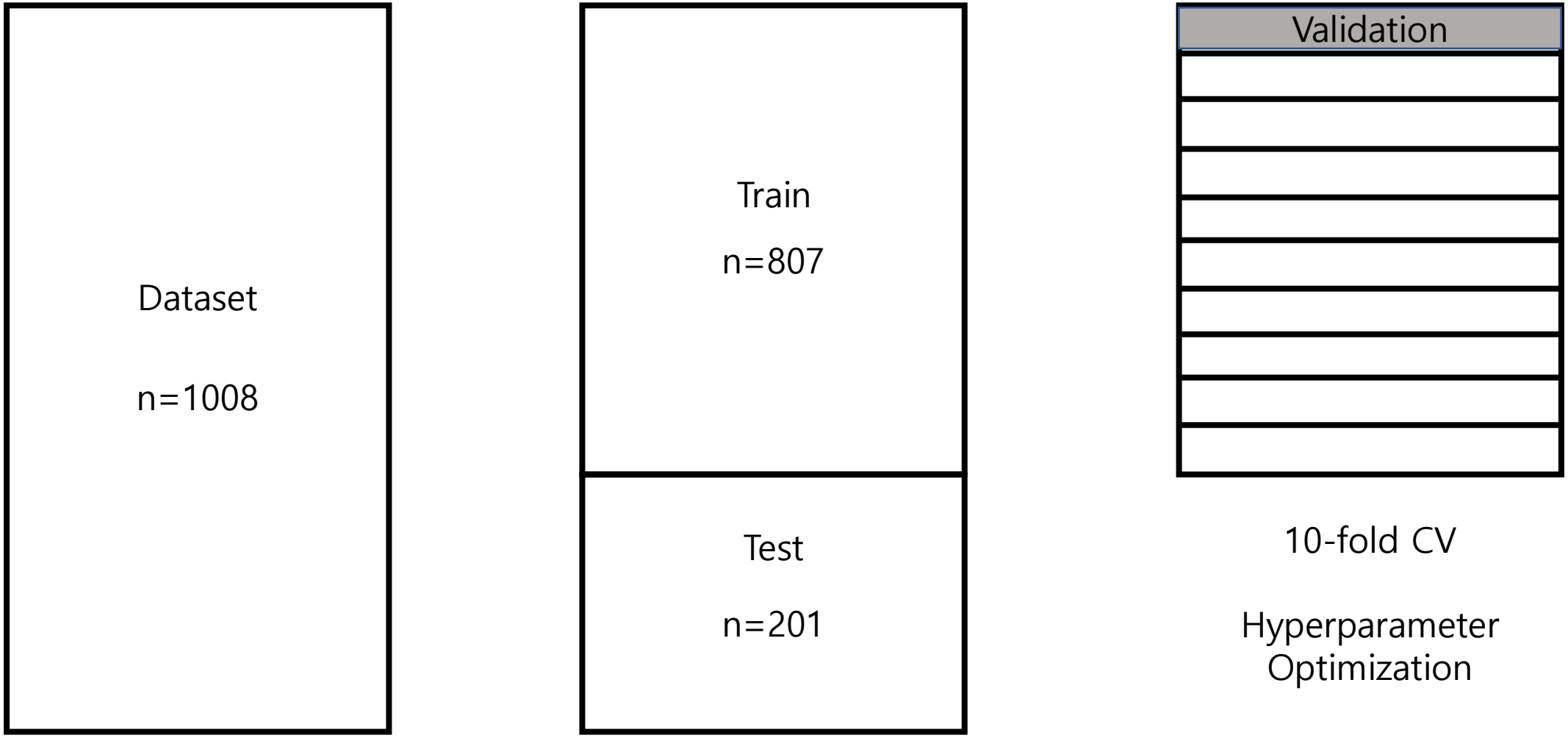
