First Model – Multi-Layer Perceptron

Using the TensorFlow Keras library I performed multiple grid searches & cross-validation to optimize the model's hyperparameters. The model is a multi-layer perceptron with the number of units, activation function, number of layers, and optimizer as hyperparameters. The grid search considers all combinations of these hyperparameters and trains and evaluates the model for each combination. First grid-search results:

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Units Per Layer	Activation Function	No. of Layers	Optimizer	Epochs	Batch Size	MSE	R^2
64	relu	2	adam	10	8	0.224044	0.316482
64	relu	2	adam	10	16	0.212253	0.312662
64	relu	2	adam	10	32	0.221621	0.321429
64	relu	2	adam	10	64	0.228725	0.346533
64	relu	2	adam	10	128	0.219787	0.322156
64	relu	2	adam	10	256	0.22963	0.330435
64	relu	3	adam	10	8	0.22722	0.33222
64	relu	3	adam	10	16	0.21132	0.320985
64	relu	3	adam	10	32	0.220123	0.319673
64	relu	3	adam	10	64	0.212145	0.31642
64	relu	3	adam	10	128	0.227734	0.320977
64	relu	3	adam	10	256	0.225559	0.324945
64	relu	4	adam	10	8	0.212145	0.327391
64	relu	4	adam	10	16	0.209875	0.316931
64	relu	4	adam	10	32	0.215377	0.321995
64	relu	4	adam	10	64	0.226254	0.313717
64	relu	4	adam	10	128	0.220234	0.313717
		4	1		1		0.319930
64 64	relu relu	5	adam adam	10	256 8	0.226489 0.237961	0.338178
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64	relu	<u>5</u>	adam	10	16 32	0.215081	0.319046
64	relu		adam	10		0.21513	0.324387
64	relu	5	adam	10	64	0.209051	0.318896
64	relu	5	adam	10	128	0.215715	0.322011
64	relu	5	adam	10	256	0.248842	0.360523
64	tanh	2	adam	10	8	0.215241	0.317689
64	tanh	2	adam	10	16	0.238018	0.341173
64	tanh	2	adam	10	32	0.232614	0.325855
64	tanh	2	adam	10	64	0.248103	0.338166
64	tanh	2	adam	10	128	0.251979	0.346708
64	tanh	2	adam	10	256	0.273365	0.365192
64	tanh	3	adam	10	8	0.225148	0.318866
64	tanh	3	adam	10	16	0.226702	0.332043
64	tanh	3	adam	10	32	0.235575	0.329446
64	tanh	3	adam	10	64	0.221118	0.325245
64	tanh	3	adam	10	128	0.235043	0.342608
64	tanh	3	adam	10	256	0.247696	0.353213
64	tanh	4	adam	10	8	0.243508	0.355629
64	tanh	4	adam	10	16	0.233445	0.340998
64	tanh	4	adam	10	32	0.224969	0.327489
64	tanh	4	adam	10	64	0.225109	0.322122
64	tanh	4	adam	10	128	0.238279	0.326479
64	tanh	4	adam	10	256	0.256057	0.355652
64	tanh	5	adam	10	8	0.239673	0.329573
64	tanh	5	adam	10	16	0.235766	0.34191
64	tanh	5	adam	10	32	0.221314	0.31752
64	tanh	5	adam	10	64	0.223995	0.318587
64	tanh	5	adam	10	128	0.234465	0.330605
64	tanh	5	adam	10	256	0.243001	0.338845
128	relu	2	adam	10	8	0.208366	0.305084
128	relu	2	adam	10	16	0.209042	0.310396
128	relu	2	adam	10	32	0.210125	0.307196
128	relu	2	adam	10	64	0.217805	0.311788
128	relu	2	adam	10	128	0.216145	0.326357
128	relu	2	adam	10	256	0.21918	0.326501
128	relu	3	adam	10	8	0.223651	0.335616
128	relu	3	adam	10	16	0.207523	0.308899
128	relu	3	adam	10	32	0.225145	0.326913

128	0.321558 0.328741 0.319751 0.306865 0.31956 0.323949 0.326555 0.322284 0.319643 0.320123 0.316637 0.328439 0.31016 0.326555 0.347482 0.342861 0.32177 0.319779 0.356113 0.366086 0.334883 0.336716 0.317835 0.341201 0.35016
128	0.319751 0.306865 0.31956 0.323949 0.326555 0.322284 0.319643 0.320123 0.316637 0.328439 0.31016 0.32655 0.347482 0.342861 0.32177 0.319779 0.356113 0.366086 0.334883 0.336716 0.317835 0.341201 0.35016
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128	0.346402
	0.348754
256 relu 2 adam 10 8 0.22492	0.330053
256 relu 2 adam 10 16 0.21829	0.319995
256 relu 2 adam 10 32 0.206546	0.311331
256 relu 2 adam 10 64 0.222013	0.333738
256 relu 2 adam 10 128 0.226403	0.331925
256 relu 2 adam 10 256 0.21609	0.32517
256 relu 3 adam 10 8 0.208955	0.313305
256 relu 3 adam 10 16 0.213413	0.322922
256 relu 3 adam 10 32 0.216532	0.309685
256 relu 3 adam 10 64 0.233748	0.323179
256 relu 3 adam 10 128 0.220572	0.316795
256 relu 3 adam 10 256 0.207801	0.315225
256 relu 4 adam 10 8 0.227595	0.328941
256 relu 4 adam 10 16 0.222006	0.310008
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256 relu 4 adam 10 64 0.228188	0.339168
256 relu 4 adam 10 128 0.214371	0.324241
256 relu 4 adam 10 256 0.218668	0.319749
256 relu 5 adam 10 8 0.204824	0.306975
256 relu 5 adam 10 16 0.2072	0.312006
256 relu 5 adam 10 32 0.211578	0.313068
256 relu 5 adam 10 64 0.207819	0.31816
256 relu 5 adam 10 128 0.218923	0.318841
256 relu 5 adam 10 256 0.209012	0.322161
256 tanh 2 adam 10 8 0.241161	0.332925
256 tanh 2 adam 10 16 0.236437	0.352759
256 tanh 2 adam 10 32 0.235537	0.345777
256 tanh 2 adam 10 64 0.222765	0.319905
256 tanh 2 adam 10 128 0.276093	
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256 tanh 3 adam 10 8 0.244419	0.348434
256 tanh 3 adam 10 16 0.240922	

