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Online Outlier Detection for Time-varying Time Series on Improved ARHMM in Geological Mineral Grade Analysis Process

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ABSTRACT

Given the difficulty of accurate online detection for massive data collecting real-timely in a strong noise environment during the complex geological mineral grade analysis process, an order self-learning ARHMM (Autoregressive Hidden Markov Model) algorithm is proposed to carry out online outlier detection in the geological mineral grade analysis process. The algorithm utilizes AR model to fit the time series obtained from "Online x - ray Fluorescent Mineral Analyzer" and makes use of HMM as a basic detection tool, which can avoid the deficiency of presetting the threshold in traditional detection methods. The structure of traditional BDT (Brockwell-Dahlhaus-Trindade) algorithm is improved to be a double iterative structure in which iterative calculation from both time and order is applied respectively to update parameters of ARHMM online. With the purpose of reducing the influence of outlier on parameter update of ARHMM, the strategies of detection-before-update and detection-based-update are adopted, which also improve the robustness of the algorithm. Subsequent simulation by model data and practical application verify the accuracy, robustness, and property of online detection of the algorithm. According to the result, it is obvious that new algorithm proposed in this paper is more suitable for outlier detection of mineral grade analysis data in geology and mineral processing.

Detección en tiempo real de valores atípicos sobre series de tiempo variable en ARHMM mejorado durante el proceso de análisis de grado mineralógico

RESUMEN

Existe gran dificultad para la detección en tiempo real para series de datos masivos con altos niveles de ruido de valores atípicos. Se propone un algoritmo de autoaprendizaje ARHMM (Modelo autoregresivo oculto de Markov) para llevar a cabo la detección de dichos valores atípicos en el proceso de análisis del grado mineral geológico. El algoritmo usa un modelo AR para ajustar la serie de tiempo obtenida del "analizador de fluorescencia de rayos X" y hace uso del HMM como una herramienta básica de detección, la cual puede evitar la deficiencia de predeterminar el umbral en métodos tradicionales de detección. Para actualizar los parámetros del ARHMM en tiempo real, la estructura del algoritmo BDT (Brockwell-Dahlhaus-Trindade) tradicional se mejora para ser una doble estructura iterativa en la que se aplica el cálculo iterativo en tiempo y en orden respectivamente. Con el propósito de reducir la influencia de valores atípicos (o extremos) en la actualización del parámetro de ARHMM, se adoptan las estrategias de detección-antes-que-actualización y la detección-basada-en-actualización, lo que también aumenta la robustez del algoritmo. La subsiguiente simulación por modelos de datos y aplicación práctica comprueba la precisión, fortaleza y capacidad de la detección en línea del algoritmo. De acuerdo con el resultado, es evidente que el nuevo algoritmo propuesto en este artículo es más apropiado para la detección de datos de valores atipicos para el análisis del grado mineral en geología y el procesamiento mineral.

Introduction

Mineral composition analysis is a key factor in determining whether or not to carry out mining. Over the years, many scholars have proposed some new ideas and methods for accurate mineral grade assessment, many of which are based on chemical or physical test equipment to obtain the data for ingredient grade analysis (Kameshwara, Rao, & Narayana, 2014; De'nan, Naaim, & Leong, 2017). Therefore, the accuracy of the data used for ore composition analysis is critical to the ore grade analysis. At present, automated testing equipment is used in ore grade analysis, such as "BOX-A type on-stream x-ray fluorescence analyzer", which uses spectral obtain by irradiating X-rays to the pulp to get the results of ore grade. It is worth noting that BOX-A type on-stream x-ray fluorescence analyzer by default is that the spectral data obtained is correct. But whether it is chemical or physical testing equipment are inevitably produced abnormal data. Those outliers directly affect the analysis results of the mineral products analysiser (Clarke, & Levis, 1998; Rivoirard, Demange, & Freulon, 2013). Therefore, the detection and elimination of these abnormal data is the premise and key to the above ore grade analysis work.

