Feature Selection of Hyperspectral Data Using an Improved Slime Mould Algorithm

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Keywords: Machine Learning, SMA, HYperspectral, Feature Selection.

Abstract: Hyperspectral data contains rich information but also has the problem of data redundancy, so it is necessary to extract features from the data according to the application requirements to obtain useful waveform information. Traditional hyperspectral data feature selection approaches rely on band screening and other methods, which are imprecise and inefficient. Feature selection of hyperspectral data can be viewed as an optimization process, and the Slime mould algorithm (SMA) in machine learning is an effective optimization algorithm that simulates the foraging behavior of mucilaginous bacteria. In this paper, SMA is applied to the feature selection of hyperspectral data, correlation information between the bands and the results is added to the initial sampling process of the SMA, which speeds up the convergence of SMA and reduces the error of feature selection. Based on the feature bands selected by this improved SMA, a hyperspectral soil heavy metal inversion model was constructed, and the model was evaluated using three distinct evaluation methods: root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R2). The experimental results demonstrate that the optimized model has faster convergence and less result error during the feature selection phase, and that the final inversion model is more accurate.

1 INTRODUCTION

Hyperspectral data is the reflectance data of a sample at multiple wavelengths obtained by measuring the sample using a hyperspectral device, which has hundreds of continuous bands. Since there are differences in the reflectivity of matter for different wavelengths of light, the subtle differences between substances can be expressed through these hundreds of bands (Bioucas-Dias et al., 2013). At the same time, as a type of high-dimensional data, hyperspectral data has the issue of redundant data, it is required to extract features for the useful band information within in (Xu et al., 2021).

Feature selection entails selecting the most relevant variables from the data and eliminating other variables that are weakly associated, hence enhancing the accuracy of the model. In general, the feature selection of the data is generally through two ways, The first is the direct selection method, such as Liu et al. direct selection of the feature band by the nature of the substance (Liu et al., 2019), but its band selection scheme is predefined, so its application scope is limited. The other is the application of machine learning algorithms for band selection, such as Lasso regression algorithm (Li et al., 2018), Distance Correlation (Li et al., 2012), Recursive Feature Elimination (Gregorutti et al., 2017), etc. M.,Imani et al. proposed a Fast Feature Selection Methods can achieve the image classification accuracy (M. & H., 2014), but there are still issues with the inversion of the material. Zhang et al. applied the Ant Colony Optimization to the feature selection process for soil inversion of remote sensing pictures without taking convergence speed into account (Zhang et al., 2019).

From an alternative viewpoint, the feature selection problem can be viewed as an optimization problem, i.e., selecting the few variables that have the highest correlation with the results from multiple variables; consequently, the band extraction process of Hyperspectral can be viewed as an optimization process. Li et al. proposed the Slime Mould Algorithm

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Zhou, H., Xiu, L., Hu, Y., Xiao, Y. and Zheng, Z.
Feature Selection of Hyperspectral Data Using an Improved Slime Mould Algorithm.
DOI: 10.5220/0012007000003612
In Proceedings of the 3rd International Symposium on Automation, Information and Computing (ISAIC 2022), pages 644-650
ISBN: 978-989-758-622-4; ISSN: 2975-9463
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(SMA) in 2020 as an new population intelligence optimization algorithm (Li et al., 2020). By varying the weight, they simulated the positive and negative feedback processes in the slime mold foraging process. The approach has been frequently applied to optimization problems because of its convergence precision and stability. For instance, Wei et al. successfully applied it to The Optimal Reactive Power Dispatch (ORPD) proble (Wei et al., 2021).

In response to the above problems, the improved SMA is applied to the feature selection of hyperspectral data, and a hyperspectral soil heavy metal inversion model is developed based on the feature bands extracted by the optimized algorithm in this paper.

The main contributions of this paper are as follows.

