

Result: FOLD-WISE (Test Data)

Tab. S1. Foldwise performance evaluation on the test data (one-versus-all) with all three classifiers considering k=3

KMR=3	Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
	SVM	0	0.8	0.8051	0.7255	0.7498	0.6831	0.7149	0.4532
		1	0.802	0.8068	0.7343	0.7585	0.686	0.7204	0.4707
		2	0.79	0.8033	0.7187	0.7502	0.6635	0.7042	0.4409
		3	0.794	0.8052	0.7207	0.7535	0.6684	0.7084	0.4451
		4	0.803	0.8137	0.7258	0.7507	0.6792	0.7132	0.4539
		Avg	0.798	0.8068	0.725	0.7525	0.676	0.7122	0.4528
Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC	
RF	0	0.793	0.8012	0.7287	0.7567	0.6801	0.7164	0.4601	
	1	0.792	0.7996	0.7272	0.7488	0.682	0.7139	0.456	
	2	0.784	0.7991	0.7168	0.7473	0.6631	0.7027	0.437	
	3	0.787	0.7973	0.7147	0.7528	0.652	0.6988	0.4344	
	4	0.795	0.8107	0.7192	0.7468	0.6662	0.7042	0.4411	
	Avg	0.79	0.8016	0.7213	0.7505	0.6687	0.7072	0.4457	
Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC	
KNN	0	0.765	0.7728	0.7007	0.7095	0.6874	0.6983	0.4016	
	1	0.768	0.7781	0.7057	0.7091	0.6954	0.7022	0.4114	
	2	0.753	0.7628	0.6903	0.7035	0.6678	0.6852	0.3814	
	3	0.757	0.7779	0.6905	0.7079	0.6645	0.6855	0.3822	
	4	0.765	0.7741	0.7027	0.7121	0.6842	0.6978	0.4057	
	Avg	0.762	0.7731	0.698	0.7084	0.6799	0.6938	0.3965	

Tab. S3. Foldwise performance evaluation on the test data (one-versus-all) with all three classifiers considering k=2

	Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
	SVM	0	0.793	0.7979	0.7207	0.7497	0.6689	0.707	0.4444
		1	0.795	0.8007	0.7268	0.7501	0.6787	0.7126	0.4556
		2	0.782	0.797	0.7118	0.7403	0.6608	0.6983	0.4267
		3	0.786	0.7997	0.7125	0.7456	0.6582	0.6992	0.429
		4	0.796	0.8079	0.7202	0.7438	0.6749	0.7076	0.4424
		Avg	0.79	0.8006	0.7184	0.7459	0.6683	0.7049	0.4396
Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC	
	0	0.791	0.7987	0.7247	0.7488	0.6824	0.7141	0.4515	

KMR=2	RF	1	0.792	0.7968	0.7278	0.7486	0.6844	0.7151	0.4573
		2	0.783	0.7974	0.7177	0.7467	0.6668	0.7045	0.4384
		3	0.785	0.7944	0.7162	0.7518	0.6582	0.7019	0.4368
		4	0.795	0.8089	0.7255	0.7511	0.6775	0.7124	0.4534
		Avg	0.789	0.7992	0.7224	0.7494	0.6739	0.7096	0.4475

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
KNN	0	0.755	0.7669	0.6998	0.7087	0.6864	0.6974	0.4
	1	0.759	0.7671	0.6987	0.7013	0.69	0.6956	0.3974
	2	0.755	0.7684	0.698	0.7135	0.6711	0.6916	0.397
	3	0.745	0.7607	0.6773	0.6906	0.6602	0.6751	0.3553
	4	0.755	0.7668	0.691	0.6986	0.6759	0.687	0.3823
	Avg	0.754	0.766	0.693	0.7025	0.6767	0.6893	0.3864

Tab. S5. Foldwise performance evaluation on the test data (one-versus-all) with all three classifiers considering k=1

KMR=1	SVM	0	0.776	0.7843	0.7102	0.7314	0.6712	0.7	0.4221
		1	0.778	0.7867	0.7117	0.7293	0.6713	0.6991	0.4246
		2	0.766	0.7842	0.7053	0.7332	0.6542	0.6914	0.4137
		3	0.77	0.7844	0.703	0.7332	0.6523	0.6904	0.4094
		4	0.778	0.7941	0.707	0.7289	0.6626	0.6942	0.4159
		Avg	0.774	0.7867	0.7074	0.7312	0.6623	0.695	0.4171

KMR=1	RF	0	0.777	0.7857	0.7107	0.7324	0.6709	0.7003	0.4232
		1	0.778	0.7842	0.7132	0.7305	0.6737	0.701	0.4275
		2	0.769	0.7803	0.7022	0.7296	0.6513	0.6882	0.4073
		3	0.77	0.7809	0.7052	0.7359	0.654	0.6925	0.4139
		4	0.779	0.7896	0.7102	0.7313	0.6679	0.6981	0.4221
		Avg	0.775	0.7841	0.7083	0.7319	0.6636	0.696	0.4188

KMR=1	KNN	0	0.735	0.751	0.6762	0.6827	0.6675	0.675	0.3525
		1	0.746	0.7574	0.6852	0.6835	0.6874	0.6854	0.3703
		2	0.732	0.7453	0.6792	0.6859	0.6721	0.6789	0.3585
		3	0.73	0.7482	0.6763	0.6887	0.6615	0.6748	0.3532
		4	0.741	0.7548	0.683	0.6854	0.6808	0.6831	0.366
		Avg	0.737	0.7513	0.68	0.6852	0.6739	0.6794	0.3601

Result: FOLD-WISE (HoldOut Data)

Tab. S2. Foldwise performance evaluation on holdout test with all three classifiers considering k=3