A new algorithm is proposed here to especially do outlier detection for ore inspection data which obtain from chemical or physical testing equipment. The algorithm utilizes AR model to fit the time series and makes use of HMM as a basic detection tool, which can avoid the deficiency of presetting the threshold in traditional detection methods. To update parameters of ARHMM online, the structure of traditional BDT (Brockwell-Dahlhaus-Trindade) algorithm is improved here, and a double iterative structure in which iterative calculation from both time and order is applied respectively. With the purpose of reducing the influence of outlier on parameter update of ARHMM, the strategies of detection-before-update and detection-based-update are adopted, which also improve the robustness of the algorithm. Subsequent simulation by model data and practical application verify the accuracy, robustness, and property of online detection of the algorithm.

In this paper our innovations are shown as follow:

1. Unlike other outlier detect method (such as the traditional AR model detection method), the outliers detect method proposed in this paper does not need to set the detection threshold.

2. Considering the problem that the model order of chemical or physical testing equipment's hard to be determined, the new detected method which is based on residual error has the function of model order self-learning.

3. In a view to avoid the influence of outliers on the test results, this paper proposes a detection-before-update and detection-based-update strategies.

The Predecessors' Achievements on Outlier detection

Many good ideas and methods are put forward for the research of outliers detection problem, such as that Barnett and Lewis proposed an outliers detected method based on statistics in their word named 'Outlier in Statistical Data (Barnett & Lewis, 1994). Outlier detection method based on distance is proposed by Knorr and Raymond (Knorr & Ng, 1999; Edwin & Raymond, 1998), an new detected method based on density is suggested by Ramaswamy et al. (2000). But for ore inspection data, the detection methods based on distance, density or variance is a lack of feasibility since an online real-time detection method be needed for the ore test data. With the research of anomaly data detection technology, many new ideas and techniques are introduced, such as clustering analysis (Almeida & Barbosa, 2007) and neural network method (Bullen, Cornford, & Nnbney, 2003; Prakobphol, & Zhan, 2008). But clustering analysis method is also not suitable for online outlier detection for extensive test data, and neural network method requires a lot of data to model learning. In 1995, Ragaran and Argrawal put forward the concept of "sequence anomaly" (Han & Micheline, 2001) and proposed the detection method based on deviation (Takeuchi, & Yamanishi, 2006). Because this method needs to know the order of the model, it can not be directly used for the outlier detection of mineral grade analysis data.

Structure of Double iteration in BDT

To make the BDT algorithm can be calculated online, the improved BDT algorithm with double repetition structure is proposed in this paper.

Traditional BDT algorithm

The traditional BDT algorithm is improved by Levinson-Durbin algorithm which is proposed by Brockwell et al. (2002). For traditional BDT algorithm, using all the data to the iterative calculation of model order, in a view to obtain the order of the forward and backward AR model.

x_t, $t = 1, 2, \cdots$ is the test data waiting for detection, where x_t is m-dimension vectors. So forward AR model can be express as Equation 1.

$$x_t = \sum_{i=1}^{k} a_k(i) x_{t-i} + \varepsilon_k(t) \tag{1}$$

In which, ε_k, (t) is forward residual under k order model, which obeys Gauss distribution with zero means. $a_k(i)$ is the coefficient of forwarding AR model under k order model. So backward AR model can be written as Equation 2.

$$x_t = \sum_{j=1}^{k} b_k(j) x_{t+j} + \eta_k(t) \tag{2}$$

With Minimizing all data forward and backward residual as the target, so the generalized objective function written as Equation 3 (Trindade, 2003).

$$\min \sum_{t-k+1}^{n} [\hat{\varepsilon}_k(t)' \omega_1 \hat{\varepsilon}_k(t) + \hat{\eta}_k(t-k)' \omega_2 \hat{\eta}_k(t-k)] \tag{3}$$

n is the number of the data. ω_1 and ω_2 are weighted coefficient matrix for forwarding and backward AR model, and in BDT algorithm, the values of ω_1 and ω_2 is 1. $\hat{\varepsilon}_k(t)$ and are Estimated residual values for forward and backward AR model individually.