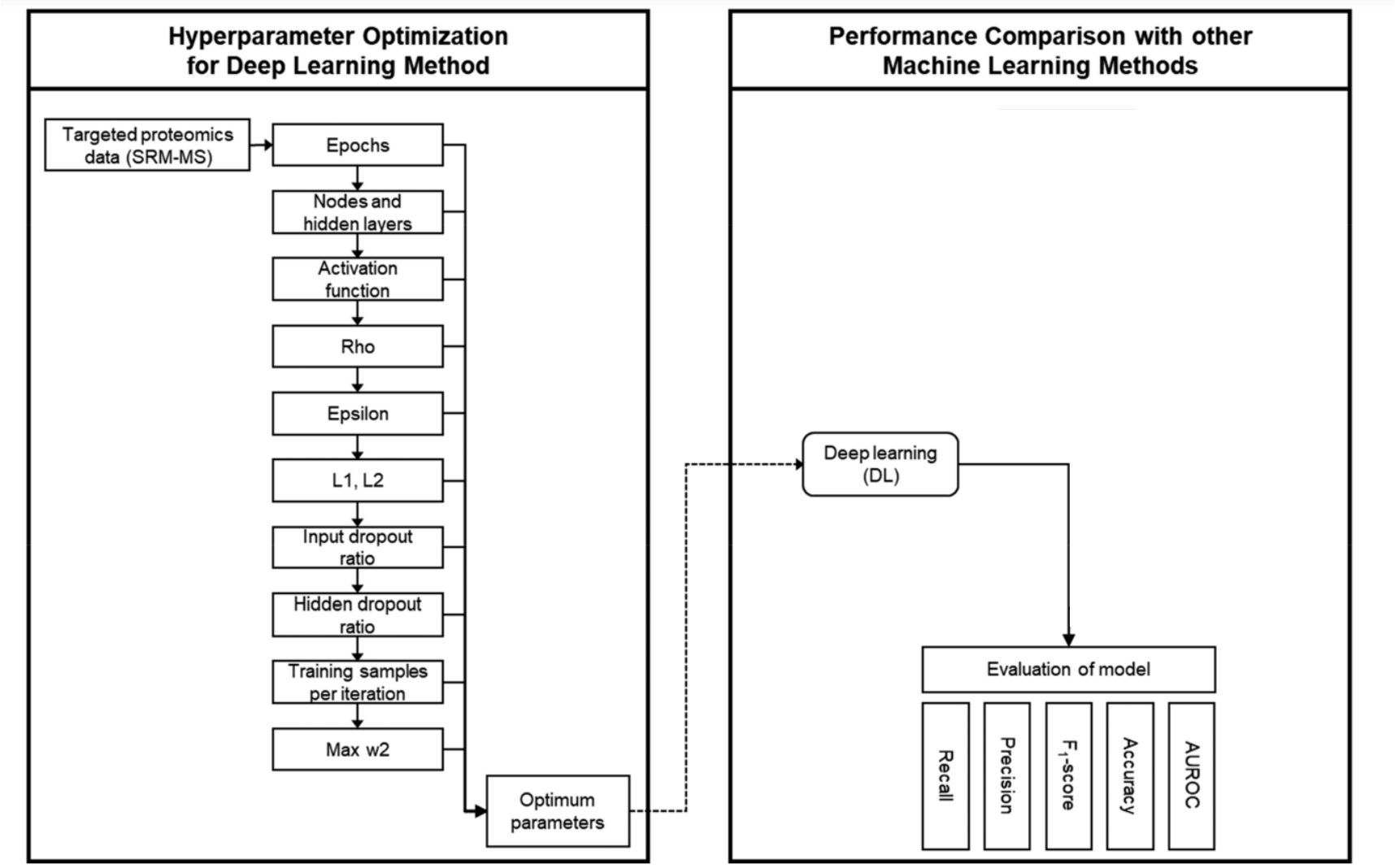
DL Algorithm Using MRM data

