

Alternative Methods for Constructing of Linear Regressions

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Received: May 30, 2017; Accepted: October 17, 2017

DOI: 10.17721/moca.2017.105-111

Different approaches to solution of linear regression problem have been implemented and tested with Python programming language. The described methods are based on two concepts: the minimization of deviation of calculated value from experimental one of the dependent variable (methods OLS, Ordinary Least Squares, and LAD, Least Absolute Deviation) and the minimization of the errors perpendicular to the regression line (methods ODR, Orthogonal Distance Regression, and LADOD, Least Absolute Deviation of Orthogonal Distances). The significant influence of the chosen function on the regression equation has been demonstrated. The set of examples, including the model problems as well as the experimental datasets, shows the importance of appropriate selection of regression model when the spread in data is significant. In such a situation, the proposed in article new method LADOD “Least absolute deviations of Orthogonal Distances” demonstrated adequate description of the system.

Keywords: QSAR, regression, least square method, least absolute deviation, orthogonal distance regression