Electronic Supplementary Material (ESI) for Analytical Methods.

Multicomponent hyperspectral grade evaluation of ilmenite using spectral-spatial joint features

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Fig. S1 The selection condition of different ROI areas.

S1. Dendrite Net modeling methodology

DD is a white-box machine learning algorithm for regression, classification and system identification proposed by Liu [1] in 2021. Given that the commonly used algorithms in the past were black-box models with uncontrollable tuning of the parameters inside the model, DD emerged as the times require in order to tune the parameters in a targeted manner and obtain superior results. The DD's main idea is that if the output logical expression contains the logical relationship (and, or, not) of the corresponding class with respect to the input expression, then the algorithm can recognize that class after learning. Since the traditional neural network (defined as a cell body net) does not consider the information processing process of dendrites but directly performs weighted summation, DD uses matrix multiplication and Hadamard product instead of a nonlinear activation function, making it computationally efficient and easy to train. For the regression problem, the DD is compared with the cell body net on nine datasets, and the results show that the DD outperforms the cell body net both with a small number of samples and with a large number of sample data. Considering the novelty of DD and the properties of multiple regression, this study verifies the reliability of the model based on the ilmenite dataset.

The previous cell body structural model expression is $f(Wx+b)$, while DD uses the Hadamard product expression ($WX \circ X$) to cleverly change the expansion into a logical expression between features, automatically realizing the function of higher powers instead of nonlinear mapping. The whole DD model contains a DD module and a linear module, and its DD module formula is as follows:

$$A^l = W^{l,l-1} A^{l-1} \circ X \qquad \text{* MERGEFORMAT (1)}$$

where A^{l-1} and A^l are the inputs and outputs of the modules. X is the original input. $W^{l,l-1}$ are the linearly transformed weights of the (l-1)-th module to the l-th module. $\circ$ denotes Hadamard product. Hadamard product is a binary operation that takes two matrices of the same dimensions and produces another matrix of the same dimension as the operands, where each element i, j is the product of elements i, j of the original two matrices.

The architecture of DD can be represented according to the following formula:

$$Y = W^{L,L-1}\left[\cdots W^{1,1-1}\left(\cdots W^{21}\left(W^{10}X \circ X\right) \circ X \cdots\right) \circ X\right] \qquad \text{* MERGEFORMAT (2)}$$

where X and Y denote the input space and output space, respectively. $W^{l,l-1}$ is the weight matrix from (l-1)-th to the l-th module. The last module is linear. L denotes the number of modules.

However, the DD learning rule differs from the previous cell body structure in that it uses half of the mean square error as the loss function. Similar to the previous structure, a learning rule based on error back propagation is also described, but the DD learning rule is simpler and easier to use. In order to interface with the cell body structure, the gradient descent method is still used for parameter optimization selection. The following set of equations describes the learning rule associated with the gradient descent method.

The forward propagation of DD modules and linear modules:

$$\begin{cases} A^l = W^{l,l-1} A^{l-1} \circ X \\ A^L = W^{L,L-1} A^{L-1} \end{cases} \qquad \text{* MERGEFORMAT (3)}$$

The error backpropagation of DD modules and linear modules:

$$dA^L = \hat{Y} - Y \quad \text{* MERGEFORMAT (4)}$$

$$\begin{cases} dZ^L = dA^L \\ dZ^l = dA^l \circ X \end{cases} \quad \text{* MERGEFORMAT (5)}$$

