



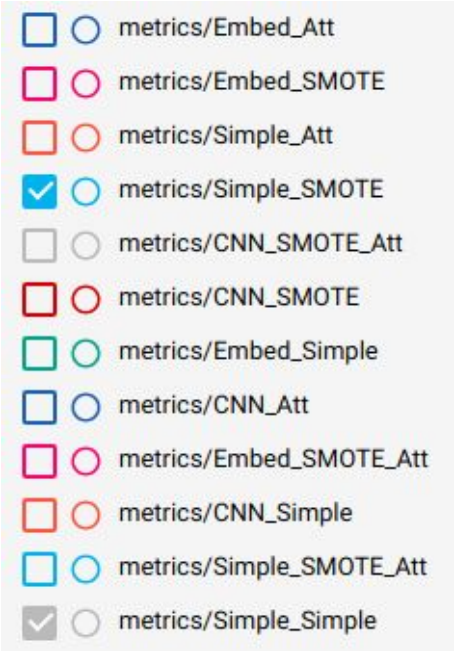
confusion mse



recall

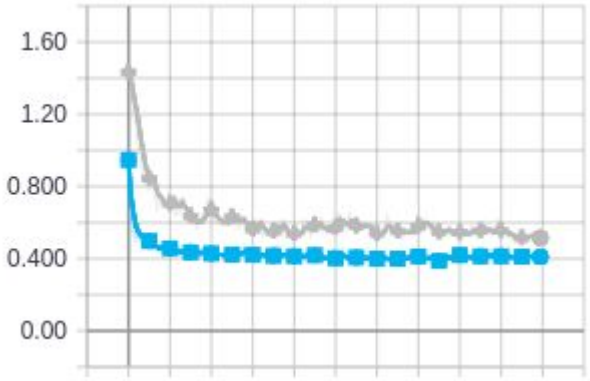


memory

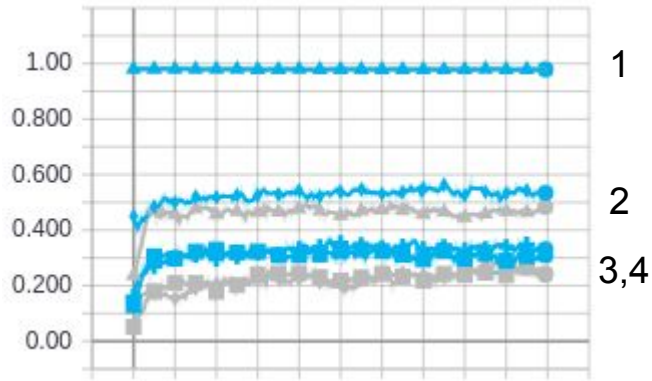


1. default (92%)
2. 18k-20k (4%)
3. 2k-9k (2%)
4. 10k-16k (1.2%)

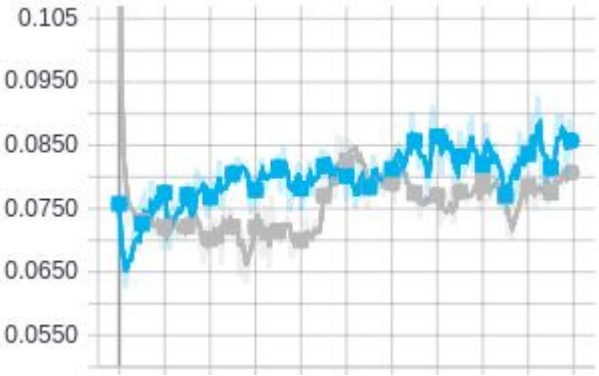
CE loss



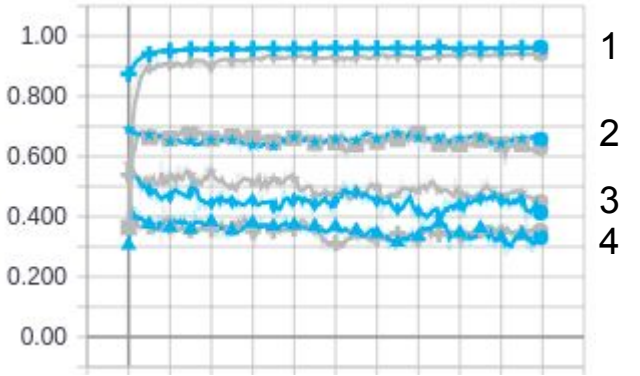
precision



confusion mse



recall



memory

- metrics/Embed_Att
- metrics/Embed_SMOTE
- metrics/Simple_Att
- metrics/Simple_SMOTE
- metrics/CNN_SMOTE_Att
- metrics/CNN_SMOTE
- metrics/Embed_Simple
- metrics/CNN_Att
- metrics/Embed_SMOTE_Att
- metrics/CNN_Simple
- metrics/Simple_SMOTE_Att
- metrics/Simple_Simple

1. default (92%)
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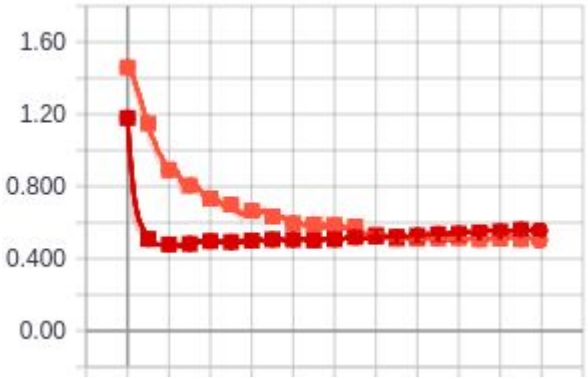
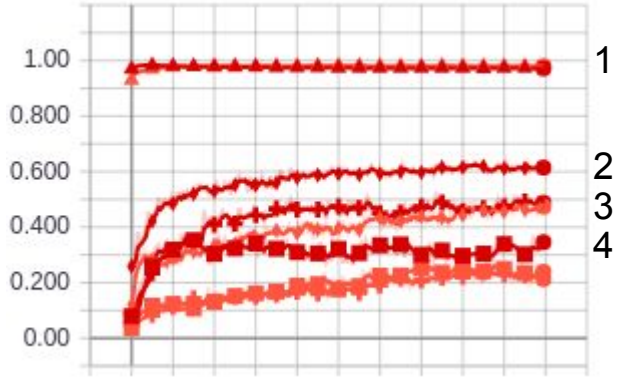
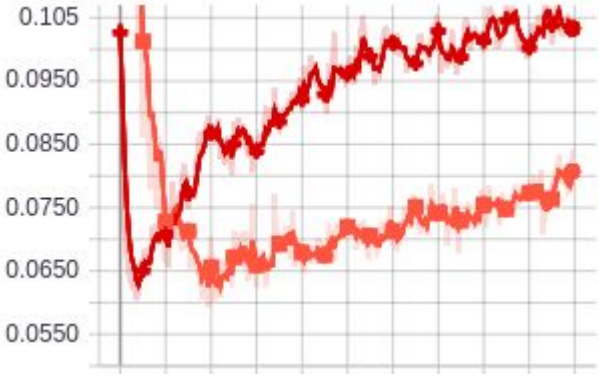
CE loss