최정인

Experimental Design



Experimental Design



Hyperparameter Tuning : 10-fold CV

Activation function : Rectifier / Tanh

Input dropout ratio : 0 / 0.05 / 0.1 / 0.2

Epochs : 20 /30 /40 /50 /60 /70 /80 /90 /100 /200 / 300 / 400 / 500 / 600 / 700 / 800

Epsilon : 1e-4 /1e-5 /1e-6 / 1e-7 / 1e-8 / 1e-9 / 1e-10

Train sample per iteration : 0 / -1 / -2

To specify one epoch, enter 0. To specify all available data, enter -1. To use the automatic values, enter -2.

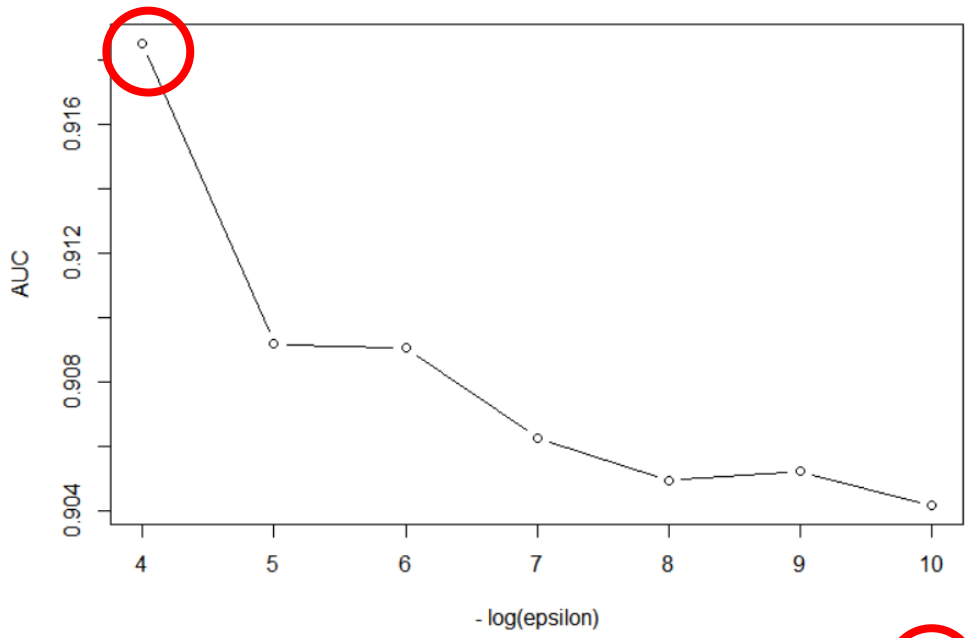
=> 2688 combinations

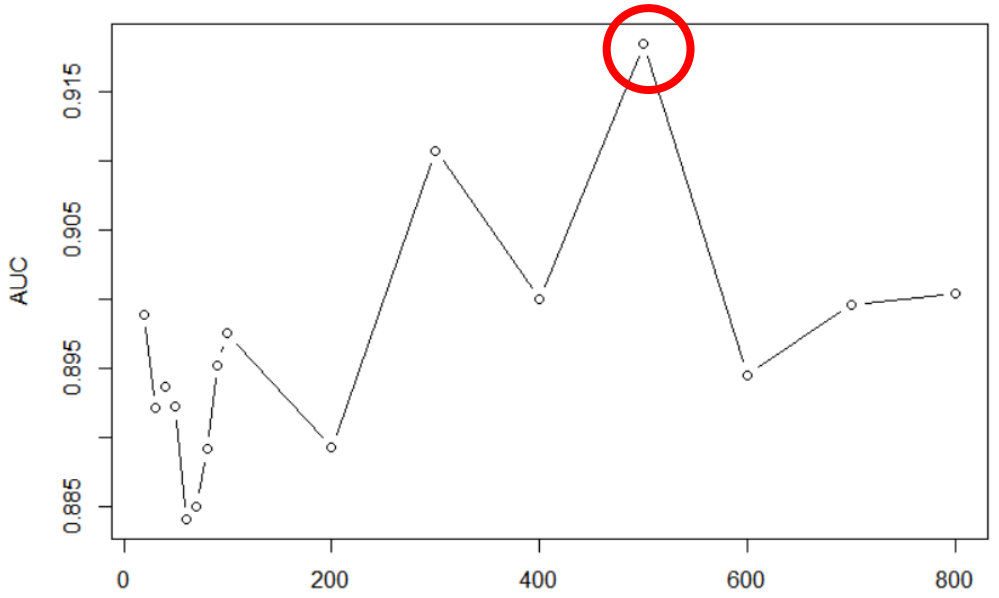
Hyperparameter Tuning : 10-fold CV

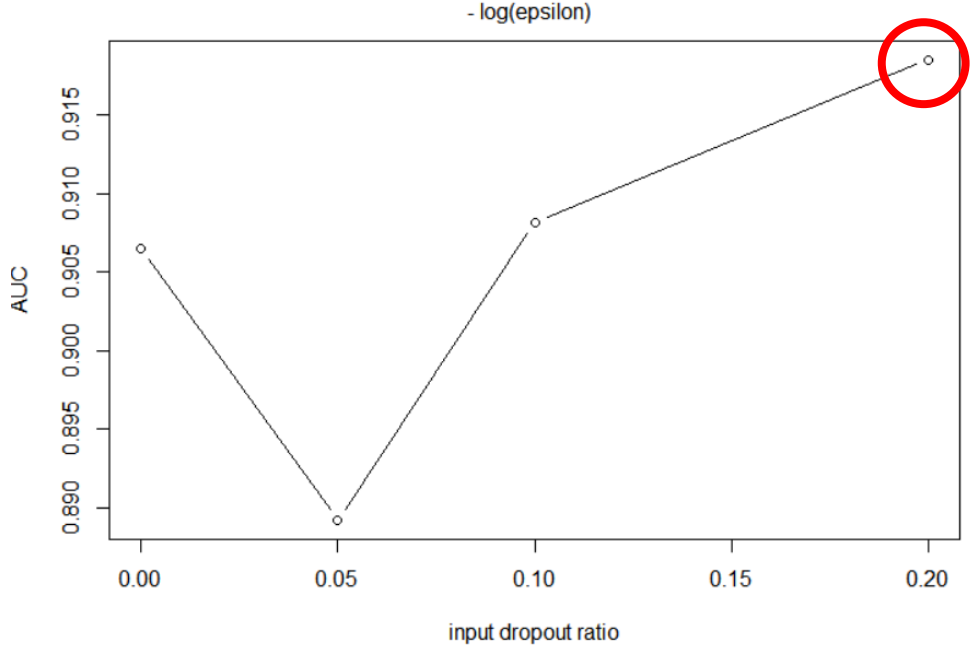
	X	activation	input_dropout_ratio	epochs	train_samples_per_iteration	epsilon	AUC
1	1	Rectifier	0.00000	20	0	0.00010	0.89184
2	2	Rectifier	0.00000	20	0	0.00001	0.90836
3	3	Rectifier	0.00000	20	0	0.00000	0.90455
4	4	Rectifier	0.00000	20	0	0.00000	0.90223
5	5	Rectifier	0.00000	20	0	0.00000	0.90575
