Machine Learning Methods for Predicting Coordination Number from EXAFS Spectra

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Abstract

X-ray absorption fine structure (XAFS) is an important structural analysis technique widely applied in investigating the oxidation state, coordination environment, and neighboring atomic characteristics of amorphous materials and disordered systems. However, due to the complexity of XAFS spectra, their interpretation relies on experienced researchers and is susceptible to inaccuracies. This study employs machine learning methods, specifically neural networks, bagged decision tree models, and random forest models, to analyze XAFS data for predicting the coordination numbers of absorbing elements. The research collected EXAFS data for fourth-period transition metal elements from the Materials Project database, encompassing diverse coordination environments, totaling 13,374 valid data entries. The results indicate that both neural network and random forest models achieve high accuracy in coordination number prediction. By enhancing model generalization capability and interpretability, this study provides a more efficient and reliable approach for XAFS data analysis.

Full Text

Preamble

Machine Learning Approach for Predicting Coordination Numbers from EXAFS Spectra

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Abstract

[**Background**] X-ray Absorption Fine Structure (XAFS) is a vital technique for structural analysis, widely employed to investigate the oxidation state, coordination environment, and neighboring atom properties of amorphous mate-

rials and disordered systems. However, the complexity of XAFS spectra often requires interpretation by experienced researchers, which can still lead to inaccuracies. [**Purpose**] This study aims to use machine learning approaches to analyze XAFS data and predict the coordination number of absorbing atoms. [**Methods**] First, a dataset of 13,374 valid EXAFS spectra of fourth-period transition metal elements was sourced from the Materials Project database. Second, this data was utilized to train three machine learning models: neural networks, bagging models, and random forest models. Finally, these models were applied to predict coordination numbers of the absorbing atoms in the spectra. [**Results**] The study achieved an average prediction accuracy of approximately 70%. Feature importance analysis revealed that data points within R $<$ 3.0 Å were critical for predictions, consistent with the prominence of short-range atomic interactions in EXAFS theory. [**Conclusions**] This research enhances the efficiency and reliability of XAFS data analysis by improving model generalizability and interpretability.

Key Words: EXAFS, Coordination Number, Bagging, Random Forest

Introduction

X-ray Absorption Fine Structure (XAFS) can be divided into two main regions: X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS). XAFS is highly sensitive to the oxidation state of the absorbing atom, its coordination environment, and the types and distances of neighboring atoms. Consequently, it finds widespread application across physics, chemistry, materials science, and biology. However, due to the complexity of XAFS spectra, their interpretation typically relies on experienced researchers, and even then may yield inaccurate conclusions [1]. Therefore, developing more efficient and reliable analytical methods to improve the accuracy of XAFS data interpretation has become an important research direction.

Machine learning, as a representative data-driven research method in recent years, has emerged as a significant focus in scientific research. Neural networks, in particular, have attracted attention for their high prediction accuracy and have been widely applied to extended-edge spectral analysis and near-edge structure feature extraction. For example, Tetef et al. (2021) demonstrated that unsupervised methods such as t-distributed Stochastic Neighbor Embedding (t-SNE) and Variational Autoencoders (VAE) can effectively classify sulfur organic compounds based on XANES and valence-to-core X-ray emission spectroscopy (VtC-XES), revealing detailed chemical properties such as oxidation state and aromaticity [2]. Timoshenko et al. (2018) developed a neural network approach to extract radial distribution functions (RDF) directly from EXAFS spectra without relying on prior structural assumptions. This method was successfully applied to analyze the high-temperature bcc-fcc phase transition in iron (Fe) and was extended to cobalt (Co) and nickel (Ni) systems [3].

Nevertheless, existing studies are typically limited to analyzing simple material

systems of specific materials or material classes under varying parameters (such as temperature changes), presenting challenges for model generalization. Furthermore, due to the complexity and "black-box" nature of neural networks, researchers often struggle to decipher the specific basis for model-generated parameters and cannot intuitively understand the decision-making process. This lack of interpretability limits the application of neural networks in research scenarios requiring explicit feature importance analysis [4]. To improve the interpretability of machine learning models, researchers have developed various techniques, including Ridge Regression (RR) [5], LASSO regression [6], the SISSO method [7], and Decision Trees (DT) [8]. Among these, decision trees have attracted widespread attention due to their simple structure and high interpretability. Building upon Ensemble Learning (EL) [9], researchers have further developed Bagging [10], Random Forest (RF) [11], and Boosting [12] methods. Decision tree models have already demonstrated potential in XAFS spectroscopy research. For instance, Torrisi et al. (2020) used random forest machine learning models to analyze XANES spectra, predicting coordination numbers, nearest-neighbor distances, and Bader charges of absorbing atoms in transition metal oxides. Their study improved model interpretability through multi-scale polynomial featurization, revealing key spectral regions associated with different properties [13].