$$\hat{\varepsilon}_k(t) = x_t - \sum_{i=1}^{k} a_k(i) x_{t-i} \tag{4}$$

$$\hat{\eta}_k(t-k) = x_{t-k} - \sum_{j=1}^{k} b_k(j) x_{t-k+j} \tag{5}$$

In which, $a_k(i), i = 1, 2, \cdots, k$、$b_k(j), j = 1, 2, \cdots, k$ are m-dimension matrix. The traditional BDT algorithm can be written in full as followed:

$$a_k(k) = \left(\frac{1}{n} \sum_{t=1}^{n+k} \hat{\varepsilon}_{k-1}(t) \hat{\eta}_{k-1}(t-k)' \right) \hat{V}_{k-1}^{-1} \tag{6}$$

$$a_k(i) = a_{k-1}(i) - a_k(k) b_{k-1}(k-i), \ i = 1, \cdots, k-1 \tag{7}$$

$$b_k(k) = \hat{V}_{k-1} a_k(k)' \hat{U}_{k-1}^{-1} \tag{8}$$

$$b_k(j) = b_{k-1}(j) - b_k(k) a_{k-1}(k-j), \ j = 1, 2, \cdots, k-1 \tag{9}$$

$$\hat{U}_k = \hat{U}_{k-1} - a_k(k) \hat{V}_{k-1} a_k(k)' \tag{10}$$

$$\hat{V}_k = \hat{V}_{k-1} - b_k(k) \hat{U}_{k-1} b_k(k)' \tag{11}$$

$$\hat{\varepsilon}_k(t) = \hat{\varepsilon}_{k-1}(t) - a_k(k) \hat{\eta}_{k-1}(t-k) \tag{12}$$

$$\hat{\eta}_k(t) = \hat{\eta}_{k-1}(t) - b_k(k) \hat{\varepsilon}_{k-1}(t+k) \tag{13}$$

In Equation 6 to Equation 13, $\hat{U}_k$ and $\hat{V}_k$ are estimated variance for forwarding and backward noise. The initial condition for traditional BDT algorithm are:

$$\hat{\varepsilon}_0(t) = \hat{\eta}_0(t) = \begin{cases} x_t, & t \in \{1, 2, \cdots, n\} \\ 0, & \text{others} \end{cases} \tag{14}$$

$$\hat{U}_\phi = \hat{\Gamma}(0) = \hat{V}_\phi \qquad (15)$$

$$\hat{\Gamma}(0) = \frac{1}{n}\sum_{t=1}^{n} x_t x_t' \text{。} \qquad (16)$$

The subscript ø express that when the initial iteration, the model order set is empty.

• Double iteration BDT algorithm

The objective function of improved BDT algorithm also is Equation 3. The dynamic performance of the algorithm is enhanced by the forgetting factor . The improved BDT algorithm has double loop structure which model order is inner loop and time is the outer loop.

We set $R_k = \frac{1}{n}\sum_{t=1}^{n+k}\hat{\eta}_{k-1}(t)\hat{\eta}_{k-1}(t-k)'$ which is part of Equation 6. So:

$$R_i = \frac{1}{n}\sum_{t=1}^{n+i}\hat{\varepsilon}_{i-1}(t)\hat{\eta}_{i-1}(t-i)', i=1,2,\cdots k,\cdots K \qquad (17)$$

In Equation 7, k a set maximum value for model order. Considering the time-varying characteristics of the model parameters, the forgetting factor is added to the outer loop(time loop) updates.

$$R_i^t = r \times R_i^{t-1} + (1-r) \times \hat{\eta}_{i-1}(t)\hat{\eta}_{i-1}(t-i), \quad i=1,2,\cdots k,\cdots,K \qquad (18)$$

$$\hat{\Gamma}(0)^t = r \times \hat{\Gamma}(0)^{t-1} + (1-r) \times x_t x_t' \qquad (19)$$

