Electronic supplementary Information (ESI)

Partial Least Squares-Discriminant Analysis (PLS-DA) for Classification of high-dimensional (HD) data: a review of contemporary practice strategies and knowledge gaps

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Supplementary Table 1

Summary results of several practical aspects in PLS-DA modeling.[1-68] Dash bar (-) indicates no information is provided by the manuscript.

Year [1](Data)	[2]Dataset			[3]Acronym (local *)	[4]DP		[5]MV			[6]DR			[7]#PLS	[8]FOM
	N	J	G (*) a		SD	SI	I	E	O	Max	COP	BL		
2017 (NIR)[1]	210	~1k	*3	PLS2-DA	MSC	-	AP Random CV	RS (7:3)	-	-	-	-	-	SENS, SPEC, ER, ROC
2017 (NIR)[2]	360	14991-3996 cm⁻¹	*2	PLS-DA	-	-	-	RS (6:4) KS (5:5)	-	-	0.5 (0,1)	-	1-20	ER
2017 (MS)[3]	20	50-1200 Da	2	PLS-DA	2MC 3PS	1NM	-	-	PT (n=1k, robustness)	-	-	-	-	R2, Q2
2017 (2DE)[4]	25	11333	*2	PLS-DA	-	-	CV7	-	PT (n=40)	-	-	-	-	R2X, R2Y, Q2
2017 (MS)[5]	43	50-6000 m/z	*3	PLS-DA	VS	-	CV7	-	-	-	-	-	-	Q2, R2
2017 (NMR)[6]	71	64k	*2	PLS-DA	2AS	1NM	-	-	PT (n=2k, Significance; overfitting)	-	-	-	-	R2, Q2, ROC, AUC
2017 (GC)[7]	200	180	*4	PLS-DA	AS	-	LO	RS (7:3)	-	-	-	-	LOOCV (9 PLS)	ER,Q2,R2
2017 (Raman)[8]	80	3200-500 cm⁻¹	*2	*PLS-DA	2MC	1SG	LO	? (5:5)	-	-	0.0 (-1,1)	-	-	RMSE, SENS, SPEC, R2
2017 (UV-Vis)[9]	73	190-1100 nm	*7	PLS-DA	1MC	21D-SG	LO	? (7:3)	-	-	BT	-	VB-CV	RMSE, SPEC, SEN

															S,ER
2017 (NIR)[10]	161	700-25000 nm	*2	PLS-DA/ PLSDA	-	SNV 1D-SG	LO	? (7:3)	-	-	-	-	-		R2, RMSE
2017 (NIR)[11]	54	700-2500 nm	*2	PLS-DA	-	1D-SG	LO	? (7:3)	-	-	-	-	-		R2, RMSE
2017 (MIR)[12]	190	400-4000 cm^{-1}	*2	PLS-DA	-	-	LO	? (6:4)	-	-	-	G1={-0.5, 0.5} G2={0.5, 1.5} (0,1)	-		R2, RMSE, ROC, AUC
2017 (MIR)[13]	221	3100-1000 cm^{-1}	2	PLS-DA	PSMC	2D-SG SNV	CV	IRS (1/3: 2/3) n=40	-		-	0.5	-	8 PLS	ROC, AUC, SPEC, SENS
2017 (IM & FS)[14]	88	350-600 nm 256 colour level	*2	PLS-DA	PDSDS	SG	CV	KS (7:3)	-		-	0.5	-	-	ER
2017 (IA)[15]	107	48	*2	PLS-DA	-	-	LNO		PT (several)	-		0.5 ROC	-		AUC, ROC
2017 (MS)[16]	45	10	*2	PLS-DA	-	-	LO	? (7:3)	-	-	-	-		3 PLS	ER
2017 (SR)[17]	384	350-2500 nm	2	PLS-DA	MC	-	CV 10	-	-	-	-	-		1-20	R2, RMSE
2017 (MS)[18]	38	1032	*3	PLS-DA	-	-	CV 10	-	-	-	-	-	-	-	AUC, SENS, SPEC, R2Y
2017 (MS)[19]	18	?	*2	PLS-DA	-	-	CV n=100	-	-	-	-	-	-	-	ROC, AUC, SENS, SPEC
2017 (MIR)[20]	135	650-4000	*3	PLS-DA	RS	-	LO	RS (8:2) n=1k	-	-	-	-		LOOCV	ER, R2
2017 (MIR/ Raman)[21]	264	4000-550 cm^{-1} / 200-2000 cm^{-1}	*4/ *10	PLS-DA	-	¹SNV ²SG	LO	-	-	-	-	-	-		ER
2017 (MIR)[22]	120	4000-400 cm^{-1}	5	*PLS-DA	AS		LO	? (7:3)	-		-	0.5 (0,1)	-	LOOCV 4 PLS	RMSE R2, Q2
2017 (MIR/ IRMS)[23]	45	4000-650 cm^{-1}	*2/ *3	*PLS-DA	MCBS	SG	CV	? (5:5)	-		-	YS	-	6 PLS	SENS. SPEC
2017 (MS)[24]	240	230-880 nm	2	PLS-DA	-	NS	LOAP	OT (7:3)	-		-	-	-	LOOCV 6/7 PLS	ER
2017	34	-	3	PLS-...	VS	-	CV7	-	PT (n=20)	-	-	-	-		R2Y