Addressing the two core constraints of machine learning in XAFS analysis—model generalization difficulties and lack of interpretability—this study constructed a large-scale EXAFS dataset covering multiple fourth-period transition metal elements across different material categories and diverse coordination environments using the Materials Project database. Based on this dataset, the developed neural network and random forest models demonstrated generalization capability in predicting coordination numbers with high accuracy. Furthermore, the interpretability analysis of the random forest model successfully identified the spectroscopic feature region that determines coordination number: the low-R region after Fourier transformation. This study provides a scalable, highly generalizable XAFS data analysis tool, laying a solid foundation for high-throughput, automated XAFS structural analysis across broad material systems, with significant methodological value and practical prospects.

The workflow of this study is illustrated in Figure 1 [Figure 1: see original paper]. We collected a total of 15,498 XAFS data entries for fourth-period transition metal elements from the Materials Project. After screening, 13,374 data points with integer coordination numbers were retained. Subsequently, we transformed these XAFS data from E-space to R-space and imported them into both fully connected neural networks and decision tree ensemble learning models (Bagging and Random Forest). For each element, we trained and evaluated separate models.

1.1 X-ray Absorption Fine Structure (XAFS) and Extended X-ray Absorption Fine Structure (EXAFS)

The XAFS phenomenon was first discovered and scientifically documented in 1920 by Friche and Hertz. A breakthrough in XAFS research came from the innovative method proposed by Sayers, Stern, and Lytle—using Fourier transform techniques to effectively analyze EXAFS oscillation signals in photoelectron wave vector space [14]. This milestone work marked the formal entry of XAFS technology into quantitative analysis and initiated its systematic development for materials characterization [15].

XAFS technology provides detailed structural information about the local chemical environment surrounding absorbing atoms. In recent years, atomic-level local property analysis based on XAFS has become an important approach in materials science and catalysis research. Specifically, XAFS techniques have been applied to investigate the coordination environments of metal clusters, explore local structural distortions in ferroelectric materials, and analyze catalytic mechanisms in single-atom catalysts.

XAFS spectra are obtained by measuring how a material' s X-ray absorption coefficient varies with incident photon energy. XAFS spectra are typically divided into two characteristic regions: X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS). The theoretical expression for EXAFS can be written as:

$$\chi(k) = S_0^2 \sum_j \frac{N_j f_j(k)}{kR_j^2} e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2} \sin[2kR_j + \delta_j(k)]$$

where k represents the photoelectron wave vector, N_j denotes the coordination number of the j-th coordination shell, R_j represents the average distance from the absorbing atom to neighboring atoms in the j-th shell, σ_j characterizes the disorder of the j-th shell, $f_j(k)$ denotes the scattering ability of neighboring atoms for photoelectrons, $\delta_j(k)$ represents the phase shift, $\lambda(k)$ denotes the mean free path of photoelectron propagation, and S_0^2 represents the amplitude reduction factor.

The above theoretical expression indicates that Fourier transform can convert the EXAFS oscillation function from k-space to R-space, thereby obtaining radial distribution information about the local structure around absorbing atoms. However, due to the simultaneous presence of multiple coupled variable parameters in the EXAFS formula and the possible superposition of multiple scattering paths, precise structural determination relying solely on EXAFS spectra faces a severe ill-posed problem. Therefore, in practical EXAFS data analysis, researchers typically adopt a "fingerprint comparison" approach, obtaining relative models of material local structures by comparing experimental data with reference spectra of known structures or theoretical simulation results.

Although directly inverting all structural parameters from XAFS spectra presents inherent difficulties, calculating theoretical XAFS spectra based on known structural models has become a reliable research method. In XAFS research, FEFF[16] and FDMNES[17] are two widely adopted computational software packages. Both are based on first-principles (ab initio) calculation methods, precisely simulating XAFS spectral features by solving the Schrödinger equation. FEFF employs Real-Space Multiple Scattering (RSMS) theory, while FDMNES is based on the Finite Difference Method (FDM), providing reliable theoretical references for experimental data analysis.