In Equation 18, R_i^t is the mean of the covariance matrix for $\hat{\varepsilon}_{i-l}(t)$ and $\hat{\eta}_{i-l}$ $(t-i)$ in time . Similarly, Equation 13 can be rewritten as:

$$\hat{\eta}_k(t-k) = \hat{\eta}_{k-1}(t-k) - b_k(k)\hat{\varepsilon}_{k-1}(t) \qquad (20)$$

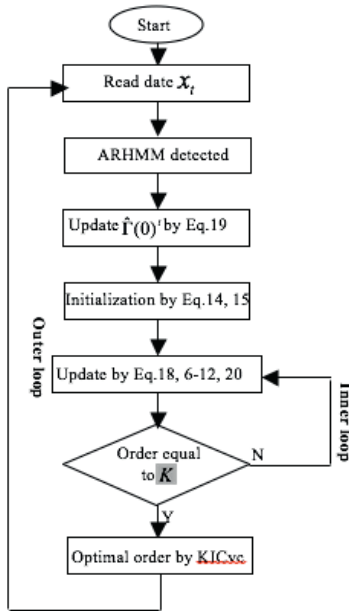So the calculation process of double iteration algorithm is illustrated in Figure 1.

Figure 1. Flow chart of double iteration algorithm

Implementation of Order Self-learning ARHMM Detection Algorithm

The traditional ARHMM structure is composed of two parts (Wang, & Chiang, 2008): one is Markov chain, which is expressed as initial state probability π and state transition matrix $A=(a_{ij})_{N\times N}, a_{ij}=P(S_t=s_j|S_{t-1}=s_i), 1\le i,j\le N$ in which S_t is the state at time t, N is the total state for HMM, and $P(\cdot)$ is a conditional probability. The other is expressed as observation probability matrix $B=(b_{ij})_{N\times N}$ calculated by AR model.

$$b_{tj} = p(\hat{x}_t|S_t=s_j) = N(\hat{x}_t|\sum_{i=1}^{k}a_k(i)x_{t-i},\hat{\Sigma}_k) \qquad (21)$$

In Equation 21, $N(\bullet)$ is Gauss function, and $\hat{\Sigma}_k$ is estimated the variance of Gauss distribution.

ARHMM outlier detection algorithm also composed of two steps:

One step-- Preliminary detection

From Equation 1, we can see that there is a deviation between estimated process data by AR model and real process data.

$$x_t = \hat{x}_t + \varepsilon_k(t) \qquad (22)$$

If the deviation $\varepsilon_k(t)$ is only noise, it obeys Gauss distribution. So the preliminary criteria for outlier detection are to determine the probability that the deviation follows Gauss distribution.

$$P\{x_t|s_t=1\} = \exp\{-\frac{1}{2}\hat{\varepsilon}_p(t)'\hat{U}^{t-1}_p\hat{\varepsilon}_p(t)\} \qquad (23)$$

In Equation 23, $s_t=1$ indicates that the real data detected is normal, $s_t=0$ means it is the outlier. So the detection criteria can be expressed that:

$$if \quad P\{x_t|s_t=1\} \ge 0.5, \quad then \quad s_t=1;$$
$$if \quad P\{x_t|s_t=1\} < 0.5, \quad then \quad s_t=0; \qquad (24)$$

In Equation 23, the subscript p is the optimal model order calculated by KICvc criteria whose expression is:

$$KIVvc(i) = n\ln\left(ave\,\hat{\Sigma}_i^t\right) + \frac{nm(2im+m+1)}{n-im-m-1}$$
$$+ \frac{nm}{n-im-(m-1)/2} + \frac{2m^2i+m^2-m}{2n}, \quad i=1,2,\cdots K \qquad (25)$$