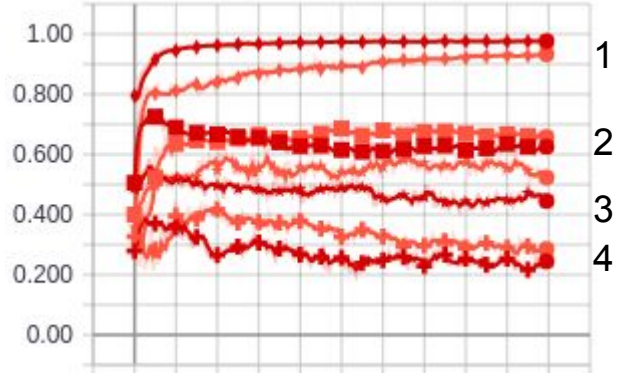
precision



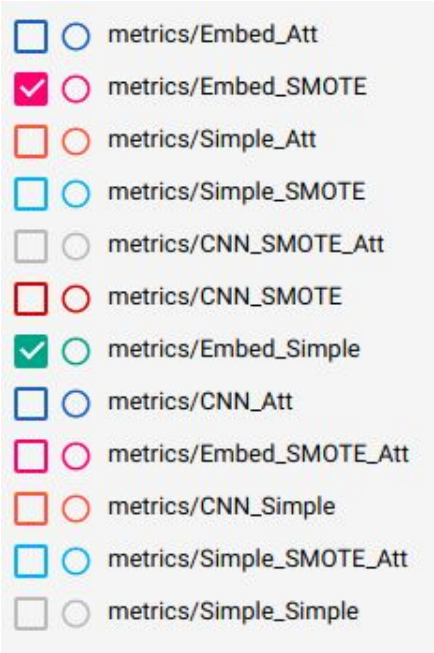
confusion mse



recall



memory



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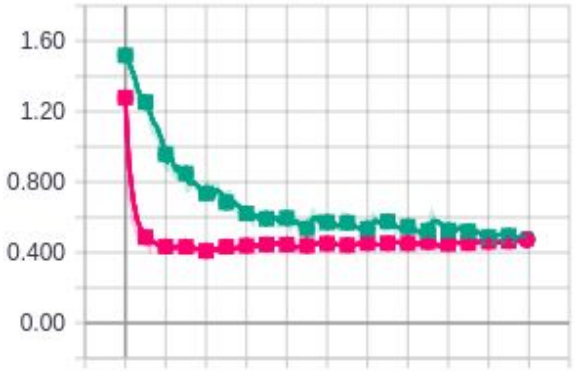
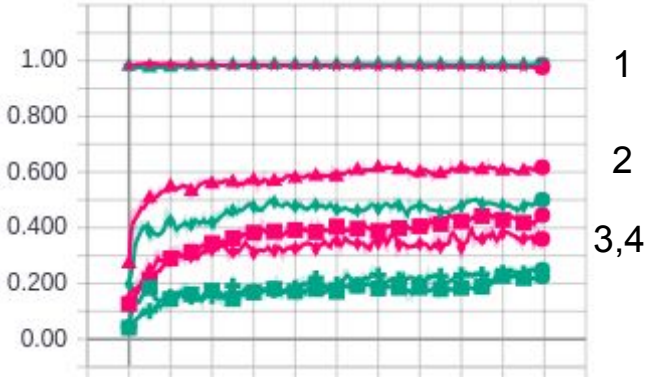
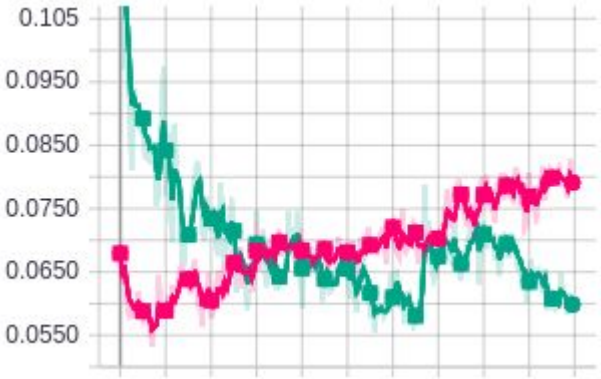
CE loss