1.2 Larch[18]

Larch is a comprehensive toolkit specifically designed for XAFS and related spectroscopic data analysis. Compared to the IFEFFIT software package developed in FORTRAN, Larch was reconstructed using Python, significantly enhancing large-scale data processing capabilities and data visualization functions. In this study, we utilized core functions from the Larch toolkit for data processing: the autobk function performs background subtraction and normalization, converting EXAFS spectra from E-space to k-space; the xftf function executes Fourier Transform (FT), converting EXAFS spectra from k-space to R-space.

1.3 Coordination Number

Coordination number is a key structural parameter describing the local coordination environment of atoms in materials and is of paramount importance for studying material properties. In traditional research, coordination numbers were typically determined through intuitive judgment of coordination conditions for individual atoms. However, with the development of high-throughput materials computing technology and the generation of large-scale datasets, developing reliable and automated coordination number calculation algorithms has become an urgent research need.

Currently, multiple coordination number calculation methods have been proposed in materials science [19]. Among the simpler algorithms are those based on interatomic distances and empirical tolerance parameters, such as BrunnerNN[20] and MinimumOKeeffeNN[21]. These methods determine coordination numbers by comparing actual interatomic distances in models with their tolerance values. Although these algorithms are relatively simple and intuitive, they are sensitive to small atomic perturbations and changes in empirical tolerance parameters, where minor atomic variations may lead to different coordination number assignments.

The VoronoiNN algorithm proposed by O' Keeffe[22] provides an alternative solution. Based on geometric principles, this algorithm employs Voronoi decomposition[23] to treat the environment around a central atom as a polyhedron and further performs weighted processing according to spatial angles to determine the number of neighboring atoms. Similarly, this study utilizes the

CrystalNN[24] algorithm. The CrystalNN method is also based on Voronoi decomposition and is widely recognized for its high computational accuracy. This method calculates the probability of possible coordination environments through Voronoi decomposition and ultimately selects the result with the highest probability as the atom' s coordination environment. In this paper, we systematically calculated the coordination numbers of absorbing atoms in various material systems using the CrystalNN algorithm from the pymatgen materials computing package[25].

1.4 Neural Networks

As an important branch of machine learning, neural networks (deep learning) have become one of the core fields in current scientific research and technological applications due to their excellent performance in regression and classification tasks. Neural network models achieve feature extraction and pattern recognition through numerous adjustable parameters, which are automatically optimized during training via backpropagation algorithms. Researchers primarily optimize model performance by tuning hyperparameters (including batch size, learning rate, and network layer structure).

A single hidden layer feedforward neural network model can be formally defined by the following mathematical expression:

$$f(X) = \beta_0 + \sum_{k=1}^{K} \beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right)$$

where $X = (X_1, X_2, \ldots, X_p) \in \mathbb{R}^p$ represents the p-dimensional input feature vector. The model parameters include:

- w_{kj}: connection weight from the j-th feature in the input layer to the k-th neuron in the hidden layer
- β_k: weight coefficient from the k-th neuron in the hidden layer to the output layer
- w_{k0} and β_0: bias terms for the corresponding linear transformations

Although this model architecture appears as a linear superposition in form, nonlinear activation functions $g(\cdot)$ must be introduced to effectively approximate nonlinear functional relationships in real-world scenarios. In machine learning, the Sigmoid function and ReLU (Rectified Linear Unit) function[26] are two classic activation functions. The Sigmoid function exhibits S-shaped saturation characteristics with an output range of (0,1), which led to its widespread application in early neural network research. However, this function suffers from vanishing gradients when input values approach positive or negative infinity (derivatives approach zero), significantly reducing parameter update efficiency during backpropagation. In contrast, the ReLU function, defined as $g(x) = \max(0, x)$, guarantees a constant derivative value in the positive interval

due to its piecewise linear nature, thereby effectively alleviating the vanishing gradient problem. Moreover, the computational complexity of the ReLU function is significantly lower than that of the Sigmoid function, enabling superior computational efficiency and convergence characteristics in deep neural network training.

1.5 Decision Trees

Despite the significant predictive performance advantages of neural networks, their inherent "black-box" characteristics result in insufficient model interpretability. Specifically, the mechanism for setting numerous neuron parameters in neural networks is difficult to interpret clearly, prompting researchers to seek alternative analysis tools with stronger interpretability. In this study, we employ decision trees as an analytical tool due to their intuitive structure and ease of interpretation. Through decision trees, researchers can clearly identify relationships between data features and results. However, traditional decision tree methods exhibit obvious deficiencies in prediction accuracy. To overcome this limitation, researchers have developed various ensemble learning methods, including Bagging, Random Forest, and Boosting. While these ensemble methods significantly improve prediction performance, they sacrifice the intuitive interpretability of single decision trees. Nevertheless, by analyzing the Gini Index, we can effectively evaluate the importance of each feature in classification decisions.

