ABSTRACT

ENNY KERISTIANA SINAGA. Partial Least Squares Robust Regression Approach to Handle Outliers in Calibration Data. Under direction of ANIK DJURAIDAH and AJI HAMIM WIGENA.

The serious problems in the calibration multivariate estimation are multicollinearity and outliers. Partial Least Squares (PLS) is one of the statistical method used in chemometrics, to handle high or perfect multicollinearity in independent variables. Straightforward Implementation Partial Least Squares (SIMPLS) is the extension of PLS regression proposed by De Jong (1993). The SIMPLS algorithm is based on the empirical cross-variance matrix between the independent variables and the regressors. This method does not resistant toward outlier observations. Robust PLS method is used to handle the multicollinearity and outliers in the data sets. This method can be classified in two groups, there are iteratively reweighting technique and robustication of covariance matrix. Partial Regression-M (PRM) method is one of the robust PLS methods used the idea of iteratively reweighting technique that proposed by Serneels et al. (2005). Robust SIMPLS (RSIMPLS) method is one of the robust PLS methods used the idea of robustication of covariance that proposed by Huber and Branden (2003). A modified RSIMPLS used M estimator with the Huber weight function called RSIMPLS-M was proposed by Ismah (2010). These two methods (RSIMPLS-M and PRM) are applied to Fish data (Naes, 1985) to know their performances. The research results indicated that the values of $R^2$ and RMSEP of RSIMPLS-M are higher than those of PRM method. Whereas based on the confidence interval estimation of the regression coefficients by jackknife method, estimation of PRM is narrower than that RSIMPLS-M method. Therefore RSIMPLS-M method is better than PRM method for prediction, whereas PRM method is better than RSIMPLS-M method for estimation.

Keywords : Partial least squares regression robust (PLSRR), partial robust M-regression (PRM), straightforward implementation partial least squares robust (RSIMPLS)