In Equation 25, $ave\hat{\Sigma}_i^t, i=1,2,\cdots K$ is the mean of residual $\varepsilon_k(t)$ under various model order (Bilmes, 2006).

$$ave\hat{\Sigma}_i^t = \frac{sum\hat{\Sigma}_i^t}{t-1} \qquad (26)$$

$$sum\hat{\Sigma}_i^t = sum\hat{\Sigma}_i^{t-1} + \hat{\varepsilon}_i(t-1)\hat{\varepsilon}_i(t-1)' \qquad (27)$$

Two step-- Final detection

In final detection, the result of Preliminary detection is the observed value of HMM. So the final detection result obtained by Viterbi algorithm (Abd-Krim, 2006):

$$\varphi_0(k) = \ln\pi_k \cdot b_{0k}$$
$$\varphi_t(k) = \max_{i=1,\cdots N}\{\varphi_{t-1}(i) + \ln a_{ik}\} + \ln b_{tk}, k=1,\cdots N \qquad (28)$$

For improved ARHMM algorithm, when the data at t time is detected, the data before t time already is detected. So the traditional Viterbi algorithm is request into:

$$\varphi_t(1) = a_{i1} \cdot P_t(1); \qquad \varphi_t(0) = a_{i0} \cdot P_t(0)$$
$$P_t(1) = P\{x_t|s_t=1\} \text{ calculated by Eq. (23)}$$
$$P_t(0) = 1 - P_t(1) \qquad (29)$$

$$if \ \varphi_t(1) > \varphi_t(0) \ x_t \ is \ normal$$
$$if \ \varphi_t(1) \le \varphi_t(0) \ x_t \ is \ outlier \qquad (30)$$

Parameters Updating by Outlier

The parameters of order self-learning ARHMM algorithm need update online, and the parameters are estimated residual mean $ave\hat{\Sigma}_i^t$, State transition matrix A, $\hat{\varepsilon}_\phi(t), \hat{\eta}_\phi(t), \hat{\Gamma}^t(0)$ and in improved BDT algorithm. Specific update algorithm is as follows:

(A) $ave\hat{\sum}_i^t$: If x_{t-1}: If is normal data, then $ave\hat{\sum}_i^t$ maintained by Equations 30, 31, otherwise, $ave\hat{\sum}_i^t$ not updated at time t.

(B) $A = (a_{ij})_{2\times 2}$: since there are two states in ARHMM algorithm. So the updated algorithm is:

$$a_{01} = \frac{N(a_{01})}{N(a_{01}+a_{00})} \quad , \quad a_{11} = \frac{N(a_{11})}{N(a_{11}+a_{10})}$$

$$a_{00} = 1 - a_{01} \quad , \quad a_{10} = 1 - a_{11} \tag{31}$$

In Equation 31, $N(a_{ij})$ indicates the times of the situation that $S_{t-1}=i$, $S_t=j$, appears (Lou, 195).

(C) $\hat{\varepsilon}_\phi(t),\hat{\eta}_\phi(t)$: If x_t,: is normal data, then $\hat{\varepsilon}_\phi(t),\hat{\eta}_\phi(t)$, calculated by Equation(14), otherwise, Using data means to replace x_t.

(D) $\hat{\Gamma}^t(0)$: If x_t is normal data, then $\hat{\Gamma}^t(0)$ calculated by Equation 19; otherwise, it calculated by Equation (32).

$$\hat{\Gamma}(0)^t = \eta \times r \times \hat{\Gamma}(0)^{t-1} + (1 - \eta \times r) \times x_t x_t' \tag{32}$$

(E) R_i: If x_t is normal data, then $\hat{\Gamma}^t(0)$ calculated by Equation (18); otherwise, it calculated by Equation 33.

$$R_i^t = \eta \times r \times R_i^{t-1}$$
$$+ (1 - \eta \times r) \times \hat{\xi}_{-1}(t)\hat{\eta}_{-1}(t-i) \tag{33}$$
$$i = 1,2,\cdots k,\cdots K$$