6	6	Rectifier	0.00000	20	0	0.00000	0.88762
7	7	Rectifier	0.00000	20	0	0.00000	0.84456
8	8	Rectifier	0.00000	20	-1	0.00010	0.90990
9	9	Rectifier	0.00000	20	-1	0.00001	0.89463
10	10	Rectifier	0.00000	20	-1	0.00000	0.89638
11	11	Rectifier	0.00000	20	-1	0.00000	0.90045
12	12	Rectifier	0.00000	20	-1	0.00000	0.90610
13	13	Rectifier	0.00000	20	-1	0.00000	0.89057
14	14	Rectifier	0.00000	20	-1	0.00000	0.84330
15	15	Rectifier	0.00000	20	-2	0.00010	0.89256
16	16	Rectifier	0.00000	20	-2	0.00001	0.88939
17	17	Rectifier	0.00000	20	-2	0.00000	0.88959
18	18	Rectifier	0.00000	20	-2	0.00000	0.89709
19	19	Rectifier	0.00000	20	-2	0.00000	0.89237
20	20	Rectifier	0.00000	20	-2	0.00000	0.88872
21	21	Rectifier	0.00000	20	-2	0.00000	0.84788
22	22	Rectifier	0.00000	30	0	0.00010	0.89351
23	23	Rectifier	0.00000	30	0	0.00001	0.89586
24	24	Rectifier	0.00000	30	0	0.00000	0.89775
25	25	Rectifier	0.00000	30	0	0.00000	0.89521
26	26	Rectifier	0.00000	30	0	0.00000	0.90815

