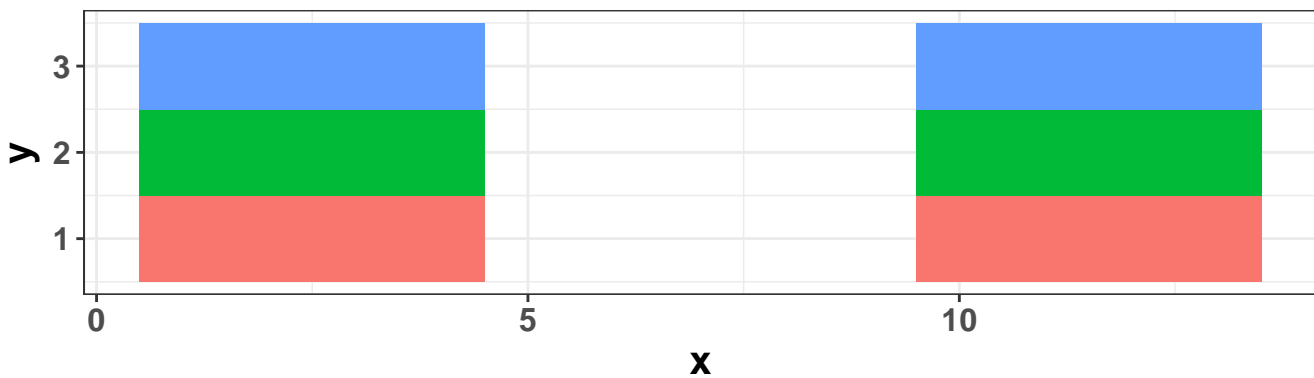


PLS for file:

testfile_squares.rdata

properties	values
Number of mz features	2718
Range of mz values	900 – 999.98
Number of pixels	24
Range of x coordinates	1 – 13
Range of y coordinates	1 – 3
Range of intensities	0 – 168
Median of intensities	3
Intensities > 0	98.75 %
Number of empty spectra	0
Preprocessing	
Normalization	FALSE
Smoothing	FALSE
Baseline reduction	FALSE
Peak picking	FALSE
Centroided	FALSE