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
SVM	0	0.7814	0.7959	0.7076	0.7361	0.6472	0.6888	0.4183
	1	0.7811	0.7958	0.7074	0.736	0.6468	0.6885	0.4179
	2	0.7808	0.7956	0.7074	0.7348	0.649	0.6893	0.4177
	3	0.781	0.7956	0.7074	0.7364	0.6459	0.6882	0.4179
	4	0.7814	0.796	0.7076	0.7363	0.6468	0.6887	0.4183
	Avg	0.7811	0.7958	0.7075	0.7359	0.6471	0.6887	0.418
	WD	0.7826	0.7968	0.7087	0.7369	0.6491	0.6902	0.4203

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
RF	0	0.7752	0.7919	0.7067	0.7379	0.6412	0.6861	0.417
	1	0.7756	0.7925	0.7075	0.7369	0.6453	0.6881	0.4181
	2	0.7749	0.7916	0.7059	0.7355	0.6432	0.6863	0.4152
	3	0.7749	0.7917	0.7069	0.7404	0.6374	0.685	0.418
	4	0.7759	0.7926	0.7073	0.7378	0.6431	0.6872	0.418
	Avg	0.7753	0.7921	0.7069	0.7377	0.642	0.6865	0.4173
	WD	0.7744	0.7916	0.7057	0.7355	0.6425	0.6859	0.4148

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
KNN	0	0.748	0.7624	0.6856	0.6964	0.6582	0.6768	0.3719
	1	0.7466	0.7635	0.6832	0.6925	0.6588	0.6752	0.3667
	2	0.7471	0.7643	0.6828	0.6951	0.6513	0.6725	0.3663
	3	0.748	0.7647	0.6881	0.7027	0.6522	0.6765	0.3772
	4	0.7456	0.7614	0.6833	0.6952	0.6527	0.6733	0.3672
	Avg	0.7471	0.7633	0.6846	0.6964	0.6546	0.6749	0.3699
	WD	0.7485	0.7656	0.6846	0.6976	0.6518	0.6739	0.3701

Tab. S4. Foldwise performance evaluation on holdout test with all three classifiers considering k=2

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
SVM	0	0.7742	0.7896	0.7037	0.734	0.6392	0.6833	0.4109
	1	0.774	0.7895	0.7023	0.7297	0.6425	0.6833	0.4074
	2	0.7741	0.7897	0.7035	0.7319	0.6422	0.6841	0.4101
	3	0.7738	0.7893	0.7036	0.7332	0.6401	0.6835	0.4105
	4	0.7742	0.7896	0.7029	0.7322	0.6399	0.683	0.4092
	Avg	0.7741	0.7895	0.7032	0.7322	0.6408	0.6834	0.4096

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
	0	0.7731	0.7911	0.7069	0.7343	0.6484	0.6887	0.4167

RF	1	0.7742	0.7913	0.7077	0.735	0.6496	0.6897	0.4182
	2	0.7732	0.7907	0.7077	0.7348	0.6502	0.6899	0.4183
	3	0.7736	0.791	0.7076	0.7383	0.643	0.6874	0.4186
	4	0.7738	0.7913	0.7067	0.7365	0.6436	0.6869	0.4166
	Avg	0.7736	0.7911	0.7073	0.7358	0.647	0.6885	0.4177

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
KNN	0	0.7361	0.755	0.6738	0.6849	0.6439	0.6637	0.3482
	1	0.7391	0.7569	0.6756	0.6836	0.654	0.6685	0.3516
	2	0.7387	0.7555	0.6753	0.687	0.644	0.6648	0.3513
	3	0.7385	0.7552	0.678	0.6873	0.6531	0.6697	0.3563
	4	0.7384	0.7556	0.6772	0.6861	0.6534	0.6693	0.3548
	Avg	0.7382	0.7556	0.676	0.6858	0.6497	0.6672	0.3524

Tab. S6. Foldwise performance evaluation on holdout test with all three classifiers considering k=1

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
SVM	0	0.7589	0.7795	0.6938	0.7166	0.6411	0.6768	0.3898
	1	0.7589	0.7795	0.6938	0.7165	0.6415	0.6769	0.3898
	2	0.759	0.7796	0.6943	0.7175	0.6407	0.677	0.3907
	3	0.7589	0.7795	0.6944	0.7177	0.6408	0.6771	0.3911
	4	0.7591	0.7797	0.6933	0.7163	0.6401	0.6761	0.3888
	Avg	0.759	0.7796	0.6939	0.7169	0.6408	0.6768	0.39

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
RF	0	0.762	0.7795	0.6944	0.7173	0.6416	0.6773	0.3909
	1	0.7624	0.779	0.695	0.7178	0.6428	0.6782	0.3922
	2	0.7621	0.7794	0.6946	0.7174	0.6419	0.6776	0.3913
	3	0.762	0.7791	0.6935	0.717	0.6396	0.6761	0.3894
	4	0.7625	0.7792	0.6948	0.7187	0.6402	0.6772	0.3919
	Avg	0.7622	0.7792	0.6945	0.7176	0.6412	0.6773	0.3911

Classifier	Fold	AUC	AUPRC	Accuracy	Precision	Recall	F1	MCC
KNN	0	0.7249	0.7432	0.6674	0.672	0.6543	0.663	0.335
	1	0.7255	0.7423	0.6674	0.6726	0.6524	0.6624	0.3351
	2	0.7266	0.7418	0.6693	0.6758	0.6508	0.6631	0.3388
	3	0.7233	0.7414	0.6658	0.6719	0.648	0.6597	0.3318
	4	0.7247	0.7398	0.6685	0.6732	0.6549	0.6639	0.3371
	Avg	0.725	0.7417	0.6677	0.6731	0.6521	0.6624	0.3356