(UV-Vis)[25]				DA										R2X Q2Y
2017 (MS)[26]	30	35-300 m/z	*2	PLS-DA	MC PS **AS**	-	CV 10 (*n*=5)	RS (7:3)	-	-	-	-	2 PLS	ER, R2, SPEC, SENS
2017 (NMR)[27]	121	-	*2 / *3	PLS-DA	MC	-	VB-CV, LO	KS (7:3)	PT (*n*=100)	-	-	-	-	AUROC, ER p-value
2017 (FS)[28]	79	250-700 nm	*3	PLS-DA	-	-	VB-CV	? (2/3: 1/3)	-	-	-	-	2 PLS	RMSE, ROC, SENS, SPEC
2017 (NMR)[29]	16	66K	*3	PLS-DA	-	-	SCV	-	-	-	-	-	2 PLS	R2 ER
2017 (NMR)[30]	54*3	32k	3	PLS-DA	AS	PQN	VB-CV7	-	PT (*n*=50)	-	-	-	-	R2, Q2
2016 (MIR)[31]	300	650-4000 cm⁻¹	*3	*PLS-DA	3MC	12D-SG 2NS	VB-CV	(5:5)	-	-	YS	-	-	SENS SPEC
2016 (GC)[32]	122	16	*2	PLS-DA	2AS	1NM	APRCV (*n*=10K)	? (6:4)	PT (*n*=10K)	-	0.5 KDF	-	-	AUROC Kappa SENS SPEC
2016 (IM)[33]	60	768	*4	PLS-DA	MC	-	CB-CV	RS (7:3)	-	-	YS	-	-	RMSE, SENS, SPEC
2016 (MIR)[34]	328	4000-600 cm⁻¹	*4	PLS-DA	2MC	1SNV	LO	RS (2/3: 1/3)	-	-	BT	-	-	SENS, SPEC, EFF, MCC, RMSE
2016 (MS)[35]	27 251	30-300 amu	*2	PLS-DA	AS	-	LO	-	-	-	-	-	-	R2, RMSE
2016 (UV-Vis)[36]	100	190-800 nm	5	PLS-DA	-	-	LO	KS (2/3: 1/3)	-	-	-	-	9 PLS	ER
2016 (MIR)[37]	170 195	4000-400 cm⁻¹	*5	PLS-DA	-	1SG 2SNV 3AS	MCCV	RS (2/3: 1/3) *n*=5k	-	-	-	-	MCCV	AUROC ER
2016 (NIR)[38]	139	4000-10000 cm⁻¹	*2	PLS-DA	MSC	SNV 2D-SG	LO	KS (7:3)	-	-	-	-	-	ER
2016 (NMR)[39]	18	32k	*3	PLS-DA	2MC	1NS	CV-ANOV	-	-	-	-	-	4 PLS	R2X, R2Y, Q2