Distribution of the response variable y



y_vector



A

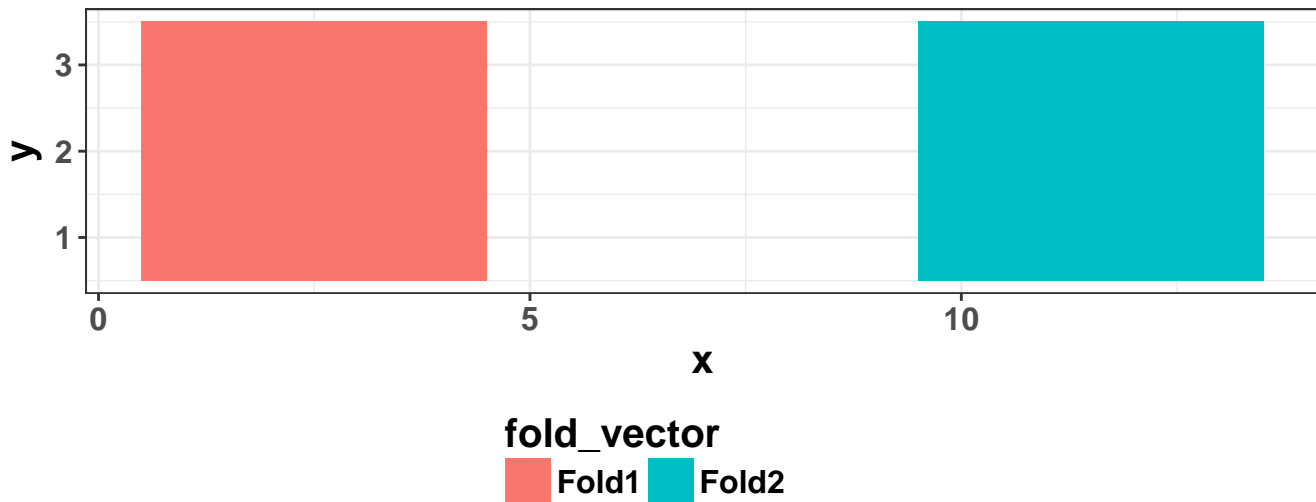


B

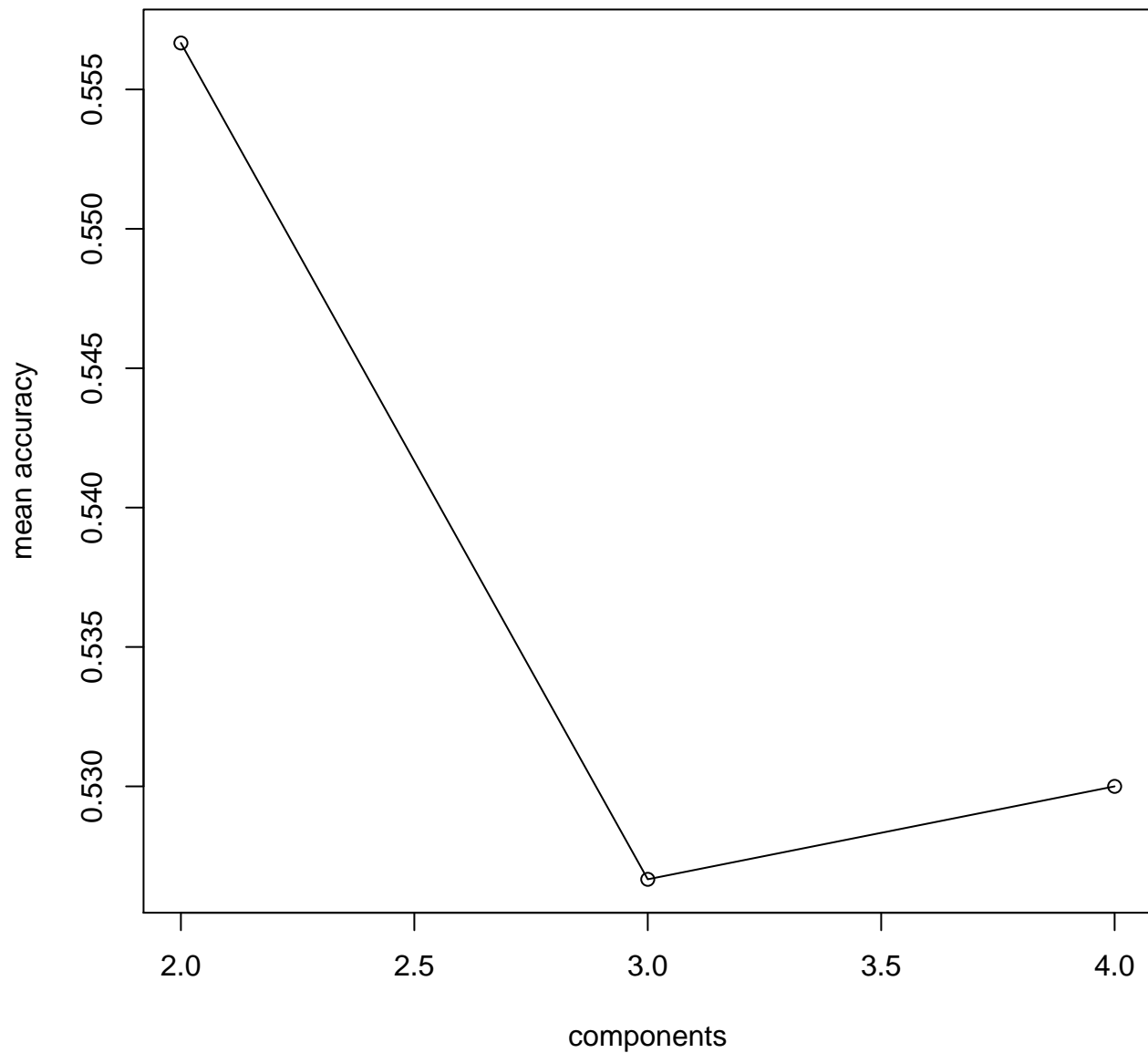


C

Distribution of the fold variable



Mean accuracy of PLS classification



Summary for the different components

ncomp = 2	Accuracy	Sensitivity	Specificity	FDR
A	0.46	0.5	0.44	0.69
B	0.54	0.5	0.56	0.63
C	0.67	0	1	NaN
ncomp = 3	Accuracy	Sensitivity	Specificity	FDR
A	0.33	0.62	0.19	0.72
B	0.58	0.25	0.75	0.75
C	0.67	0	1	NaN
ncomp = 4	Accuracy	Sensitivity	Specificity	FDR
A	0.46	0.5	0.44	0.68
B	0.46	0.38	0.5	0.83
C	0.67	0	1	NaN