The modeling mechanism of decision trees follows a recursive feature space partitioning strategy. Through preset tree-structure hyperparameters (such as maximum depth), this algorithm employs supervised learning to extract optimal splitting criteria from training datasets, thereby decomposing the p-dimensional feature space (assuming input samples are p-dimensional feature vectors) into several mutually exclusive geometric subspaces. Theoretical studies show that this model exhibits excellent classification performance on datasets with explicit hyperplane partition characteristics, but its classification effectiveness declines significantly when handling nonlinearly separable data or classification problems with complex decision boundaries. However, empirical studies demonstrate that when processing tabular data, ensemble learning algorithms derived from decision tree architectures show superior prediction accuracy compared to neural network models. Taking the XGBoost algorithm as an example, this optimized gradient boosting framework achieves significant performance breakthroughs in multiple benchmark tests through iterative decision tree integration and regularization strategies[27].

1.6 Materials Databases

Constructing robust predictive models in materials science machine learning research heavily depends on support from large-scale, high-quality datasets[28]. Current mainstream materials informatics platforms include Open Catalyst[29],

Materials Project[30], and the Open Quantum Materials Database (OQMD)[31]. This study selected Materials Project as the data source primarily based on the following considerations: the database integrates structural information for over 160,000 materials and provides FEFF-theory-calculated XAFS spectral data, which is valuable for establishing structure-property relationships. Additionally, its open Python Application Programming Interface (API) significantly improves data acquisition efficiency and enables seamless integration with high-throughput computational workflows. Data acquisition was performed through the pymatgen materials analysis toolkit, with all processed structured data stored in a MongoDB document database for efficient retrieval.

According to literature cited in the official Materials Project documentation, convergence checks and optimization tests were performed on input fields in FEFF9: in convergence checks, researchers varied the rfms1 value from 2 Å to 8 Å in 1 Å increments to alter FEFF' s self-consistent potential automatic calculations. The self-consistent potential is controlled by the Self-Consistent Field (SCF) card. Simultaneously, the rfms value was varied from 3 Å to 11 Å in 1 Å increments to determine parameters for the Full Multiple Scattering (FMS) card.

2 Dataset and Preprocessing

The data for this study were sourced from the Materials Project database, where we systematically retrieved materials containing fourth-period transition metals and extracted their EXAFS calculation data. All EXAFS data were generated through the FEFF calculation software package. To ensure data quality, we excluded samples where different absorbing atoms within the same material exhibited different coordination numbers, as such data could interfere with coordination number classification.

In this study, we utilized theoretically calculated EXAFS data from the Materials Project database rather than noise-added calculated EXAFS data. According to research by Paolo Ghigna[32] and Nicholas Marcella[33] et al., the impact of adding noise to calculated data is smaller than that of systematic factors (such as background subtraction in data processing). Therefore, we could directly use the calculated EXAFS data for machine learning.

The database contains materials from various complex systems, such as oxides, sulfides, and alloys. While this enhances model generalization capability, it also poses challenges for classification. Moreover, overly complex classification can dilute prediction accuracy for individual categories. Consequently, this study focuses solely on classifying absorbing atoms.

For periodic EXAFS data, we employed Fourier transform for preprocessing. For large-scale data processing, we implemented automated processing using the Larch toolkit combined with Python programming. Specifically, the autobk function in Larch was used to convert raw E-space data to k-space data, followed

by the xftf function to Fourier transform k^2-weighted k-space data into R-space data.

Regarding R-space data processing, we extracted intensity values at intervals of 0.030 Å as features. Additionally, we used Python' s Peak package to calculate the R coordinates and intensity values corresponding to each characteristic peak, incorporating these parameters as additional features. For comparison, we separately trained neural network models using k-space data and wavelet-transformed data. The wavelet transform employed the cauchy_{wavelet} function from the Larch toolkit with parameters set to kweight = 0, rmax_{out} = 6, transforming k-space data from k_{min} = 3 to k_{max} = 14.

3 Model Construction and Training

To accomplish the coordination number prediction task, this study constructed a prediction model based on fully connected neural networks. As shown in Figure 2 [Figure 2: see original paper], the neural network' s input layer contains 326 features corresponding to intensity values of EXAFS R-space spectra at intervals of 0.030–0.031 Å. The network employs a dual hidden-layer structure with 512 neurons in each layer. Following each hidden layer are sequentially configured ReLU activation function layers and Dropout regularization layers: the ReLU activation function enhances the model' s nonlinear expressive capability, while the introduced Dropout regularization mechanism mitigates overfitting. The parameter range k in the output layer varies according to the coordination number range corresponding to different elements. During model optimization, models with optimal validation set performance were selected as final models through five-fold cross-validation, effectively improving model generalization capability.