- By treating the feature selection problem as an optimization problem, the SMA is applied in feature selection of hyperspectral data to obtain useful bands information.
- further improvement of SMA is achieved by adding the correlation information between the bands and the results to the initial sampling process of SMA by using the Spearman's rank correlation coefficient.
- On the basis of the Support Vector Machine (SVM) regression algorithm, three hyperspectral soil heavy metal inversion models were built and evaluated using three distinct evaluation methodologies.

The rest of the paper is organized as follows. In the second section, the algorithm is optimized and an inverse model is developed. A series of experiments and analyses are given in the third section. Finally, the fourth section summarizes the paper.

2 METHOD

2.1 Slime Mould Algorithm (SMA)

The SMA is a metaheuristic algorithm with great merit-seeking abilities and rapid convergence (Li et al., 2020). The operation of the SMA consists of three main stages. The first is random diffusion to find the food with the strongest odor, then approaching diffusion toward the food with the strongest odor, and finally completing the wrapping of the target. The mathematical operation may imitate the random motion with directionality displayed by slime bacteria during their quest for food, and when this random motion tends to be stable, the slime bacteria position is the optimal value chosen by the slime bacteria algorithm. This motion's iterative pattern can be described by Eq. (1).

$$X(t+1) = \begin{cases} rand.(UB - LB) + LB, rand < z \\ X_b + v_b * (W * X_A(t) - X_B(t)), rand < p \\ v_c * X(t), rand < p \end{cases}$$
(1)

where the parameters of p are as follows :

$$p = tanh|S(i) - DF|$$
(2)

Among Eq. (2), S(i) is the fitness score of the *i*-th particle in this iteration, and DF is the optimal fitness score since the beginning of the iteration. UB and LB are the upper and lower boundaries of the optimization search space, while z is a threshold parameter with a relatively low value. X_b is the position of the slime bacteria with the highest concentration of food odor found at the current moment, i.e., the current optimal solution. v_b is a random value in the interval [-a, a], and the value of a is as follows.

$$a = \arctan((-\frac{t}{max_{t}}) + 1)$$
(3)

As the iteration count grows, v_c declines linearly from 1 to a random value between 0 and 1.

The expression for W in Eq. (1) is shown below:

$$W = \begin{cases} 1 + r \cdot \log\left(\frac{bF - S(i)}{bF - wF} + 1\right), conditons\\ 1 - r \cdot \log\left(\frac{bF - S(i)}{bF - wF} + 1\right), others \end{cases}$$
(4)

Eq. (4) is contingent on S(i)'s size being in the top half of all particles' rankings during the current iteration. The best fitness score for this iteration is bF, while the poorest fitness score is wF.

During the preceding procedure, the particle positions gradually converge to the optimal aim as the number of iterations increases.

2.2 Application of SMA to Feature Selection

The hyperspectral data can be considered as a series of high-dimensional vectors $A = [a_1, a_2 \dots a_i \dots a_n]$, where a_i is the spectral reflectance of the *i*-th band. Feature selection on hyperspectral data consists of selecting *m* elements from *n* elements to construct a new vector set $B = [b_1, b_2, \dots, b_m](m < n)$. In the ensuing modeling phase, vector *B* is modeled in place of vector A, thereby eliminating redundant data.

The application of the traditional SMA is still limited to the selection of optimal values within a certain range, whereas the feature selection problem is to select the most pertinent variables from the data. Therefore, the algorithm must be further optimized to address the feature selection problem.

In terms of the nature of the problem, the selection behavior of the data variables can be understood as a process of binarization, i.e., being selected when the value is 1 and not being picked when the value is 0. Therefore, the optimization issue can be transformed into a problem involving feature selection.

