Supplemental Digital Content 4. **Machine learning and partial least square regression (PLS).**

PLS regression, derived from artificial intelligence methods, is a robust classification method that generalizes logistic regression to multiclass problems, i.e. with more than two possible discrete outcomes. It is worth noting that PSL models are an interesting alternative to naive Bayes classifiers because they do not assume statistical independence of the random variables. In other words, contrary to multiple linear or logistic regressions, PLS models do not require data absence of multicollinearity and thus can be more accurately performed when there are more variables than observations. Furthermore, it must be highlighted that the non-linear iterative partial least squares algorithm implemented in such modelling, accurately handle missing data, frequently encountered in this setting.

PLS latent variables were calculated from the largest covariance between the independent and dependent variables (TUS data and outcome, respectively). PLS components with an Eigenvalue superior to 1 were included in the model. To avoid over-fitting risk, the data of the validation set, was used to evaluate the predictive abilities of the obtained model. The standardized coefficients and 95% confidence intervals of each parameter were determined using à bootstrap procedure (1000 permutations). Finally, a binary logistic regression was performed on the PLS components to convert PLS values of each observation into a probability score.