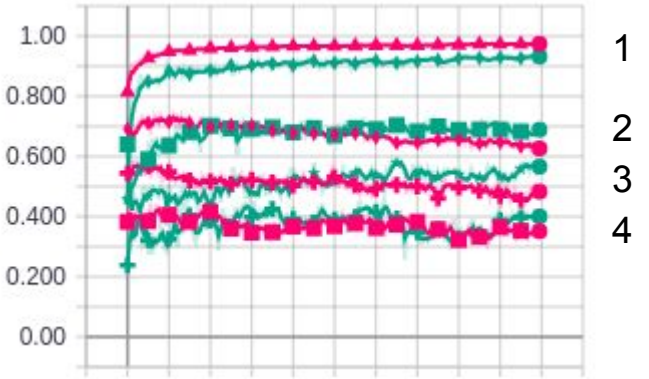
precision



confusion mse



recall

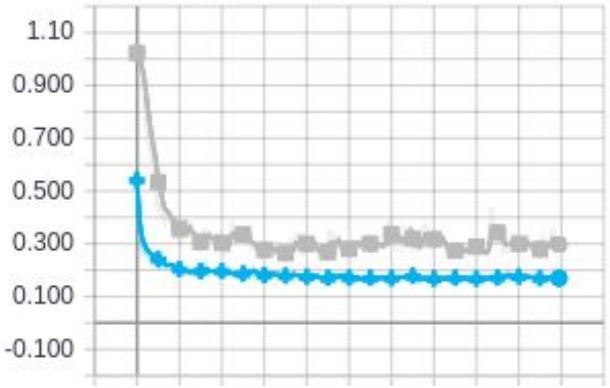


splitting

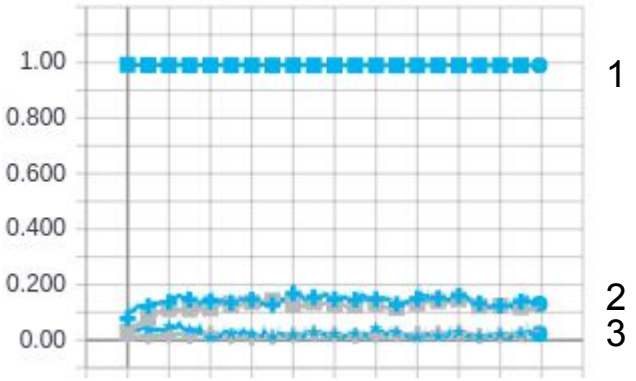
- metrics/Embed_Att
- metrics/Embed_SMOTE
- metrics/Simple_Att
- metrics/Simple_SMOTE
- metrics/CNN_SMOTE_Att
- metrics/CNN_SMOTE
- metrics/Embed_Simple
- metrics/CNN_Att
- metrics/Embed_SMOTE_Att
- metrics/CNN_Simple
- metrics/Simple_SMOTE_Att
- metrics/Simple_Simple

1. default (98%)
2. 10x-100x (1%)
3. 2x-3x (0.4%)