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2016 (Raman)[40]	45	3500-50 cm-1	*2	PLS-DA	1MC	2D-SG	CV	RS (2/3:1/3)	-	-	-	-	-	SENS SPEC, ER ROC
2016 (MIR)[41]	46	4000-600 cm-1	3	PLS2-DA	-	SG	LOAP	KS (7:3)	-	-	-	0.45-0.55 (UA)	-	RMSE R2
2016 (Raman)[42]	159	400-4000 cm-1	*2	PLS-DA	2MC	1BC	LO	-	-	-	-	-	LOOCV 3 PLS	ER ROC SENS SPEC
2016 (MIR)[43]	30	4000-500 cm-1	6	PLS-DA	-	1BC 2NS 31D-SG	-	-	-	-	-	0.5	7 PLS	R2Y Q2 ER
2016 (MIR/MS)[44]	146	50-350 amu / 4000-600 cm-1	3	PLS-DA	ASMC	SNV 1D-SG	LO	RS (2/3:1/3 n=10)	-	-	-	-	-	ER SENS SPEC
2016 (NIR-IM)[45]	576	-	*2/*3	PLS-DA	-	1SG 2DT 3BC	VB-CV 10 AP	RS (6:4)	-	-	-	-	-	RMSE
2016 (NIR)[46]	90	649	3	PLS-DA	AS	-	CV3	-	PT	-	-	-	1-10	PRESS
2015 (FS)[47]	95	270-640 nm	25	PLSDA	MC	-	VB-CV AP	-	-	-	-	-	-	SENS SPEC ER
2015 (Raman)[48]	95	1560-90 cm-1	9	*PLS-DA	-	BC NM SG	CV9/20 AP	-	-	-	-	-	-	SENS SPEC ER R2 RMSE
2015 (MS)[49]	23	50-550 m/z	*2/*3	PLS-DA	AS	-	CV7	-	-	-	-	-	-	R2X, R2Y, Q2
2015 (MIR)[50]	88	4000-600 cm-1	4	PLS2-DA	MC	-	LO	RS (2/3:1/3)	-	-	-	BT	-	SENS, SPEC
2015 (EN)[51]	407	-	*4	PLS-DA	-	-	CV10 (n=1K)	-	-	-	-	-	-	AUC SPEC SENS RMSE
2015 (MIR)[52]	125	4000-600 cm-1	5	PLS2-DA	-	-	LO	RS (2/3:1/3)	-	-	-	(0.49-0.51) UA	-	RMSE R2
2015 (LIBS)[53]	1250	-	5	PLS2-	-	-	AP CV	-	-	-	-	UA	4 PLS	SENS

				DA										SPEC ER
2015 (HI)[54]	396	966-1700 nm	*2	PLS-DA	3MC	1SNV 21D-SG	CB-CV	? (7:3)	-	-	-	-	-	SENS SPEC EFF
2015 (Raman)[55]	294	109-1810 cm-1	14	PLS-DA	-	2D NE AS	CV	KS (2/3:1/3)	-	-	BT	-	-	SENS SPEC
2015 (NIR)[56]	186	4000-10000 cm-1	2	PLS-DA	MC MSC	SNV 1D, 2D	CV	? (5:5)	-	-	-	-	-	ER
2015 (MIR)[57]	155	600-4000 cm-1	5	PLS1-DA	2MC	1D-SG	VB-CV	? (2/3:1/3)	--	-	0.5 BT	-	-	ER R2Y R2X
2014 (EN)[58]	127	12	4	PLS-DA	AS	-	CV 10 n=100	RS (6:4)	BTT (n=1k)	-	-	-	-	SPEC SENS ER
2014 (VSC)[59]	540	400-1000 nm	25	*PLS-DA	3MC	1SNV 21D-SG	LO	? (7:3)	-	-	-	-	-	RMSE
2014 (FES)[60]	75	260-860 nm	3	PLS2-DA	MC	-	LO	KS ?	-	-	-	-	-	SENS SPEC ER
2014 (NIR)[61]	180	1350-1800 nm	2	*PLS-DA	-	-	CV	KS RS (n=1k)	-	-	-	0.3-0.7 (UA)	-	ER
2014 (NIR/MIR)[62]	910	1100-2498 nm / 600-4000 cm-1	*2	*PLS-DA	-	1D-SG	CV 10	? (2/3:1/3)	-	-	-	-	-	ER SENS SLEC
2014 (NIR/Raman)[63]	32078	1000-2500 Nm / 100-3500 cm-1	2	*PLS-DA	2MC	1SNV	LO AP	OT (2/3, 1/3)	-	-	-	-	-	ER SENS SPEC
2014 (MS)[64]	113	7	2	PLS-DA	AS MC	NS	CV	RS (2/3:1/3) n=1k	-	-	-	-	-	SENS SPEC
2014 (MS)[65] [	210	40-200 m/z	5	PLS-DA	AS	-	CV	RS (7:3)	-	-	-	-	-	ER
2014 (ICP-MS)[66]	39	10ppb-100 ppm	*2	PLS-DA	-	-	LO	-	-	-	0.00 (1,-1)	-	1-15	ER
2014	58	-	*3	*PL	AS	WL	VB-	DUP	-	-	[-0.7,0.7,0	-	VB-	ER

