

CSC 4850 Team 5 Project Report

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1 Model Results

1.1 DrugOrchestra Results

Datasets	Metrics	SVM	Random Forest	STL-NN	DrugOrchestra
STITCH	AUROC	0.668±0.048	0.666±0.032	0.827±0.031	0.833±0.047
	AUPRC	0.320±0.092	0.349±0.053	0.583±0.034	0.587±0.088
Drugbank	AUROC	0.625±0.042	0.616±0.035	0.748±0.034	0.752±0.023
	AUPRC	0.260±0.098	0.269±0.055	0.530±0.041	0.540±0.012
Repur	AUROC	0.530±0.010	0.585±0.049	0.691±0.014	0.703±0.031
	AUPRC	0.125±0.018	0.221±0.066	0.293±0.023	0.321±0.036
PDX	SCC	0.491±0.015	0.436±0.017	0.468±0.094	0.465±0.014
	MSE	0.824±0.034	0.846±0.034	0.856±0.028	0.840±0.023
GDSC	SCC	0.235±0.039	0.151±0.020	0.394±0.022	0.410±0.010
	MSE	1.150±0.086	1.110±0.048	0.930±0.024	0.814±0.061
CCLE	SCC	0.206±0.016	0.118±0.012	0.394±0.022	0.410±0.010
	MSE	1.472±0.046	1.147±0.031	0.930±0.026	0.882±0.037
SIDER	AUROC	0.591±0.026	0.640±0.026	0.660±0.026	0.671±0.036
	AUPRC	0.231±0.022	0.295±0.035	0.312±0.016	0.321±0.034
OFFSIDES	AUROC	0.629±0.009	0.638±0.029	0.640±0.025	0.686±0.011
	AUPRC	0.399±0.005	0.435±0.013	0.432±0.022	0.457±0.037

1.2 Project Results

Datasets	Metrics	KNN	Linear Regression	Logistic Regression	Naive Bayes	Decision Tree	Random Forest	Gradient Boosting	SVM
STITCH	AUROC	0.659 ± 0.066	0.775 ± 0.05	0.763 ± 0.053	0.73 ± 0.069	0.592 ± 0.065	0.746 ± 0.031	0.736 ± 0.039	0.74 ± 0.013
	AUPRC	0.214 ± 0.056	0.34 ± 0.132	0.334 ± 0.108	0.303 ± 0.119	0.161 ± 0.044	0.311 ± 0.082	0.311 ± 0.087	0.295 ± 0.059
Drugbank	AUROC	0.688 ± 0.024	0.689 ± 0.062	0.665 ± 0.078	0.716 ± 0.103	0.566 ± 0.021	0.739 ± 0.056	0.652 ± 0.057	0.784 ± 0.049
	AUPRC	0.368 ± 0.119	0.503 ± 0.094	0.448 ± 0.102	0.491 ± 0.126	0.098 ± 0.009	0.388 ± 0.115	0.296 ± 0.118	0.48 ± 0.125
Repur	AUROC	0.602 ± 0.041	0.669 ± 0.009	0.672 ± 0.014	0.635 ± 0.053	0.541 ± 0.053	0.632 ± 0.027	0.604 ± 0.038	0.66 ± 0.042
	AUPRC	0.138 ± 0.018	0.196 ± 0.016	0.234 ± 0.055	0.222 ± 0.029	0.123 ± 0.018	0.217 ± 0.023	0.214 ± 0.032	0.216 ± 0.033
PDX	SCC	0.244 ± 0.073	0.231 ± 0.083	N/A	N/A	0.273 ± 0.049	0.271 ± 0.042	0.276 ± 0.054	0.266 ± 0.027
	MSE	1.049 ± 0.138	1.152 ± 0.072	N/A	N/A	1.559 ± 0.201	1.04 ± 0.045	0.958 ± 0.131	0.989 ± 0.164
GDSC	SCC	0.058 ± 0.04	0.061 ± 0.036	N/A	N/A	0.039 ± 0.018	0.092 ± 0.013	0.053 ± 0.038	0.091 ± 0.011
	MSE	1.761 ± 0.37	1.441 ± 0.182	N/A	N/A	2.721 ± 0.319	1.491 ± 0.187	1.324 ± 0.208	1.31 ± 0.2
CCLE	SCC	0.104 ± 0.022	0.177 ± 0.051	N/A	N/A	0.069 ± 0.043	0.047 ± 0.035	0.077 ± 0.05	0.148 ± 0.05
	MSE	1.432 ± 0.199	1.102 ± 0.092	N/A	N/A	2.079 ± 0.129	1.178 ± 0.117	1.093 ± 0.135	1.086 ± 0.166
SIDER	AUROC	0.567±0.084	0.541±0.088	0.544±0.068	0.701±0.019	0.549±0.036	0.691±0.025	0.673±0.023	0.672±0.026
	AUPRC	0.192 ± 0.045	0.252 ± 0.063	0.242 ± 0.064	0.359 ± 0.008	0.161 ± 0.017	0.296 ± 0.037	0.295 ± 0.019	0.33 ± 0.012
OFFSIDE	AUROC	0.544 ± 0.042	0.525 ± 0.072	0.501 ± 0.049	0.584 ± 0.075	0.545 ± 0.017	0.591 ± 0.069	0.545 ± 0.044	0.59 ± 0.061
	AUPRC	0.328 ± 0.031	0.369 ± 0.058	0.343 ± 0.037	0.419 ± 0.09	0.316 ± 0.009	0.376 ± 0.048	0.372 ± 0.044	0.383 ± 0.056

2 GitHub

Link to GitHub: <https://github.com/marendale/team-5-csc-4850>