For the band selection model of hyperspectral data, the dimensionality of the particles is first determined to ensure that the number of dimensions I of the particles equals the number of bands n of the data. In addition, the upper limit UB and lower limit LB of search seeking must be set to 1 and 0 correspondingly, and a threshold λ must be set so that each X_i satisfies Eq. (5), thereby expressing the relationship between the selection of particles and the selected ones.

$$X_i = \begin{cases} 0, \lambda < 0.5\\ 1, \lambda \ge 0.5 \end{cases}$$
(5)

By configuring this relationship, the particle values are binarized in order to select the desired band. In addition, the fitness score within the SMA must be specified. In the process of selecting features for hyperspectral data, the level of the fitness score corresponds to the merit of various band selection schemes. Here, the partial least squares regression (PLSR) model, which requires few setup parameters and is efficient, is introduced for quantitative evaluation of feature selection schemes. Specifically, the data corresponding to the specified bands are modeled with the data to be inverted using PLSR, and the root mean square error (RMSE) score of the resulting model is utilized as the fitness value. As a result, the level of the fitness score can express the advantages and disadvantages of different band selection schemes.

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)}$$
(6)

Where y_i and \hat{y}_i represent the true value and predicted value of the *i*-th sample respectively. This band selection strategy is more successful when RMSE has a smaller value.

2.3 Sampling-Optimized Slime Mould Algorithm (SO-SMA)

When band selection is performed for hyperspectral data, the initial sampling process of SMA discussed above is a uniform sampling with a threshold of 0.5. However, for hyperspectral data, the value of each band has a considerable effect on the findings. therefore the threshold needs to be continuously modified for different bands. In this research, the Spearman's rank coefficient of correlation is used to express the effect of each band on the results. In the initial sampling process of the SMA, the acceptancerejection sampling with correlation coefficient as the threshold is used in place of the original uniformly distributed sampling to improve the initial state of the algorithm and increase the directionality in the feature selection process. The algorithm after sampling optimization strategy has the potential to expedite the convergence of the algorithm for feature selection.

The Spearman's rank correlation coefficient which is denoted by the Greek letter ρ in this work is used to estimate the correlation between two variables X and Y, where the correlation between the variables can be described using a monotonic function (Schober et al., 2018). The correlation coefficient between two variables can be either +1 or -1 if one of their respective sets of values can be adequately represented by the other variable as a monotonic function (i.e., the two variables have the same trend of change).

Suppose that the two random variables are X and Y respectively, the number of their elements are both N. The *i*-th value taken by X and Y is denoted by X_i and Y_i respectively. x_i and y_i are the ordered set of elements in X and Y. d_i is a ranking difference set after the corresponding subtraction of the elements in the sets x_i and y_i . Finally, as shown in Eq. (7), a simpler procedure is used to calculate ρ .

$$\rho = 1 - \frac{6\sum d_i^2}{n(n^2 - 1)} \tag{7}$$

$$d_i = x_i - y_i, \quad 1 \le i \le N \tag{8}$$

After computing the Spearman's rank correlation coefficient independently for each band, it is necessary to linearly deflate the absolute values of the acquired correlation coefficients in order to give a more effective sampling optimization. In this paper, the maximum value of correlation coefficient after linear reduction is 0.8 and the minimum value is 0.2. Eventually, they become the selected thresholds for each band in the feature selection process. As shown in the Eq. (9).

$$X_{i} = \begin{cases} Selected, \ \lambda < thre_{i} \\ Unselected, \ \lambda \ge thre_{i} \end{cases}$$
(9)

Eq. (9) permits the selection of the band with the highest absolute correlation coefficient with an 80% chance during the initial phase of the SMA. Similarly, the band with the lowest correlation with the result has a 20% chance of being chosen in the initial procedure, which brings the algorithm's random distribution near to the distribution of the correlation coefficient.



Figure 1: The probability of each band being selected before algorithm optimization.



Figure 2: The probability of each band being selected after algorithm optimization.

In Fig. 1 and Fig. 2, p is the probability of the band being selected. As shown in the picture, the sampling-optimized SMA (SO-SMA) is more relevant for different bands and the correlation between the bands and the outcomes influences the selection of different bands.