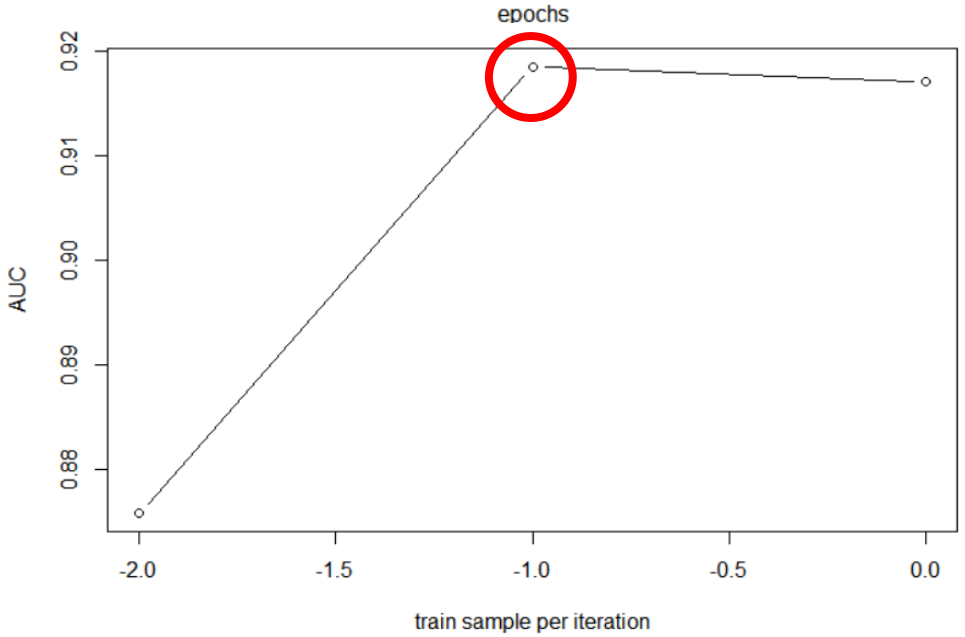
	X	activation	input_dropout_ratio	epochs	train_samples_per_iteration	epsilon	AUC
1248	9	Rectifier	0.20000	400	-1	0.00001	0.89885
1249	10	Rectifier	0.20000	400	-1	0.00000	0.89383
1250	11	Rectifier	0.20000	400	-1	0.00000	0.90380
1251	12	Rectifier	0.20000	400	-1	0.00000	0.91272
1252	13	Rectifier	0.20000	400	-1	0.00000	0.90212
1253	14	Rectifier	0.20000	400	-1	0.00000	0.89684
1254	15	Rectifier	0.20000	400	-2	0.00010	0.87128
1255	16	Rectifier	0.20000	400	-2	0.00001	0.89846
1256	17	Rectifier	0.20000	400	-2	0.00000	0.89957
1257	18	Rectifier	0.20000	400	-2	0.00000	0.90339
1258	19	Rectifier	0.20000	400	-2	0.00000	0.90089
1259	20	Rectifier	0.20000	400	-2	0.00000	0.90620
1260	21	Rectifier	0.20000	400	-2	0.00000	0.89791
1261	1	Rectifier	0.20000	500	0	0.00010	0.91701
1262	2	Rectifier	0.20000	500	0	0.00001	0.90081
1263	3	Rectifier	0.20000	500	0	0.00000	0.89562
1264	4	Rectifier	0.20000	500	0	0.00000	0.90386
1265	5	Rectifier	0.20000	500	0	0.00000	0.90493
1266	6	Rectifier	0.20000	500	0	0.00000	0.90712
1267	7	Rectifier	0.20000	500	0	0.00000	0.89810
1268	8	Rectifier	0.20000	500	-1	0.00010	0.91850
1269	9	Rectifier	0.20000	500	-1	0.00001	0.90919
1270	10	Rectifier	0.20000	500	-1	0.00000	0.90905
1271	11	Rectifier	0.20000	500	-1	0.00000	0.90628
1272	12	Rectifier	0.20000	500	-1	0.00000	0.90497
1273	13	Rectifier	0.20000	500	-1	0.00000	0.90523
1274	14	Rectifier	0.20000	500	-1	0.00000	0.90418
1275	15	Rectifier	0.20000	500	-2	0.00010	0.87580
1276	16	Rectifier	0.20000	500	-2	0.00001	0.89808
1277	17	Rectifier	0.20000	500	-2	0.00000	0.90426
1278	18	Rectifier	0.20000	500	-2	0.00000	0.88569