(NMR, EEM, HPLC)[67]				S-DA		SNM	CV10	LEX (?)			.2]		CV10	
2013 (Raman)[68]	85	3200-200 cm-1	*3	PLS2-DA	[3]MC	[1]NV [2]2D-SG	LO	RS (7:3)	BTT (n=1k)	-	BT	-	-	ER SPEC SENS EFF RMSE

[1]Data: 2DE (two-dimensional electrophoresis); HPI (Hyperspectral imaging); IM (image); FES (Flame Emission Spectroscopy); FS (fluorescence spectroscopy); IA (immunoassay); SR (spectral reflectance); VSC (Video Spectral comparator), NMR (nuclear magnetic resonance); EEM (florescence excitation-emission matrix); HPLC (High performance liquid chromatography)

[2]Dataset: N (sample sizes); J (number of variables); G (number of groups); [a]* indicates imbalanced dataset

[3]Acronym: [Local]* indicates local region is used as input variables

[4]DP (Data pre-processing): SD=set dependent (MC=mean-center; VS=variance scaling, AS=autoscaling; BS=block-scaling; PS=Pareto scaling; MSC=multiplicative scatter correction; DS=direct standardization; PDS=piecewise DS; RS=range scaling), SI=set independent (NM=normalization; SNV=standard normal variates; Der=derivatives; WLS=weighted least squares), bold indicates the chosen DP, superscript numbers indicate sequence of DP

[5]MV (Model Validation methods): I=internal VM (AP=autoprediction; CV-v=v-fold CV, VB-CV = Venetian blinds-CV; CB-CV= Contiguous block-CV; LNO=leave-n-out; LO=leave one out CV, SCV=segment CV that all replicates of one class is leave out, RCV=repeated CV), E=external VM (KS=Kennard-stone sampling; RS=random sampling; IRS=iterative RS; OT=others), O=optional (BTT=bootstrapping; PT=permutation test)

[6]DR: Max=maximum value, COP=cut-off point (BT=Bayesian theorem; YS=ypred plot; KDF=Kernel density estimate function), BL=boundary line (UA= unassigned)

[7]#PLS (method to determine number of optimum PLS): LO=leave-one-out cross-validation, 2CV=repeated CV, MCCV=Monte Carlo CV; VB-CV (Venetian blinds –CV)

[8]FOM (Figures of Merit): ER (error rate/accuracy rate); AUC (Area under curve); EFF (efficiency); F (residue); MCC (Matthews correlation coefficient); Q2 (coefficient of prediction); PREC (precision); PRESS (predictive error of sum of squares); R2 (coefficient of determination); RMSEC/CV/P (root mean squared error of calibration/cross-validation/prediction); ROC (receiver operator characteristic); SEL (selectivity); SENS (sensitivity); SPEC (specificity)

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