2.4 Inversion Method

In this study, the inversion model is built with the SVM regression algorithm, a branch of the normal SVM algorithm. The objective of the SVM regression algorithm is to locate the ideal hyperplane that brings the data closest to the hyperplane and enables regression analysis via data fitting. The advantage of the SVM regression algorithm is that only a small number of support vectors are required to establish the optimal hyperplane, and the kernel method endows the data with a nonlinear regression approach; therefore, it has a distinct advantage when dealing with small samples of high-dimensional hyperspectral data (Yuan et al., 2017). In the subsequent experiments, this paper uses the SVM regression algorithm to model the inversion of hyperspectral soil heavy metals based on the data extracted by the SMA and the SO-SMA in the previous paper.

2.5 Model Evaluation Method

In this study, three evaluation metrics, root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R2), are chosen to evaluate the inversion model constructed using SMA following the initial sampling optimization. RMSE is defined by Eq. (6), MAE and R2 are defined as follow.

$$MAE = \frac{1}{N} \sum_{j}^{N} \left| \hat{y}_{j} - y_{j} \right|$$
(10)

$$R^{2} = 1 - \frac{\sum_{j} (\widehat{y_{j}} - y_{j})^{2}}{\sum_{i} (\overline{y_{j}} - y_{j})^{2}}$$
(11)

Where y_j and \hat{y}_j represent the true value and predicted value of the *j*-th sample respectively, \overline{y}_j is the average of the true value, and *N* is the number of samples. The three evaluation indices are identified by the letters C and P in the bottom right-hand corner of the model training and prediction data sets (from the initials Calibration and Prediction, respectively). That is, we've lettered the assessments of the training data sets R_c^2 , $RMSE_c$ and MAE_c , and the assessments of the prediction data sets R_p^2 , $RMSE_p$ and MAE_p .

3 EXPERIMENTAL EVALUATION

3.1 Study Area and Datasets

As shown in Fig. 3, the area chosen for this study is situated on the northern bank of the Yangtze River in the Chinese city of Nanjing, Jiangsu Province. The presence of nearby heavy industrial facilities may result in the enrichment of heavy metals in the surrounding soil. In this paper, 134 ground soil sampling sites in the study region were selected, and modeling inversions were done based on the relevant data of laboratory-measured heavy metal concentrations and the hyperspectral data of the sample sites' corresponding locations.



Figure 3: Study area and location of sampling points.

Three different types of soil heavy metals were statistically examined. The results are displayed in Table 1.

Table 1: Descriptive statistics of heavy metal concentration.

	Cd (mg/kg)	Cu (mg/kg)	Hg (10 ⁻³ mg/kg)
Max	50.995	148.1	175.65
Min	19.3	80.0	37.3
Mean	33.34	106.38	101.49
Std	6.29	11.58	21.60

3.2 Rate of Convergence

In this paper, we use SMA and SO-SMA for feature selection of hyperspectral data of three different heavy metals. From the results of the feature selection of part (a) and part (b) in Fig. 4, it can be inferred that the SO-SMA is indeed consistent with fast convergence in terms of feature selection of spectral data, and the RMSE error is also reduced. For the convergence results of part (c) in Figure 3, SMA and SO-SMA only took a fewer number of iterations to get a smaller RMSE due to the limited data of the measured samples and the weak content of Hg in the soil, which caused SO-SMA to lack a noticeable advantage.

The intention of the Spearman's rank correlation coefficient utilized in this research for the construction process of acceptance-rejection sampling is to circumvent the inadequacies of Pearson correlation coefficients. This is due to the fact that the Pearson correlation coefficient may not fulfill the normal distribution in the case of a small sample size, and therefore fails to meet the common assumption of its correlation coefficient. The Spearman's rank correlation merely demands that the observations of the two variables be paired rank-rated information or that the rank information be derived from observations of continuous variables. Consequently, regardless of the general distribution pattern of the two variables and the sample size, the Spearman rank correlation coefficient may be utilized to assess the correlation between the two variables. In the optimization process of the SMA, this paper stretches the absolute value of the Spearman's rank correlation coefficient and applies it to the initial sampling process of the SMA, thereby transforming the uniform distribution in the band selection process into a dynamic distribution that varies according to the relationship between the band and the result. Therefore, the SO-SMA achieves superior outcomes in the hyperspectral data feature selection procedure.

