

# Ensemble Deep Kernel PLS Regression Method for Full-spectrum Multi-component LIBS Quantitative Analysis of Mars Surface Oxides

Haoyang Yu <sup>a</sup>, Haonan Xie <sup>a</sup>, Qian Huang <sup>a</sup>, Zhaohui Jiang <sup>a</sup>, Dong Pan <sup>a,\*</sup>, Weihua Gui <sup>a</sup>

<sup>a</sup> School of Automation, Central South University, 410083, Changsha, China

\* Corresponding author: pandong@csu.edu.cn

To assess the impact of kernel matrix dimension  $m$  on model performance, preliminary tuning experiments were performed over a defined search range as outlined in Table S1, testing values of 256, 512, 1024, and 2048. The results were recorded as shown in Figure S1, indicating a notable improvement in model performance as  $m$  increases from 256 to 1024 while further gains become marginal while computational cost rises substantially beyond 1024. Therefore,  $m$  was set to 1024 as the optimal setting, achieving a balance between predictive performance and computational efficiency.

TABLE S1. The selection range and determination of hyperparameter for the quantitative model

Hyperparameter	LVs in the first layer	Layers	LVs in subsequent layers
Range of values	[80, 100]	[4, 5]	[30, 40]

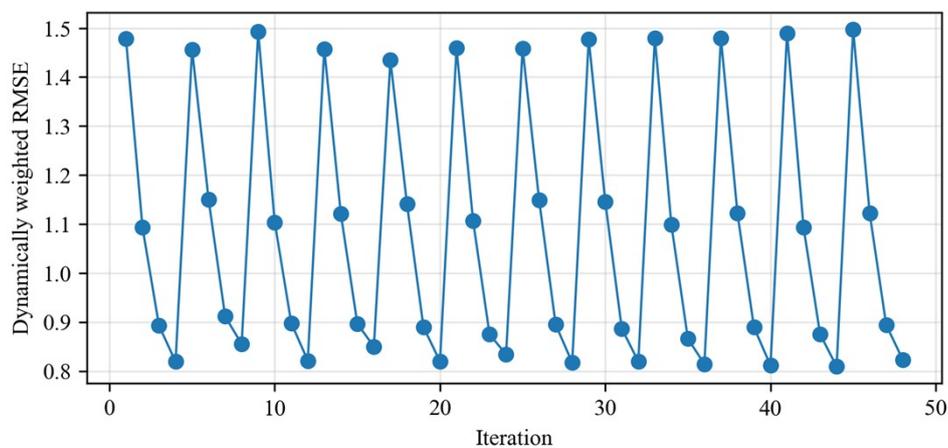


Fig S1. Impact of the kernel matrix dimension on model performance under different hyperparameter configurations