25.0	41-	2	- 1	10	22	0.224020	0.22041
256 256	tanh tanh	3	adam adam	10 10	32 64	0.234029 0.253037	0.32941 0.358586
256	1	3		10	128	0.233037	0.336360
256	tanh tanh	3	adam adam	10	256	0.247423	0.341739
256	tanh	4	adam	10	8	0.236934	0.339330
256	tanh	4	adam	10	16	0.246199	0.343001
256	tanh	4	adam	10	32	0.250844	0.354546
256	tanh	4	adam	10	64	0.230844	0.343142
-	1	4		10		0.248201	
256 256	tanh tanh	4	adam adam	10	128 256	0.24273	0.352775 0.353073
256	1	5	adam	10	8	0.27193	0.333073
	tanh	5				0.289563	
256 256	tanh tanh	5	adam adam	10 10	16 32	0.289303	0.393264
256	1	5		10	64	0.262953	0.36383
256	tanh tanh	5	adam adam	10	128	0.202933	0.355329 0.427542
256	tanh	5	adam	10	256	0.250764	0.340192
512	relu	2	adam	10	8	0.230704	0.326564
512	relu	2	adam	10	16	0.22466	0.320304
512	relu	2	adam	10	32	0.207466	0.306897
512	relu	2	adam	10	64	0.207400	0.308437
512	relu	2	adam	10	128	0.204488	0.334703
512	relu	2	adam	10	256	0.225631	0.326718
512	relu	3	adam	10	8	0.223631	0.326718
512	relu	3	adam	10	16	0.212703	0.313481
512	relu	3	adam	10	32	0.210349	0.330387
512	relu	3	adam	10	64	0.209336	0.309705
512	relu	3	adam	10	128	0.218821	0.321909
512	relu	3	adam	10	256	0.218821	0.321303
512	relu	4	adam	10	8	0.216645	0.30532
512	relu	4	adam	10	16	0.218291	0.322156
512	relu	4	adam	10	32	0.219542	0.3255
512	relu	4	adam	10	64	0.210059	0.324888
512	relu	4	adam	10	128	0.240048	0.330429
512	relu	4	adam	10	256	0.213656	0.320748
512	relu	5	adam	10	8	0.21028	0.315247
512	relu	5	adam	10	16	0.215092	0.333958
512	relu	5	adam	10	32	0.205468	0.317355
512	relu	5	adam	10	64	0.215524	0.326526
512	relu	5	adam	10	128	0.218851	0.331722
512	relu	5	adam	10	256	0.211248	0.317664
512	tanh	2	adam	10	8	0.26916	0.371122
512	tanh	2	adam	10	16	0.249523	0.359523
512	tanh	2	adam	10	32	0.251282	0.347249
512	tanh	2	adam	10	64	0.249699	0.33647
512	tanh	2	adam	10	128	0.252707	0.335468
512	tanh	2	adam	10	256	0.24265	0.338714
512	tanh	3	adam	10	8	0.24744	0.345029
512	tanh	3	adam	10	16	0.260181	0.351524
512	tanh	3	adam	10	32	0.24503	0.352272
512	tanh	3	adam	10	64	0.239263	0.332768
512	tanh	3	adam	10	128	0.26393	0.350336
512	tanh	3	adam	10	256	0.240569	0.344233
512	tanh	4	adam	10	8	0.312941	0.399384
512	tanh	4	adam	10	16	0.276091	0.358734
512	tanh	4	adam	10	32	0.26419	0.363237
512	tanh	4	adam	10	64	0.272449	0.370399
512	tanh	4	adam	10	128	0.271018	0.368783
512	tanh	4	adam	10	256	0.261508	0.356
512	tanh	5	adam	10	8	0.438602	0.483205
512	tanh	5	adam	10	16	0.292322	0.408722
512	tanh	5	adam	10	32	0.264102	0.377943
512	tanh	5	adam	10	64	0.260966	0.357417
512	tanh	5	adam	10	128	0.271158	0.383269
512	tanh	5	adam	10	256	0.252574	0.367451
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