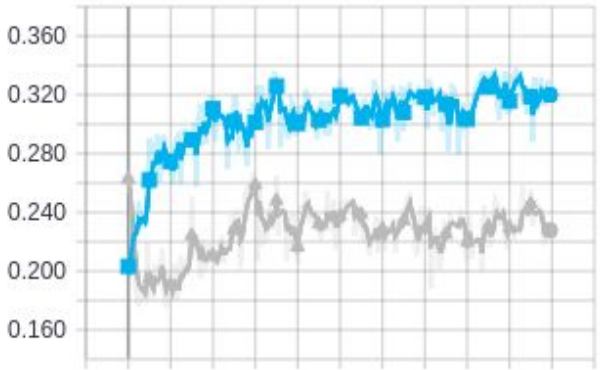
CE loss



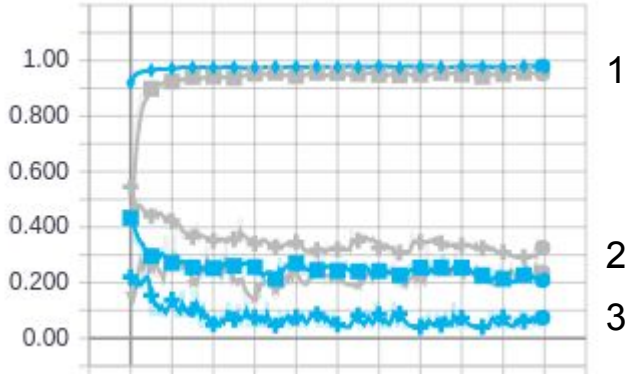
precision



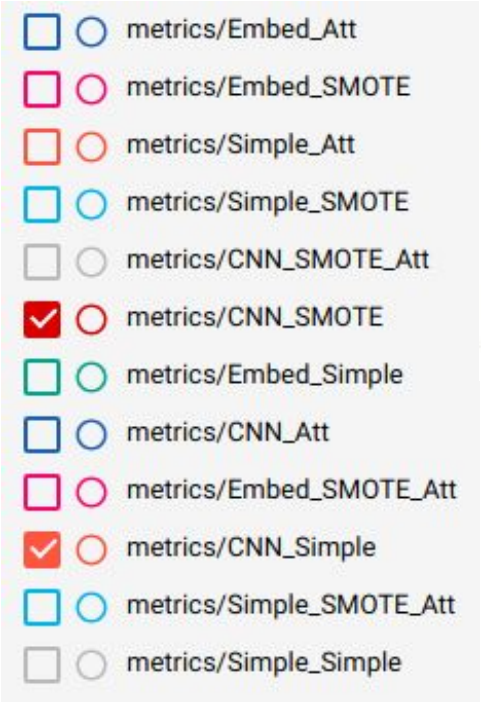
confusion mse



recall



splitting



1. default (98%)
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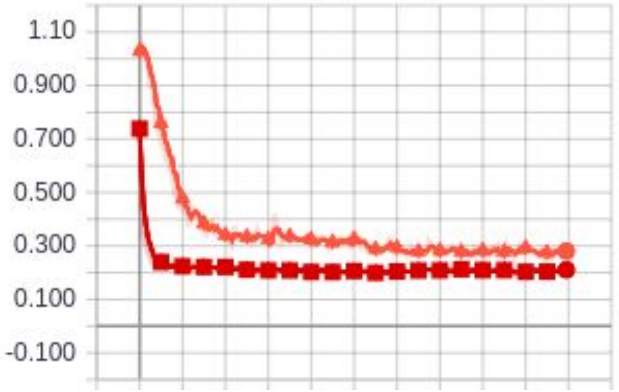
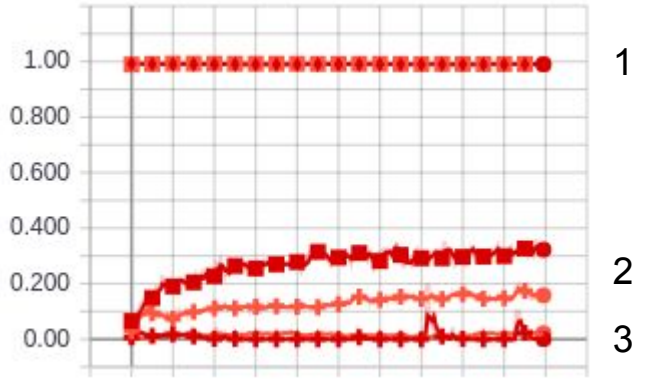
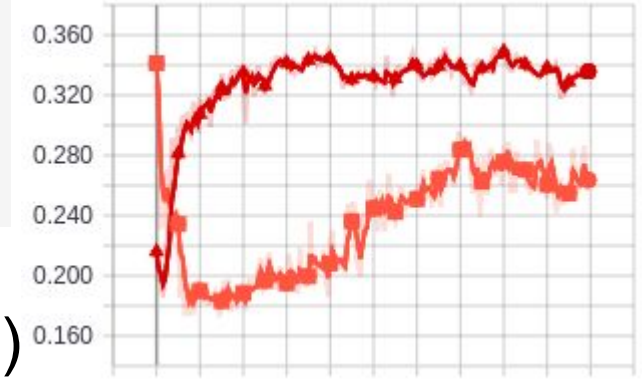
CE loss



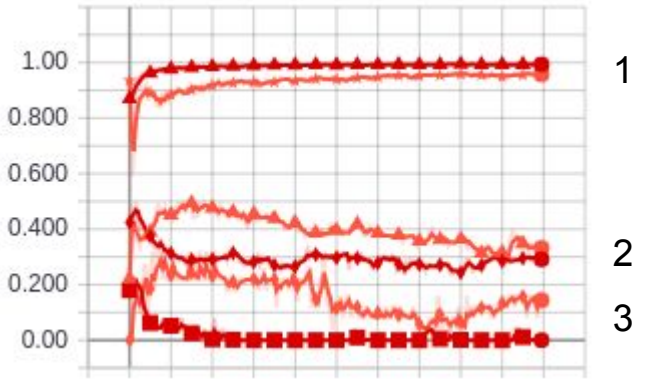
precision



confusion mse



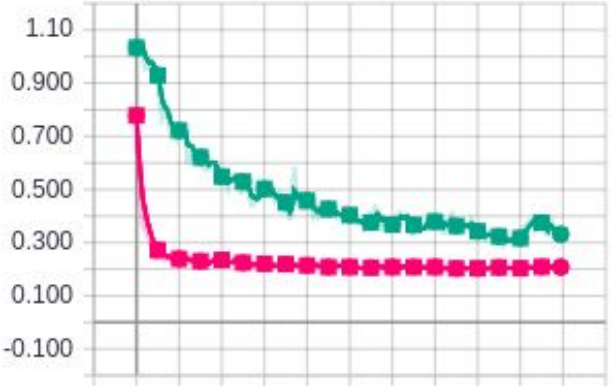
recall



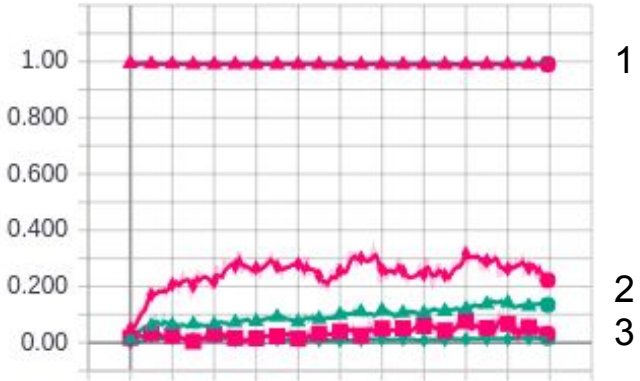
splitting

- metrics/Embed_Att
- metrics/Embed_SMOTE
- metrics/Simple_Att
- metrics/Simple_SMOTE
- metrics/CNN_SMOTE_Att
- metrics/CNN_SMOTE
- metrics/Embed_Simple
- metrics/CNN_Att
- metrics/Embed_SMOTE_Att
- metrics/CNN_Simple
- metrics/Simple_SMOTE_Att
- metrics/Simple_Simple

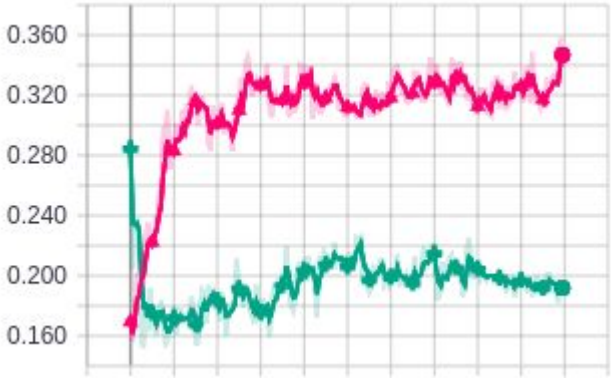
CE loss



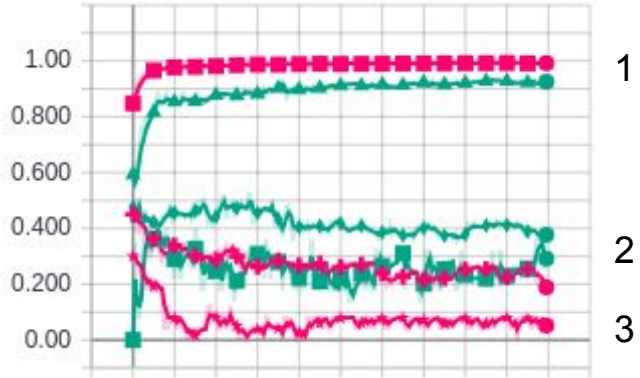
precision



confusion mse



recall

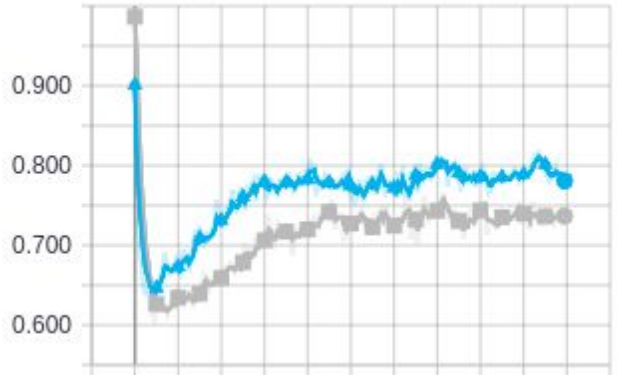


1. default (98%)
2. 10x-100x (1%)
3. 2x-3x (0.4%)

