

Table 1: **KPLS-SVC**: In all cases the Gaussian kernel was used. The unknown parameters (width of the Gaussian kernel (h), number of PLS score vectors (p), ν and C parameters for ν -SVC and C-SVC, respectively) were selected based on the minimum classification error using five-fold cross validation on the first five training sets.

DATA SET	NUMBER OF SCORE VECTORS	GAUSSIAN KERNEL WIDTH (h)	ν AND C PARAMETER FOR ν -SVC AND C-SVC
BANANA	$p = 9$	$h = 0.7$	$\nu = 0.7$
B.CANCER	$p = 7$	$h = 60$	$C = 10$
DIABETES	$p = 2$	$h = 55$	$\nu = 0.6$
GERMAN	$p = 1$	$h = 20$	$\nu = 0.5$
HEART	$p = 1$	$h = 15$	$\nu = 0.55$
IMAGE	$p = 27$	$h = 8$	$\nu = 0.1$
RINGNORM	$p = 1$	$h = 15$	$\nu = 0.25$
F.SOLAR	$p = 4$	$h = 70$	$\nu = 0.75$
SPLICE	$p = 4$	$h = 55$	$\nu = 0.6$
THYROID	$p = 5$	$h = 9$	$\nu = 0.1$
TITANIC	$p = 7$	$h = 15$	$C = 1000$
TWONORM	$p = 1$	$h = 45$	$\nu = 0.45$
WAVEFORM	$p = 3$	$h = 25$	$\nu = 0.2$

Table 2: **KPLS_{class}-SVC**: In all cases the Gaussian kernel was used. The unknown parameters (width of the Gaussian kernel (h), number of PLS score vectors (p), ν and C parameters for ν -SVC and C-SVC, respectively) were selected based on the minimum classification error using five-fold cross validation on the first five training sets. (*Remark: On the Waveform data set, when using $\nu = 0.1$ parameter selected by cross validation, increased classification error rates were observed in five cases out of 100 test sets. Using $\nu = 0.2$ this was not observed. See results in Table 4.*)

DATA SET	NUMBER OF SCORE VECTORS	GAUSSIAN KERNEL WIDTH (h)	ν AND C PARAMETER FOR ν -SVC AND C-SVC
BANANA	$p = 8$	$h = 0.6$	$\nu = 0.75$
B.CANCER	$p = 7$	$h = 65$	$C = 7.5$
DIABETES	$p = 2$	$h = 65$	$\nu = 0.6$
GERMAN	$p = 2$	$h = 10$	$\nu = 0.45$
HEART	$p = 1$	$h = 15$	$\nu = 0.55$
IMAGE	$p = 26$	$h = 8$	$\nu = 0.05$
RINGNORM	$p = 2$	$h = 15$	$\nu = 0.6$
F.SOLAR	$p = 6$	$h = 95$	$\nu = 0.6$
SPLICE	$p = 4$	$h = 55$	$\nu = 0.05$
THYROID	$p = 5$	$h = 10$	$\nu = 0.1$
TITANIC	$p = 7$	$h = 15$	$C = 1000$
TWONORM	$p = 1$	$h = 45$	$\nu = 0.45$
WAVEFORM	$p = 3$	$h = 15$	$\nu = 0.1(0.2)$

Table 3: **KPLS-Regression**: In all cases the Gaussian kernel was used. The unknown parameters (width of the Gaussian kernel (h), number of PLS score vectors (p)) were selected based on the minimum classification error using five-fold cross validation on the first five training sets.

DATA SET	NUMBER OF SCORE VECTORS	GAUSSIAN KERNEL WIDTH (h)
BANANA	$p = 9$	$h = 0.7$
B.CANCER	$p = 4$	$h = 50$
DIABETES	$p = 2$	$h = 50$
GERMAN	$p = 1$	$h = 40$
HEART	$p = 1$	$h = 20$
IMAGE	$p = 29$	$h = 8$
RINGNORM	$p = 1$	$h = 15$
F.SOLAR	$p = 2$	$h = 50$
SPLICE	$p = 4$	$h = 55$
THYROID	$p = 4$	$h = 6$
TITANIC	$p = 8$	$h = 5$
TWONORM	$p = 1$	$h = 45$
WAVEFORM	$p = 3$	$h = 40$

Table 4: Comparison of the mean and standard deviation test set classification errors between kernel Fisher DA (KFD), C-SVC, kernel PLS-SVC (asterisks indicate data sets where C-SVC was used in contrast to ν -SVC used on the remaining data sets), kernel PLS_{class}-SVC ('classical' scaling of score vectors) and kernel PLS-Regression (KPLS-R).

DATA SET	KFD	C-SVC	KPLS-SVC	KPLS _{class} -SVC	KPLS-R
BANANA	10.8±0.5	11.5±0.5	10.5±0.4	10.4±0.5	10.5±0.4
B.CANCER	25.8±4.6	26.0±4.7	25.1±4.5*	25.3±4.5*	26.2±4.4
DIABETES	23.2±1.6	23.5±1.7	23.0±1.7	23.1±1.7	23.2±1.8
GERMAN	23.7±2.2	23.6±2.1	23.5±2.0	24.4±2.2	23.8±2.2
HEART	16.1±3.4	16.0±3.3	16.5±3.6	16.5±3.6	16.4±3.7
IMAGE	4.76±0.58	2.96±0.60	3.03±0.61	3.08±0.62	2.94±0.57
RINGNORM	1.49±0.12	1.66±0.12	1.43±0.10	1.46±0.11	1.40±0.07
F.SOLAR	33.2±1.7	32.4±1.8	32.4±1.8	32.4±1.7	33.2±1.6
SPLICE	10.5±0.6	10.9±0.7	10.9±0.8	10.9±0.7	10.9±0.8
THYROID	4.20±2.07	4.80±2.19	4.39±2.10	4.31±2.20	4.16±2.20
TITANIC	23.2±2.06	22.4±1.0	22.4±1.1*	22.5±1.1*	22.5±1.2
TWONORM	2.61±0.15	2.96±0.23	2.34±0.11	2.34±0.11	2.33±0.11
WAVEFORM	9.86±0.44	9.88±0.43	9.58±0.36	9.85±1.74 (9.67±0.39)	9.76±0.41