

Supp Table 1: Different hyperparameter values for 964 side effect of each model

Method	No. hidden layers	No. neurons	Activation function	Dropout rate	Learning rate	Momentum
Model-1	1	300	relu, sigmoid	0.1	0.01	0.9
Model-2	2	300,200	relu,relu,sigmoid	0.1	0.01	0.9
Model-3	3	300,200,100	relu,relu,relu,sigmoid	0.1	0.01	0.9
Model-4	3	100,200,300	relu,relu,relu,sigmoid	0.1	0.01	0.9
Model-5	3	300,200,200	relu,relu,relu,sigmoid	0.1	0.01	0.9
Model-6	3	300,100,100	relu,relu,relu,sigmoid	0.1	0.01	0.9
Model-7	3	300,200,100	tanh,tanh,tanh,sigmoid	0.1	0.01	0.9
Model-8	3	300,200,100	sigmoid,sigmoid,sigmoid,sigmoid	0.3	0.01	0.9
Model-9	3	300,200,100	tanh,tanh,tanh,tanh	0.5	0.01	0.9
Model-10	3	300,200,200	relu,relu,relu,sigmoid	0.1	0.001	0.9
Model-11	3	300,200,200	relu,relu,relu,sigmoid	0.1	0.01	0.7

Supp Table 2: AUROC results of NNPS and Decagon on best performance side effects in NNPS

Best performance side effects in NNPS	AUROC (NNPS)	AUROC (Decagon)
Arachnoiditis	1.0	0.744
MPD	1.0	0.746
Sinus arrest	1.0	0.832
Colon neoplasm	1.0	0.826
Sarcoma	1.0	0.791
Carcinoma of the cervix	1.0	0.879
Pneumoconiosis	1.0	0.856
Malignant hypertension	1.0	0.906
Epidural hematoma	1.0	0.936
Oophorectomy	1.0	0.917

Supp Table 3: AUPRC results of NNPS and Decagon on best performance side effects in NNPS

Best performance side effects in NNPS	AUPRC (NNPS)	AUPRC (Decagon)
Arachnoiditis	1.0	0.694
MPD	1.0	0.685
Sinus arrest	1.0	0.776
Colon neoplasm	1.0	0.788
Sarcoma	1.0	0.789
Carcinoma of the cervix	1.0	0.810
Pneumoconiosis	1.0	0.834
Malignant hypertension	1.0	0.858
Epidural hematoma	1.0	0.906
Oophorectomy	1.0	0.911

Supp Table 4: AUPRC results of NNPS and Decagon on best performance side effects in Decagon

Best performance side effects in Decagon	AUPRC (Decagon)	AUPRC (NNPS)
Mumps	0.964	0.981
Carbuncle	0.949	0.963
Coccydynia	0.943	0.995
Tympanic membrane perforation	0.941	1.0
Dyshidrosis	0.938	0.995
Spondylosis	0.929	0.929
Schizoaffective disorder	0.919	0.920
Breast dysplasia	0.918	0.999
Ganglion	0.909	0.999
Uterine polyp	0.908	1.0

Supp Table 5: AUROC results of NNPS and Decagon on worst performance side effects in NNPS

Worst performance side effects in NNPS	AUROC (NNPS)	AUROC (Decagon)
Corneal abrasion	0.913	0.820
Eosinophilic pneumonia	0.916	0.854
Haemarthrosis	0.886	0.868
Aplasia pure red cell	0.883	0.848
Patent ductus arteriosis	0.889	0.708
Lung adenocarcinoma	0.933	0.724
Glomerulonephritis	0.879	0.842
Endocarditis	0.919	0.865
Transfusion reaction	0.913	0.723
Hypoglycaemia neonatal	0.862	0.903

Supp Table 6: AUPRC results of NNPS and Decagon on worst performance side effects in NNPS

Worst performance side effects in NNPS	AUPRC (NNPS)	AUPRC (Decagon)
Corneal abrasion	0.759	0.783
Eosinophilic pneumonia	0.780	0.802
Haemarthrosis	0.797	0.813
Aplasia pure red cell	0.801	0.793
Patent ductus arteriosis	0.802	0.649
Lung adenocarcinoma	0.811	0.720
Glomerulonephritis	0.816	0.739
Endocarditis	0.818	0.803
Transfusion reaction	0.830	0.716
Hypoglycaemia neonatal	0.835	0.884

Supp Table 7: AUPRC results of NNPS and Decagon on worst performance side effects in Decagon

Worst performance side effects in Decagon	AUPRC (Decagon)	AUPRC (NNPS)
Bleeding	0.679	0.931
Increased body temperature	0.680	0.950
Emesis	0.693	0.943
Renal disorder	0.694	0.951
Leucopenia	0.695	0.898
Diarrhea	0.705	0.942
Icterus	0.707	0.936
Nausea	0.711	0.940
Itch	0.712	0.952
Anaemia	0.712	0.945