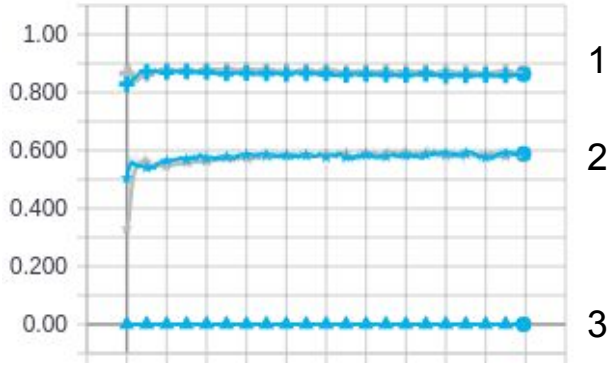
xrootd

- metrics/Embed_Att
- metrics/Embed_SMOTE
- metrics/Simple_Att
- metrics/Simple_SMOTE
- metrics/CNN_SMOTE_Att
- metrics/CNN_SMOTE
- metrics/Embed_Simple
- metrics/CNN_Att
- metrics/Embed_SMOTE_Att
- metrics/CNN_Simple
- metrics/Simple_SMOTE_Att
- metrics/Simple_Simple

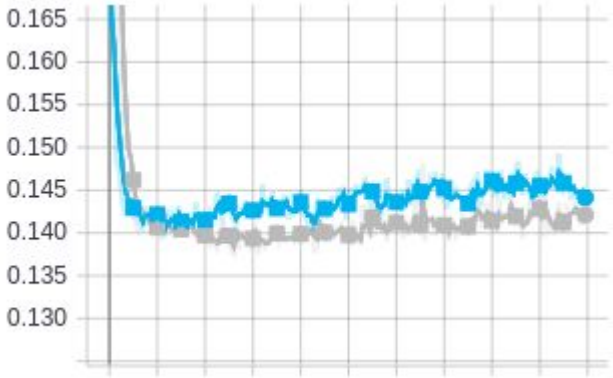
CE loss



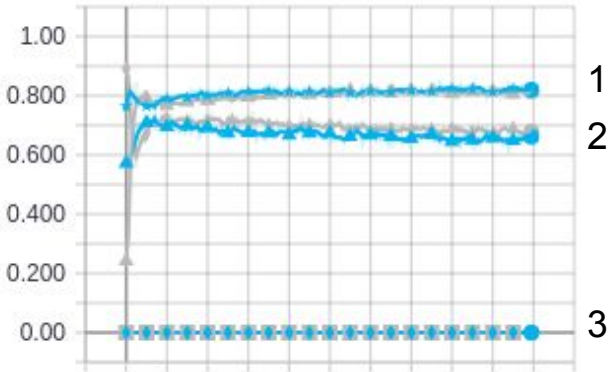
precision



confusion mse



recall

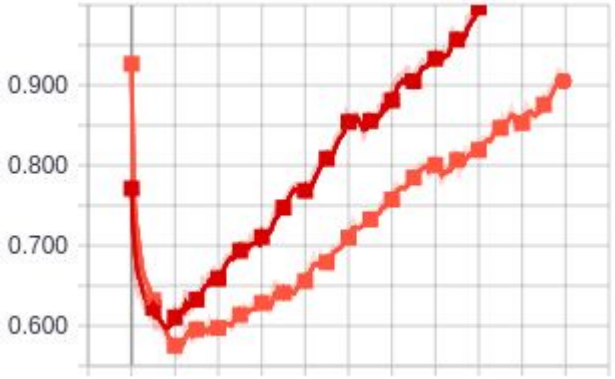


1. default (72%)
2. enabled (28%)
3. disabled (0.01%)

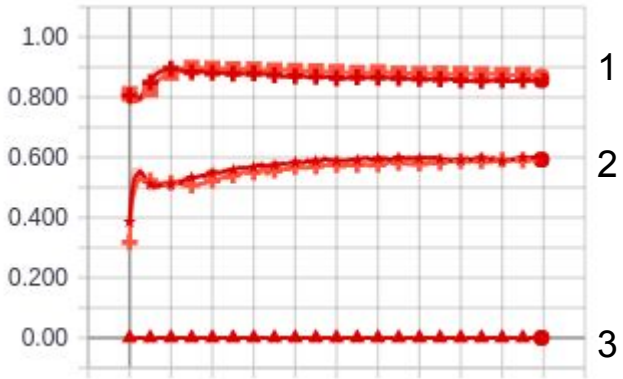
xrootd

- metrics/Embed_Att
- metrics/Embed_SMOTE
- metrics/Simple_Att
- metrics/Simple_SMOTE
- metrics/CNN_SMOTE_Att
- metrics/CNN_SMOTE
- metrics/Embed_Simple
- metrics/CNN_Att
- metrics/Embed_SMOTE_Att
- metrics/CNN_Simple
- metrics/Simple_SMOTE_Att
- metrics/Simple_Simple