Results and Discussion

Model-Based Validations

To verify the accuracy of the algorithm to detect the order of the model, the three order model which reacting ore detection interference process are used to generate the data. The data is shown in Figure 2-(a), and the order detection results are shown in Figure 2-(b).
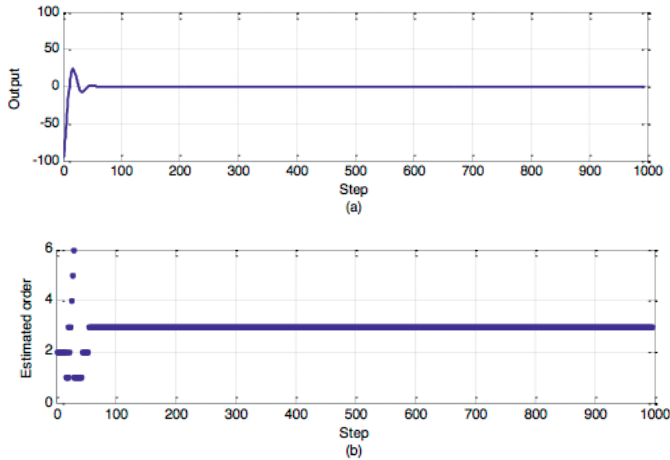

Figure 2. Data and results of order detection

As can be seen from the order detection results, the proposed algorithm can accurately detect the model order through the short-term adjustment process.

With a view to verify that the proposed algorithm not only can identify the optimal model order but also can detect the abnormal data accurately. We modified the open-loop model mentioned in the Alex Alexandridis paper to get the second set of data (Alexandridis, Sarimveis, & Bafas, 2003). Rabiner 1989). The modified model is as follows:

$$y(k) = \{y(k-1)y(k-2)y(k-3)u(k-2)$$
$$\times (y(k-3)-1)+u(k-1)\}/\{1$$
$$+0.2\sin(2\pi k/25)+y(k-2)^2+y(k-3)^2\} \tag{34}$$

In which:

$$u(k) = \begin{cases} \sin(\dfrac{2\pi k}{250}), & k \le 500 \\ 0.8\sin(\dfrac{2\pi k}{250})+0.2\sin(\dfrac{2\pi k}{25}), & k > 500 \end{cases} \tag{35}$$

As can be seen from (34), there are time vary parameters on the denominator. To verify the robustness of the algorithm, we add 10% of the white noise and eight anomalies. The data is shown in Figure 3-(a), and the order detection results and outliers detected results are shown in Figure 3-(b) and Figure 3-(c).
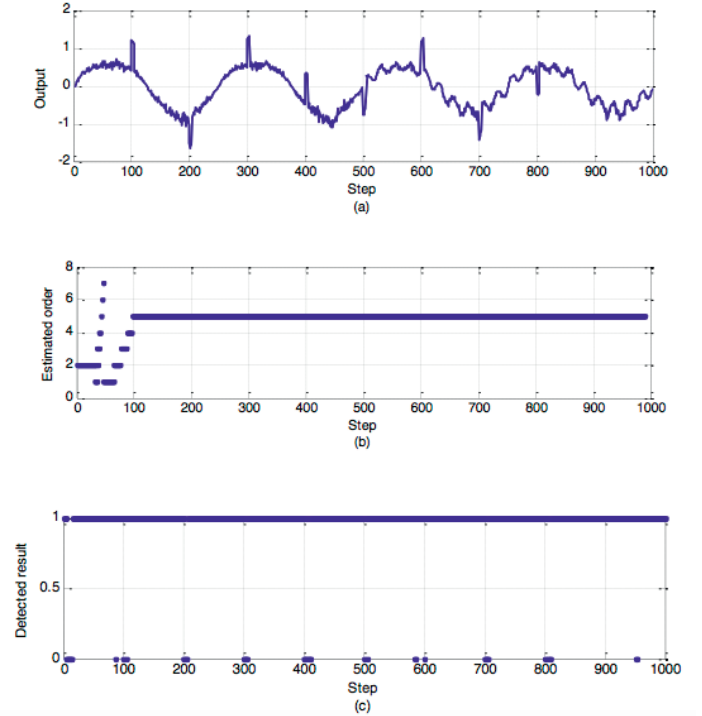

