A genetic-algorithm-based neural network approach for EDXRF analysis (Postprint)

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Abstract

In energy dispersive X-ray fluorescence (EDXRF), quantitative elemental content analysis becomes difficult due to the existence of the noise, the spectrum peak superposition, element matrix effect, etc. In this paper, a hybrid approach of genetic algorithm (GA) and back propagation (BP) neural network is proposed without considering the complex relationship between the elemental content and peak intensity. The aim of GA-optimized BP is to get better network initial weights and thresholds. The starting point of this approach is that the reciprocal of the mean square error of the initialization BP neural network is set as the fitness value of the individuals in GA; and the initial weights and thresholds are replaced by individuals, then the optimal individual is searched by selecting, crossover and mutation operations, finally a new BP neural network model is established with the optimal initial weights and thresholds. The quantitative analysis results of titanium and iron contents in five types of mineral samples show that the relative errors of 76.7% samples are below 2%, compared to chemical analysis data, which demonstrates the effectiveness of the proposed method.

Full Text

Preamble

A Genetic-Algorithm-Based Neural Network Approach for EDXRF Analysis

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Abstract: In energy-dispersive X-ray fluorescence (EDXRF) spectroscopy, quantitative elemental analysis becomes challenging due to spectral noise, peak overlap, and matrix effects. This paper proposes a hybrid genetic algorithm (GA) and back-propagation (BP) neural network approach that circumvents the need to model the complex relationship between elemental content and peak intensity. The GA-optimized BP network aims to obtain superior initial weights and thresholds. The methodology sets the reciprocal of the mean-square error of the initialized BP network as the fitness function for GA individuals. The initial weights and thresholds are encoded as individuals, and selection, crossover, and mutation operations are performed to search for the optimal individual. A new BP neural network model is then established using these optimal initial weights and thresholds. Quantitative analysis of titanium and iron in five mineral sample types demonstrates that 76.7% of samples achieve relative errors below 2% compared to chemical analysis data, validating the effectiveness of the proposed method.

Keywords: EDXRF, Quantitative analysis, BP neural network, Genetic algorithm
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Introduction

Vanadium-bearing titanomagnetite represents an important source of iron and titanium oxides with significant comprehensive utilization value. Its complex elemental composition necessitates accurate elemental analysis for mineral species identification in industrial applications. While traditional chemical analysis offers high accuracy, it is time-consuming and costly. Energy-dispersive X-ray fluorescence (EDXRF) provides a non-destructive alternative that is widely employed in the mining industry.

EDXRF-based instruments have been commercialized for diverse applications including cement and mineral production, ore exploration, environmental monitoring, mine mapping, and process control. However, matrix effects—particularly absorption-enhancement interactions among elements—represent a critical factor limiting analytical accuracy for complex samples. These effects substantially interfere with fluorescence count rates, causing significant errors between measured intensities and actual elemental concentrations. Consequently, developing effective methods to correct matrix effects and improve analytical accuracy remains an important research focus in X-ray spectroscopy.

Traditional correction methods, whether experimental or mathematical, largely depend on the availability of accurate standard samples. Fundamental parameter (FP) methods face challenges in obtaining precise basic physical parameters. Recent work using radial basis function (RBF) neural networks to adjust for matrix effects has shown promising results. This paper proposes a hybrid GA-BP

approach that avoids explicit modeling of the complex concentration-intensity relationship. The GA optimization seeks superior network initial weights and thresholds by using the reciprocal of the mean-square error of the initialized BP network as the fitness value. Initial weights and thresholds are encoded as individuals, and genetic operations identify the optimal individual for establishing an improved BP network model.

The paper is organized as follows: Section II describes model formulation, Section III presents computational results and model validation, and Section IV provides concluding remarks.

Methodology

The GA-BP model employs a three-layer architecture with m input nodes, h hidden nodes, and n output nodes. The implementation determines a basic state space for the connection weight matrix, with hidden node counts and weight matrices encoded into mixed strings containing integer and real values. Experimental data are partitioned into training and testing subsets.

The algorithm proceeds through eight steps:

Step 1: A three-layer BP neural network estimates the basic state space of connection weights initialized within [-1, 1] using training samples.

Step 2: Connection weights and hidden node numbers are encoded. Hidden nodes use binary coding: 1 indicates connection to input/output nodes, while 0 indicates no connection. Weights are encoded as floating-point strings with length $H = m \times h + h + h \times n + n$, where m, n, and h represent input, output, and hidden nodes, respectively. Each string corresponds to a chromosome comprising multiple gene sections: A (hidden neuron count, binary), B (input-hidden weights), C (hidden neuron thresholds), D (hidden-output weights), and E (output neuron thresholds). Sections B through E use real-valued encoding that evolves during training.

Step 3: Initialize a population of chromosomes with length $L = G + H$, where G is the binary code length for hidden node numbers and H is the real-valued code length for connection weights.

Step 4: Calculate individual fitness using Equation (1):

$$f(x) = \frac{1}{\text{sse}(T' - T)} = \frac{1}{\sum_{i=1}^{n}(t'_i - t_i)^2}$$

where $T' = \{t'_1, t'_2, \cdots, t'_n\}$ is the desired output and $T = \{t_1, t_2, \cdots, t_n\}$ is the actual data.