3.3 Model Evaluation

Based on the original data, the data after feature selection by SMA, and the data after feature selection by SO-SMA, and using the SVM regression algorithm, hyperspectral soil heavy metal inversion models (SVM, SMA-SVM and SO-SMA-SVM) were built in this paper. In addition, Recursive Feature Elimination (REF), a classic feature selection approach in machine learning, is also frequently utilized in band extraction of hyperspectral data; therefore, this study establishes an RFE-SVM inversion model based on this algorithm. Firstly, all of the samples were separated into training sets and test sets. The training set was used to tweak the model's parameters and establish the model, while the test set was used to assess the model's generalization capacity. Tabulated in Table 2 are the precisions of the 4 models. Finally, the inversion model was evaluated using the RMSE, MAE, and R2 assessment indices.

From the inversion model accuracy table, it is clear that the SVM regression method suffers from overfitting throughout the inversion model development process and is therefore incapable of completing the soil heavy metal inversion accurately and effectively. In addition, the REF-SVM model developed based on REF can only partially mitigate the overfitting issue, and the accuracy is low, so the effect of the inversion process is not adequate. In contrast, the SMA-SVM and SO-SMA-SVM models built by using the SMA for feature selection of hyperspectral data both weakened the overfitting phenomenon. Comparing the SMA-SVM and SO-SMA-SVM models, the SO-SMA-SVM model generated after the initial sampling optimization provides more accurate end findings than the SMA-SVM model.



Figure 4: Comparison of optimal RMSE changes in every iteration.



Figure 5: Inversion scatter diagram of SO-SMA-SVM model.

Metal	Method	R_c^2	RMSE _c	MAE _c	R_p^2	$RMSE_p$	MAE_p
Cd	SVM	0.99	0.09	0.09	0.48	3.60	2.96
	REF-SVM	0.99	0.09	0.08	0.51	3.41	2.84
	SMA-SVM	0.97	0.15	0.12	0.53	3.53	2.77
	SO-SMA-SVM	0.89	2.03	1.69	0.61	3.02	2.06
Cu	SVM	0.84	4.35	2.26	0.43	6.39	8.28
	REF-SVM	0.83	4.28	2.15	0.47	6.37	7.75
	SMA-SVM	0.83	4.21	2.35	0.59	6.33	6.98
	SO-SMA-SVM	0.81	4.85	2.74	0.62	6.21	6.35
Hg	SVM	1.00	0.10	0.10	0.49	11.49	9.31
	REF-SVM	0.99	0.10	0.10	0.49	11.12	9.02
	SMA-SVM	0.95	0.11	0.12	0.51	10.45	8.77
	SO-SMA-SVM	0.94	0.14	0.16	0.63	9.34	7.21

Table 2: Regression results of SVM, SMA-SVM and SO-SMA-SVM.

4 CONCLUSIONS

This work employs the SMA method for feature selection of hyperspectral data in order to overcome the problem of data redundancy encountered during the information extraction process of hyperspectral data. This paper replaces the uniformly distributed sampling in the initial randomization process of the SMA with acceptance-rejection sampling during the feature selection procedure, thereby incorporating the relationship between the waveband and the result into the algorithm during the optimization phase and enhancing the algorithm's convergence speed and precision. In addition, we applied the SO-SMA to the hyperspectral soil heavy metal inversion modeling procedure, and the final experimental results demonstrated that the final results of the optimized sampling feature selection algorithm were superior to those of the most fundamental uniformly distributed sampling feature selection scheme, and diminished the overfitting phenomenon in the conventional SVM model. Therefore, before selecting features for the bands of hyperspectral data, it is essential to consider the correlation coefficient of each band for the outcomes.

ACKNOWLEDGEMENTS

This work was supported by Jiangsu Province Natural Resources Development Special Fund (Marine Science and Technology Innovation) Project (Grant No. JSZRHYKJ202007) and Jiangsu Province Frontier Leading Technology Basic Research Project (Grant No. BK20192003).

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