Train AUC – mean AUC of 10-fold CV







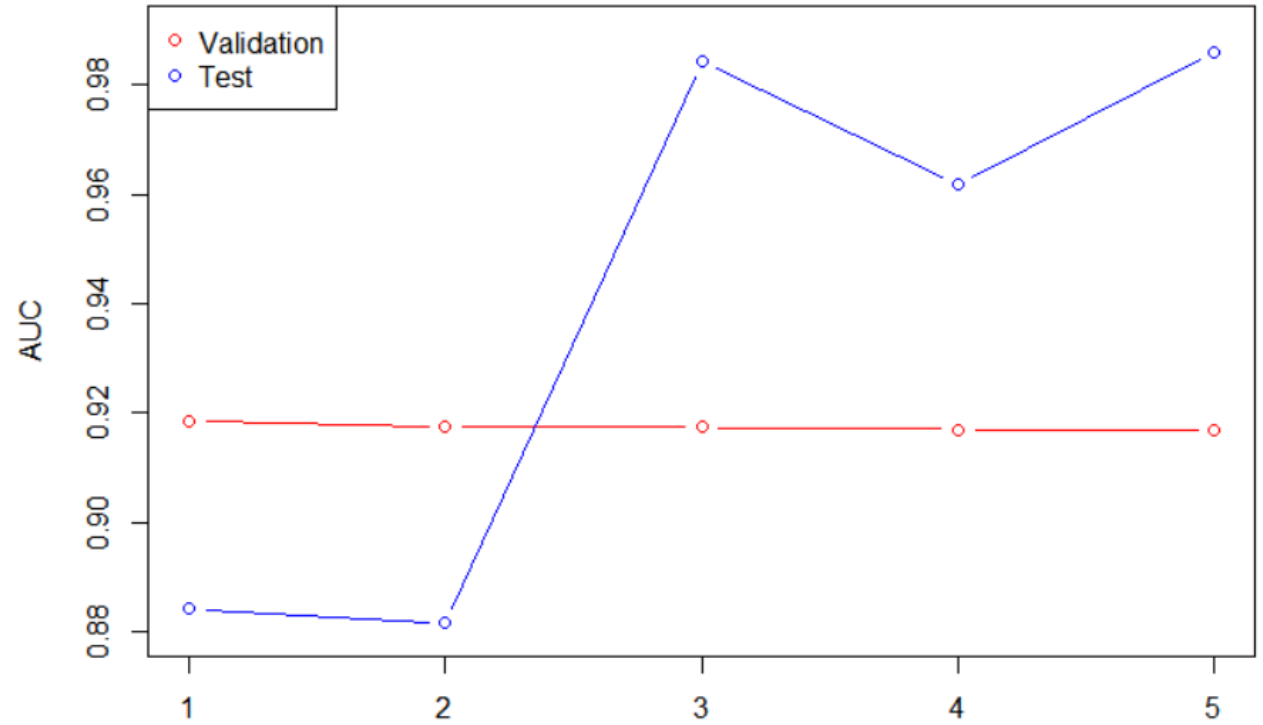


Best 5 models based on train AUC

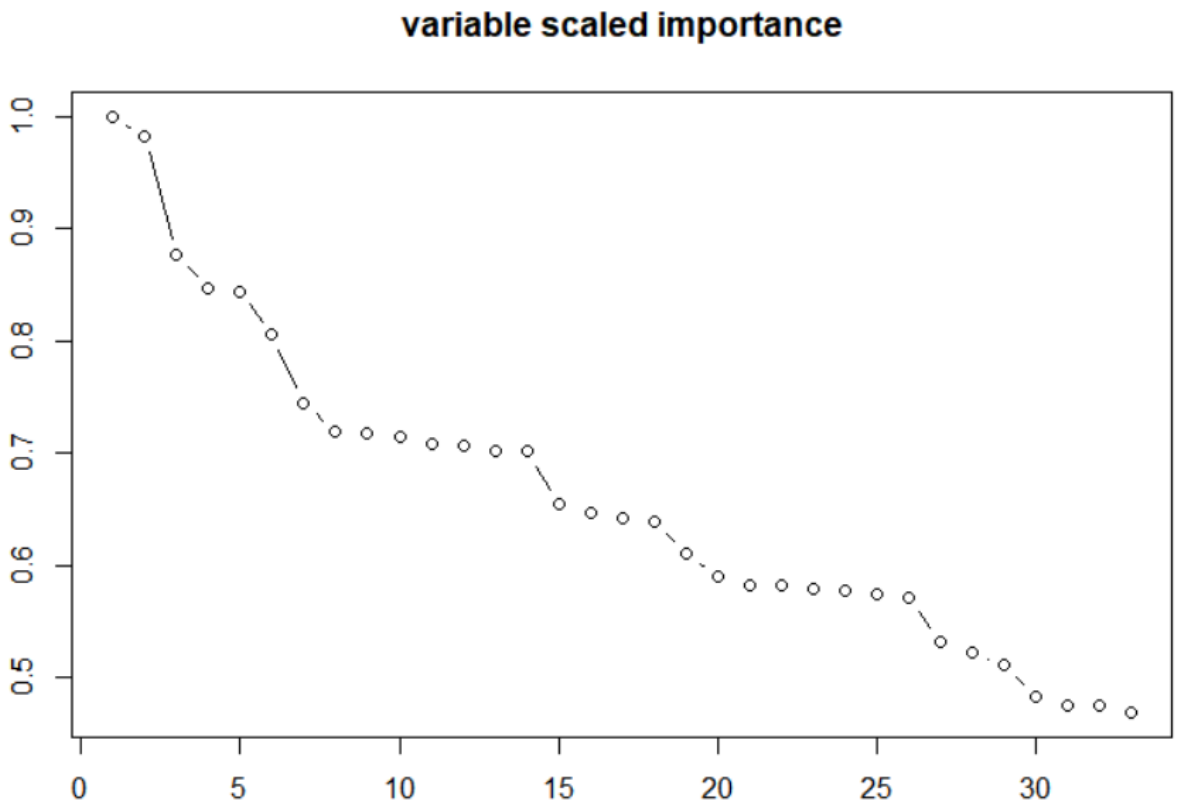
	X	activation	input_dropout_ratio	epochs	train_samples_per_iteration	epsilon	AUC
1268	8	Rectifier	0.20000	500	-1	0.00010	0.91850
379	1	Rectifier	0.05000	40	0	0.00010	0.91738
432	12	Rectifier	0.05000	60	-1	0.00000	0.91738
1261	1	Rectifier	0.20000	500	0	0.00010	0.91701
665	14	Rectifier	0.05000	800	-1	0.00000	0.91679

Test AUC of Best 5 models

	activation	input_dropout_ratio	epochs	epsilon	AUC	test_AUC
1268	Rectifier	0.20000	500	0.00010	0.91850	0.88414
379	Rectifier	0.05000	40	0.00010	0.91738	0.88156
432	Rectifier	0.05000	60	0.00000	0.91738	0.98433
1261	Rectifier	0.20000	500	0.00010	0.91701	0.96174
665	Rectifier	0.05000	800	0.00000	0.91679	0.98596



Variable Importance : Gedeon method



Variable Importance : Gedeon method

Variable Importances:

	variable	relative_importance	scaled_importance	percentage
1	VAAGAFQGLR	1.000000	1.000000	0.045900
2	AADDTWEPFASGK	0.982147	0.982147	0.045080
3	EWFSETFQK	0.877037	0.877037	0.040256
4	ELLALIQLER	0.847206	0.847206	0.038887
5	DGYLFQLLR	0.844421	0.844421	0.038759

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	variable	relative_importance	scaled_importance	percentage
28	LSNNALSGLPQGVFGK	0.521897	0.521897	0.023955
29	IQPSGGTNINEALLR	0.511345	0.511345	0.023471
30	YGQPLPGYTTK	0.482897	0.482897	0.022165
31	DLLLPQPDLR	0.475694	0.475694	0.021834
32	GGSASTWLTAFALR	0.474624	0.474624	0.021785
33	AGFSWIEVTFK	0.468733	0.468733	0.021515