Step 5: Compute the total fitness of the population and each individual' s relative fitness using Equation (2) as the inheritance probability. The highest-

fitness individual is copied directly to the offspring, with remaining individuals selected via roulette-wheel selection.

$$P_i = \frac{f(X_i)}{\sum f(X_i)}$$

Step 6: Apply crossover and mutation operations. For control codes, mutation adds or deletes hidden nodes by toggling between 0 and 1. Weight operations follow these rules:

(a) Crossover with probability p_c:

$$X_i^{t+1} = c_i X_i^t + (1 - c_i) X_{i+1}^t X_{i+1}^{t+1} = (1 - c_i) X_i^t + c_i X_{i+1}^t$$

where X_i^t and X_{i+1}^t are parent individuals, X_i^{t+1} and X_{i+1}^{t+1} are offspring, and c_i is a random value in [0,1].

(b) Mutation with probability p_m:

$$X_i^{t+1} = X_i^t + c_i$$

where X_i^t is the pre-mutation individual, X_i^{t+1} is the post-mutation individual, and c_i is a random value in [0,1].

Step 7: Generate the new population and replace the current one. Repeat Steps 4-7 until convergence criteria are met.

Step 8: Decode the highest-fitness individual to obtain optimal thresholds and connection weights, retrain the network with these parameters, and output predictions.

Model Implementation and Results

Mineral samples were collected from two mining plants in Panzhihua, Sichuan Province, China, comprising 40 sample groups from each location. The five mineral types included iron concentrate, iron gangue, titanium concentrate, titanium gangue, and raw ore. Each 4 kg sample group was crushed and ground in an agate mortar for 30 minutes to ensure homogeneity and reduce particle size effects. Powders were sieved to 180 mesh and dried at 105-110°C for one hour to minimize moisture effects before tablet preparation for EDXRF measurement.

Analysis employed a standard EDXRF setup with a vacuum chamber (to reduce argon interference), X-ray tube, sample holder, and detector. The X-ray tube operated at 12.25 keV and 25.56 μA. Fluorescent X-rays were detected by an electrically cooled Si(PIN) semiconductor detector with 180-190 eV energy resolution at 5.9 keV. Each sample group was measured three times for three minutes per measurement, with final spectra derived from mean count rates.

The five mineral types contained ten metallic elements (Ca, V, Cr, Ni, Cu, Zn, As, Pb, Ti, Fe), with Ti and Fe as major components. Count

rates in the 4.038-8.364 keV spectral region (channels 280-580 after energy calibration) served as primary indicators of elemental content. This region includes Kα peaks for Ti (4.510 keV), Fe (6.403 keV), V (4.951 keV), Ni (7.477 keV), and Cu (8.046 keV). The competitive layer structure employed a $9\$\times 2 architecture(9 hiddennodes, 2 outputneurons), withhiddennodecountdeterminedbytheempiricalformula$ (where n is input neuron count). Channel count rates formed the input vector, while Ti and Fe concentrations served as outputs. The input-to-hidden activation function was logsig, hidden-to-output was purelin, and the training function was traincgb. Model parameters are summarized in Table 1 .

Thirty training and prediction cycles were performed for each mineral type, with average relative prediction error, standard deviation, and coefficient of variation (CV) calculated as accuracy and precision metrics. Table 2 shows that for 76.7% of samples, GA-BP predictions of Ti and Fe content matched chemical analysis results with relative errors below 2%. Table 3 and Figure 1 [Figure 1: see original paper] illustrate the genetic algorithm' s convergence process, demonstrating rapid convergence and efficient fitness evolution.

Conclusion

Accurate EDXRF analysis requires advanced data processing techniques to address absorption-enhancement effects among elements. Building on previous research, this study proposes a hybrid GA-BP approach for processing EDXRF spectra of complex samples such as vanadium-bearing titanomagnetite. The GA-BP model exhibits capabilities for memorizing new patterns, associating existing patterns, learning unknown patterns, and achieving effective prediction for complex samples, thereby reducing matrix effects and improving measurement accuracy.

Future work will expand the sample collection from the Panzhihua region to further validate model effectiveness and assess generalization capability across all available sample types in the field.

References

[1] Li Z, Tuo X G, Yang J B, et al. Nucl Sci Tech, 2012, 23: 289-
[2] Frangi J P and Richard D. Sci Total Environ, 1997, 205: 71-79.
[3] Sumpun W, Phadoong B, Thippawan S. Hydrometallurgy, 1997, 45: 161-167.
[4] Orhan M K, Zafer U, lknur O, et al. J Quant Spectrosc Ra,
[5] GonzalezFern O, Queralt I, Carvalho M L, et al. Nucl Instrum Meth B, 2007, 262: 81-86.
[6] Natarajan V, Porwal N K, Babu Y, et al. Appl Radiat Isotopes, 2010, 68: 1128-1131.
[7] Richard M. Rousseau. Spectrochim Acta B, 2006, 61: 759-
[8] Sherman J. Spectrochim Acta, 1955, 7: 283-306.
[9] Lachance G R and Traill R J. Can Spectrosc, 1966, 11: 43-48.

[10] Cao L G. Nucl Tech, 1987, 10: 15-21. (in Chinese)
[11] Cao L G, Ding Y M, Huang Z Q. Method of Energy Dispersive X-ray Fluorescence. Chengdu: Chengdu University of Science and Technology Press, 1998, 182-274.
[12] Li Z, Tuo X G, Mu K L. Nucl Sci Tech, 2009, 32: 35-40.
[13] Kima G H, Yoona J E, An S H, et al. Build Environ, 2004, 39:
[14] Ozkaya B, Demi A, Bilgili M S. Environ Modeling Software, 2007, 22: 815-822.
[15] Messai N, Thomas P, Lefebvre D, et al. A neural Network Approach for freeway Traffic Flow Prediction. In Proceedings of the 2002 IEEE International Conference on Control Applications, Glasgow, Scotland, U.K, September 2002, 18-20.

Note: Figure translations are in progress. See original paper for figures.