

Supporting Information

S5 Table. Classification Performance without subjects over 60.

KPLS-Poly(2) followed by LDA significantly outperformed direct LDA and OLS followed by LDA in accuracy (adjusted for multiplicity using the Bonferroni-Holm method with significance level $\alpha = 0.05$).

	accuracy (%)	sensitivity (%)	specificity (%)
direct LDA	66.1±4.27	66.7±6.19	65.6±5.89
direct SVM	67.8±4.21	74.1±5.75	62.3±6.01
OLS+LDA	61.7±4.38	61.1±6.40	62.3±6.01
PLS+LDA	70.4±4.11	72.2±5.88	68.9±5.74
KPLS-Poly(2)+LDA	78.3±3.72	77.1±5.29	80.0±5.22
KPLS-Poly(3)+LDA	73.9±3.96	68.5±6.10	78.7±5.08
KPLS-Gauss+LDA	70.4±4.11	68.5±6.10	72.1±5.56