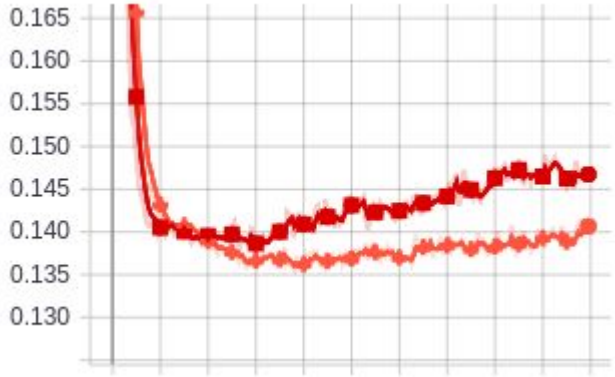
CE loss



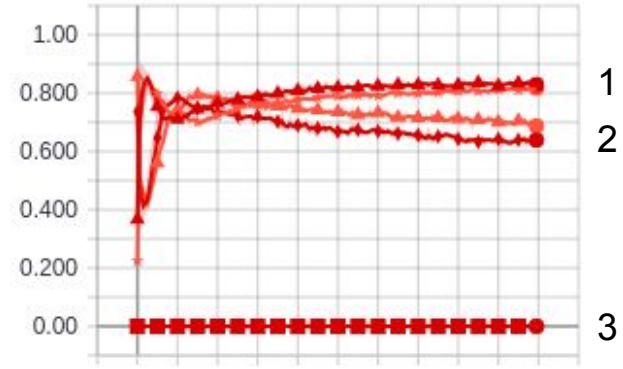
precision



confusion mse



recall



1. default (72%)
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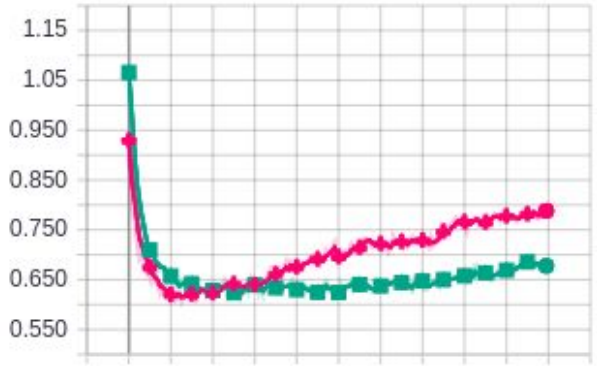
3. disabled (0.01%)

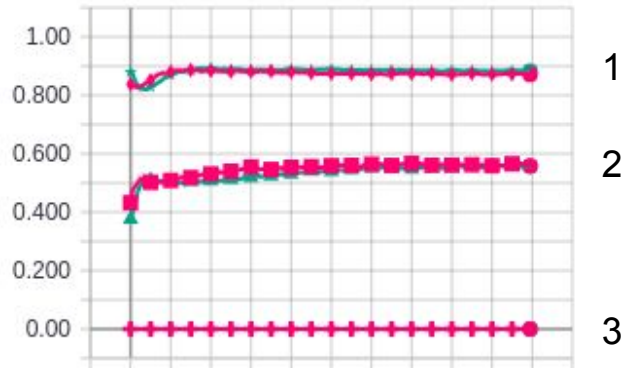
xrootd

- [ ] metrics/Embed_Att
- [x] metrics/Embed_SMOTE
- [ ] metrics/Simple_Att
- [ ] metrics/Simple_SMOTE
- [ ] metrics/CNN_SMOTE_Att
- [ ] metrics/CNN_SMOTE
- [x] metrics/Embed_Simple
- [ ] metrics/CNN_Att
- [ ] metrics/Embed_SMOTE_Att
- [ ] metrics/CNN_Simple
- [ ] metrics/Simple_SMOTE_Att
- [ ] metrics/Simple_Simple

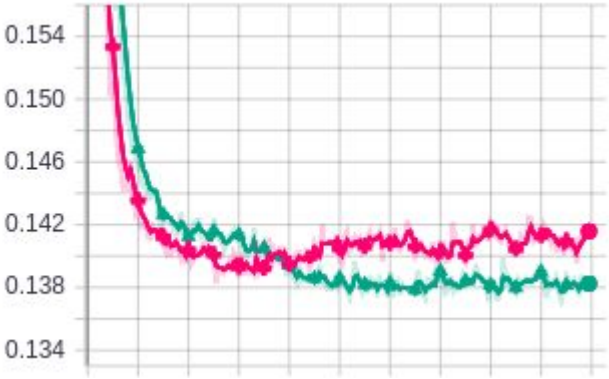
CE loss



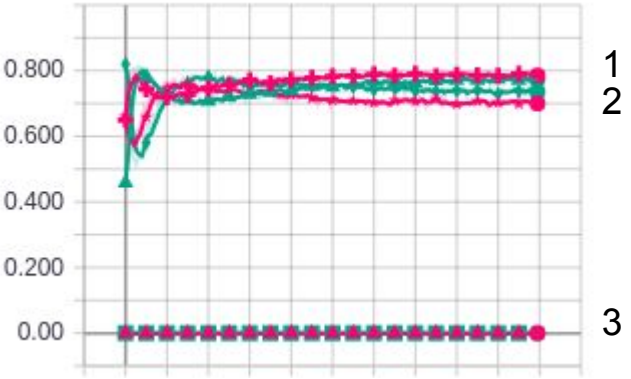
precision



confusion mse



recall



1. default (72%)
2. enabled (28%)
3. disabled (0.01%)

Attention vs no Attention (confusion matrices)