Figure 3. Data and detection results for model data

Fig.3-(a) is the data waiting for detecting. Fig.3-(b) is the order estimated result, and Fig.3-(c) is the outlier detection result. As can be seen from the result, for the third-order nonlinear time-varying system, the model-order self-learning algorithm proposed in this paper can find its optimal model order and accurately detect all the anomaly data.

Application

To further verify the practicality of the improved ARHMM outlier identified method, it is applied to the on-stream x-ray fluorescence analyzer, which, first of all, in the last century 70's by the Finotec Outotec company successfully developed and implemented to mineral processing practice. So far, Finland Outotec company still has more than 80% market share. In China, the Beijing Institute of Mining and Metallurgy following its analytical principles, developed in 2014 with the same function grade analyzer - BOXA type on-stream x-ray fluorescence analyzer (Hekimoglu, Eernoglu, & Kalina, 2009). According to foreign reports, the measurement accuracy of the analyzer increased by 1%, will effectively improve the metal recovery rate of 0.2 or more, and now from the hardware to improve measurement accuracy has been very difficult, or input-output serious disproportionate, so more scholars turn to the analysis of the modeling technology to improve research. Based on this situation, the accuracy of the data for the model of learning is essential

Our comparative tests are as follows:

The first set of data is obtained as follows: first of all, we use the improved ARHMM outlier detection algorithm proposed in this paper to pre-process the spectral signal which as the input of the analyzer, and get the ore grade results as the first set of data.

The second set of data is obtained as follows: we use the traditional AR outlier detection algorithm proposed in paper by Northey, Mohr, & Mudd (2014) to pre-process the spectral signal which as the input of the analyzer, and get the ore grade results as the second set of data.

Finally, the two sets of data are compared with the results of the ore grade laboratory test, the error of the two groups of test results as shown in table 1.

Table 1. The result of Comparison between with outlier detection process and without outlier detection process

		Relative error(%)by traditional AR method	Relative error(%)By Improved ARHMM method
Lead concise ore	Pb	3.25	2.31
	Zn	4.43	3.32
Lead Tailings	Pb	5.21	4.52
	Zn	4.17	3.07
Zinc concise ore	Pb	5.89	4.21
	Zn	1.75	1.02
Ore	Pb	3.21	2.52
	Zn	3.75	2.57
Total tailings	Pb	5.27	4.72
	Zn	4.87	3.25

It can be seen from the table that there is higher accuracy when using the improved ARHMM outlier detection algorithm proposed in this paper to do the pre-processing of the spectrum compared to tradition AR outlier detected method, which since the improved ARHMM outlier detected algorithm have more robustness and more suitable for non-linear systems.

Conclusions

Taking into account the lack of ARHMM algorithm for ore grade analysis process, an order self-learning ARHMM algorithm is proposed in this paper, whose innovation points are summarized as: first, unlike other outlier detection method (such as the traditional AR model detection method), the outliers detection method proposed in this paper does not need to set the detection threshold. Second, considering the problem that the model order of control system's hard to be determined, the new detected method which is based on residual error has the function of model order self-learning. And third, to avoid the influence of outliers on the test results, this paper proposes a detection-before-update and detection-based-update strategies. So under above improving, ARHMM algorithm can more accurately use to analysis the data in the geological mineral grade analysis process. In other words, the application field of ARHMM algorithm has been expanded. Subsequent simulation by model data and practical application verify the accuracy, robustness, and property of online detection of the algorithm. According to the result, it is evident that new algorithm proposed in this paper is more suitable for outlier detection in the geological mineral grade analysis process.

Acknowledgments

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