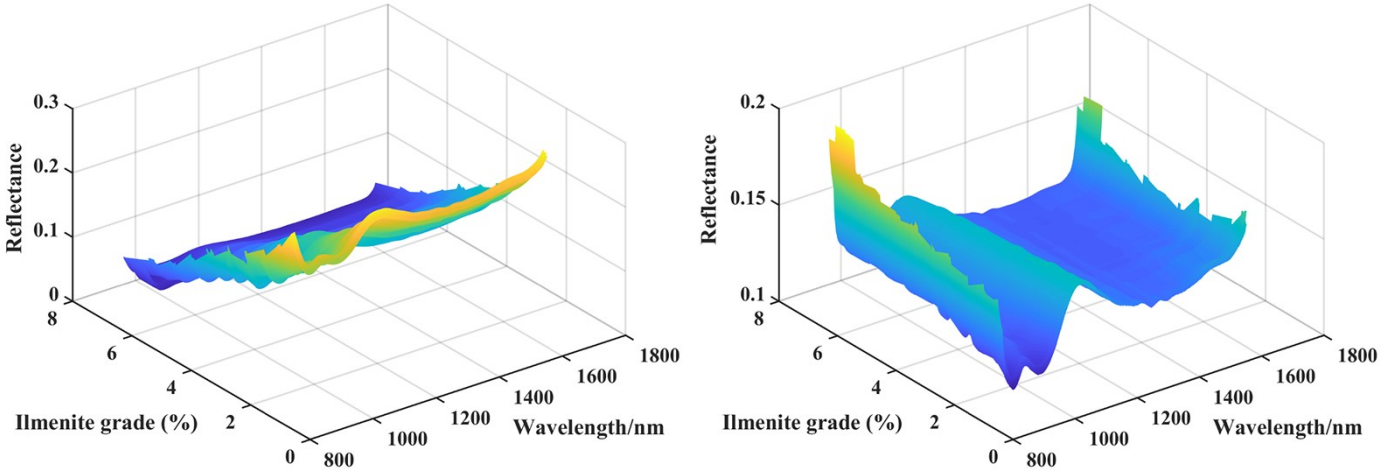
$$dA^{l-1} = (W^{l,l-1})^T dZ^l \quad \text{* MERGEFORMAT (6)}$$

The weight adjustment of DD modules:

$$dW^{l,l-1} = \frac{1}{m} dZ^l (A^{l-1})^T \quad \text{* MERGEFORMAT (7)}$$

$$W^{l,l-1(\text{new})} = W^{l,l-1(\text{old})} - \alpha dW^{l,l-1} \quad \text{* MERGEFORMAT (8)}$$

where $\hat{Y}$ and Y are the outputs and labels of the DD, respectively. m is the number of training samples in a batch. The learning rate α can either vary over time or be fixed to a small value according to the heuristic.



(a) Spectra after SG pretreatment (b) Spectra after MSC pretreatment

Fig. S2 Pretreatment spectra of SG and MSC.

Table S1 Characteristic wavelength selection based on iPLS-VCPA-IRIV and iPLS-VIP-IRIV.

Selection methods	No.	Characteristic wavelength (nm)
iPLS-VCPA-IRIV	28	924.23,927.55,954.15,962.46,964.12,1007.33,1022.29,1027.28,1038.91, 1042.24,1043.9,1110.38,1122.02,1228.39,1268.29,1269.95,1271.61, 1274.93,1356.38,1389.62,1487.68,1491.01,1492.67,1520.93,1524.25, 1602.37,1604.03,1638.94
iPLS-VIP-IRIV	38	897.63,897.63,899.3,919.24,920.9,1015.64,1017.31,1018.97,1082.13, 1083.79,1087.12,1095.43,1097.09,1098.75,1240.03,1243.35,1328.12, 1363.03,1374.66,1399.59,1401.25,1495.99,1499.32,1519.26,1572.45, 1574.11,1577.44,1590.73,1592.4,1594.06,1595.72,1607.36,1609.02, 1614,1615.67,1633.95,1635.61,1643.92

No.: number of variables.

Table S2 Pretreatment analysis of image data.

Pretreatment methods	Calibration set		Prediction set			
	R^2_C	RMSEC	R^2_P	RMSEP	RPD	RPIQ
RAW	**0.9686**	**0.3245**	**0.9723**	**0.3085**	**5.5278**	**4.2656**
SG	0.7835	0.8751	0.8042	0.8519	2.0358	2.1512
MSC	0.9258	0.5019	0.9157	0.5347	3.8512	3.0353
CR	0.8943	0.5676	0.8672	0.7217	2.7645	2.8798
SD	0.9206	0.5234	0.9085	0.5468	3.1568	4.0426
MSC+SG	0.8704	0.6205	0.8516	0.7451	2.3836	3.1002

1. G. Liu and J. Wang, *IEEE Transactions on Cybernetics*, 2022, **52**, 13774-13787.