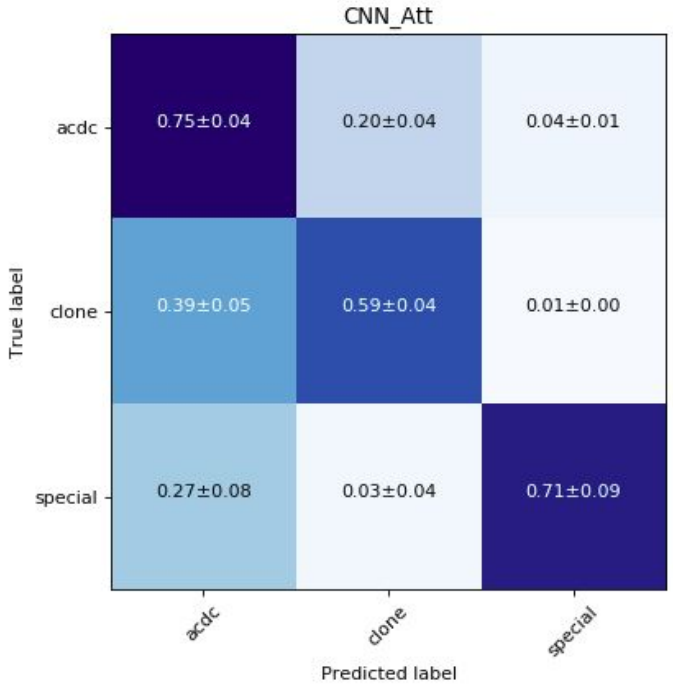
Following slides show:

- Best confusion matrix on each Y target on validation dataset (averaged across 5 folds) using Attention (left matrix) and comparison on right with model without using Attention

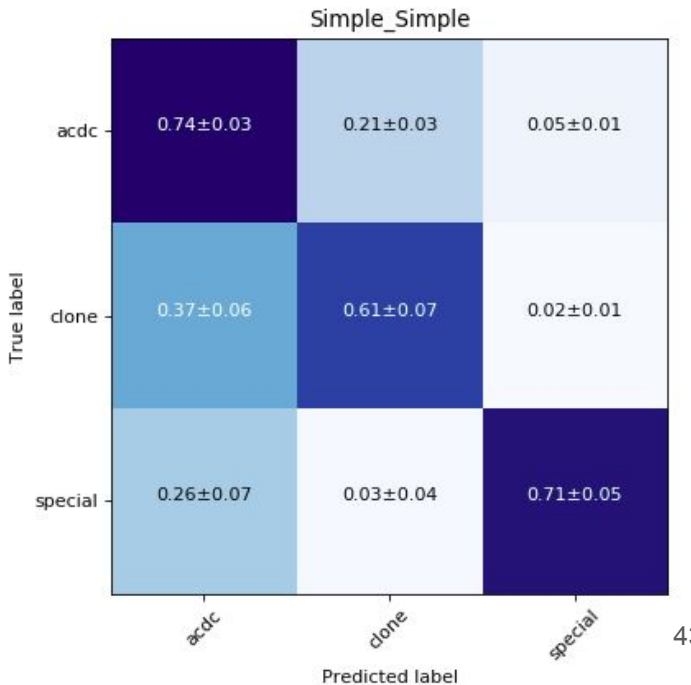
action

1. acdc (88%)
2. clone (10%)
3. special (2%)

best: CNN model
w/ weighted CE
w/out SMOTE



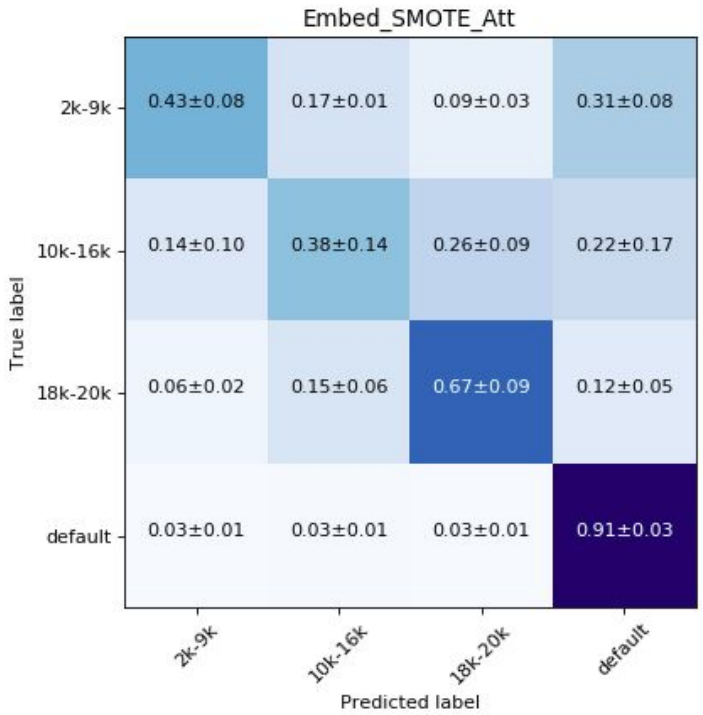
comparison w/ best model
w/out Attention:
Simple w/ weighted CE
w/out SMOTE



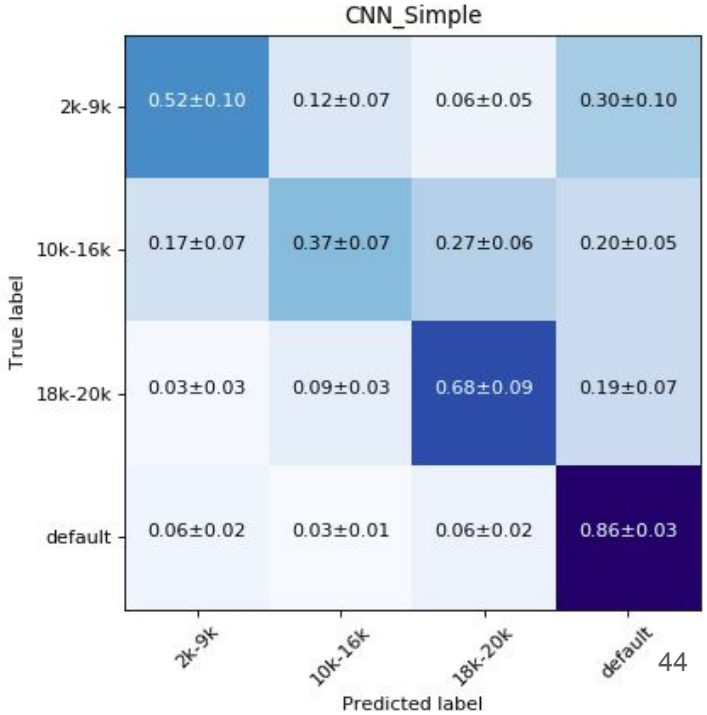
memory

1. default (92%)
2. 18k-20k (4%)
3. 2k-9k (2%)
4. 10k-16k (1.2%)

best: Embed model w/ SMOTE



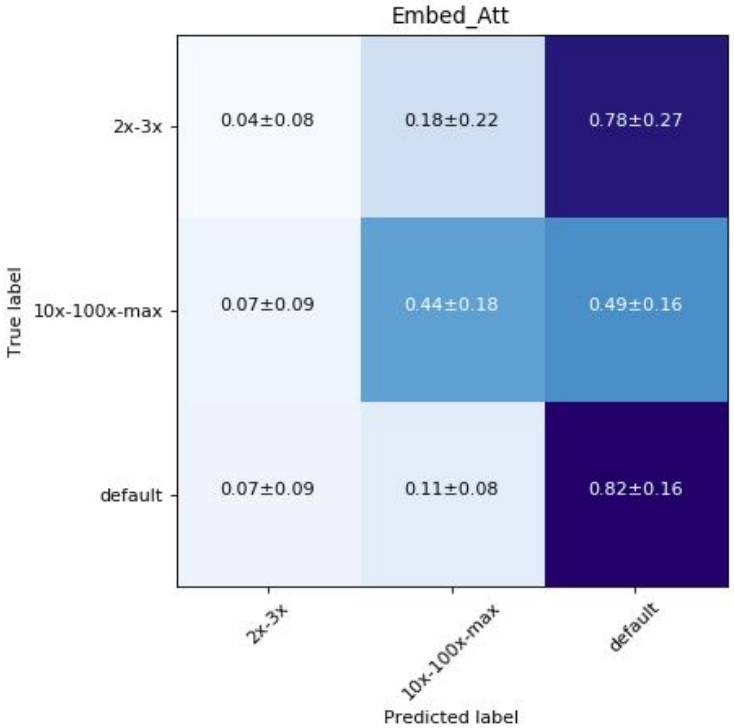
comparison w/ best model w/out Attention:
CNN w/ weighted CE w/out SMOTE



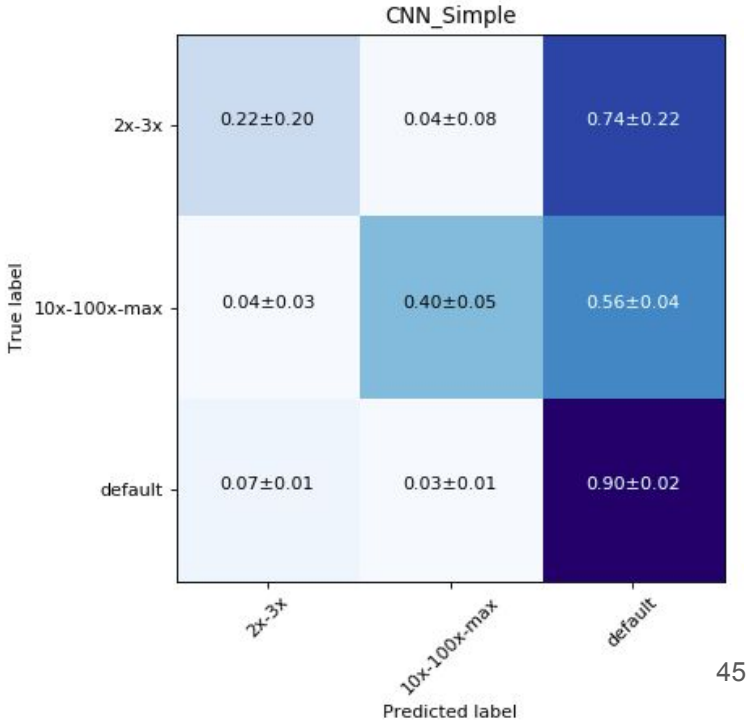
splitting

1. default (98%)
2. 10x-100x (1%)
3. 2x-3x (0.4%)

best: Embed model
w/ weighted CE
w/out SMOTE



comparison w/ best model
w/out Attention:
CNN w/ weighted CE
w/out SMOTE



xrootd

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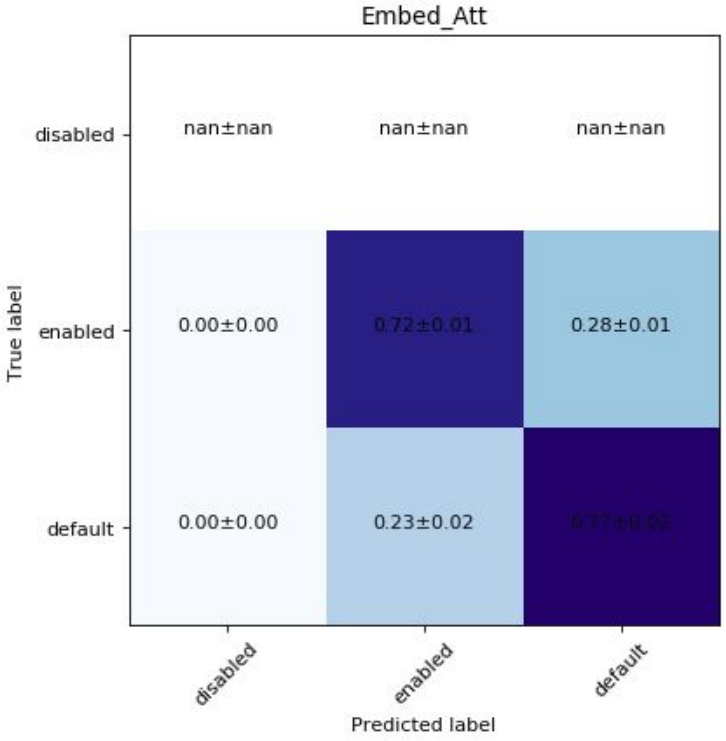
best: Embed model
w/ weighted CE
w/out SMOTE



comparison w/ best model
w/out Attention:
CNN w/ weighted CE
w/out SMOTE