To enhance model interpretability and verify neural network predictions, this study simultaneously constructed ensemble learning models based on decision trees. First, we implemented two ensemble models using the Scikit-learn[34] machine learning framework: decision tree ensembles based on Bagging and Random Forest. Bagging generates sub-training sets equal in size to the original dataset through bootstrap sampling, trains independent decision tree models on each subset, and integrates predictions through a voting mechanism. Random Forest introduces feature randomness on top of Bagging—during each node split, only sqrt(d) features (d being the total feature count) are randomly selected for optimal partitioning, thereby enhancing model diversity. Both models use the Gini index as the splitting criterion. As shown in Figure 3 [Figure 3: see original paper], each box in the diagram represents a split node. "Freq_r" in the box indicates the intensity corresponding to coordinate r in R-space of the EXAFS spectrum, while "samples" indicates the quantity of data contained in that node before splitting.

This study systematically analyzed EXAFS spectra of fourth-period transition metal materials using neural networks and decision tree algorithms. As shown

in Figure 4 [Figure 4: see original paper], for each metal, the models from left to right are: neural network model, Bagging model, Random Forest model, Bagging model incorporating peak height and position, and Random Forest model incorporating peak height and position. The results indicate that both methods achieved prediction accuracies around 70%, with neural network models showing slightly superior performance compared to decision tree models. Notably, the accuracies of the two methods exhibit significant correlation, showing synchronized increase or decrease trends with varying element types. In the application of ensemble learning methods, Random Forest models improved prediction accuracy by approximately 1–3 percentage points on average compared to Bagging models. Additionally, this study examined feature datasets incorporating peak position and intensity information, finding that decision tree model prediction accuracies on this dataset showed no significant difference compared to the original dataset.

The results demonstrate that model prediction accuracy exhibits significant element dependence in coordination number classification. Vanadium (V) showed the best prediction performance in the neural network framework, reaching 81.74% accuracy, while cobalt (Co) exhibited relatively low prediction accuracy at only 67.39%. Further analysis revealed that this difference may be related to the coordination number distribution characteristics of elements in the database. Specifically, V maintains a relatively stable six-coordinate structure in most materials, whereas Co shows more diverse coordination number variations, which may be the primary reason for its lower prediction accuracy.

As shown in Figure 5 [Figure 5: see original paper], we plotted each element' s prediction rate against the information entropy of coordination number distribution. The scatter plot was fitted using least squares linear regression, revealing the relationship between these variables, with the R-squared value indicating the strength of the fit. The results show that prediction accuracy exhibits certain correlation with coordination number distribution characteristics.

Simultaneously, this study compared prediction accuracies based on k-space and q-space (wavelet transform) data. As shown in Figure 6 [Figure 6: see original paper], prediction accuracies vary across the three spaces, but the overall trend is similar: prediction rates show common upward or downward trends with element changes. R-space prediction accuracy is superior to k-space and q-space in most cases, leading us to recommend using R-space for neural network learning.

To demonstrate model bias characteristics, we used Zn as an example to create a confusion matrix comparing true and predicted coordination numbers.

This study further constructed feature importance distribution maps for each element' s EXAFS spectra based on the Gini index from decision tree ensemble models. Figure 8 [Figure 8: see original paper] shows the feature importance and its correspondence to R-space for Co and Mn elements in Bagging and Random Forest models. Here, (a) represents Co element Bagging Gini index;

(b) represents Co element Random Forest Gini index; (c) represents Mn element Bagging Gini index; (d) represents Mn element Random Forest Gini index. Since the R-space dataset contains intensity values at 326 equally spaced coordinate points, the maximum single feature importance value is generally below 0.1. Based on experience in EXAFS spectral processing, we only discuss the region where $R < 6.0$ Å. Through comparative analysis of relative importance distribution, we find that feature importance weights are primarily concentrated in the short-range interaction region of $R < 3.0$ Å, which aligns with the empirical understanding in existing EXAFS theory that short-range atomic interactions dominate spectral features.

For distant coordination shells with $R > 6.0$ Å, current models struggle to reliably establish direct correspondence between high-shell coordination numbers and R-space parameters. Because high-shell signal intensities are low, prediction errors increase significantly, failing to meet accuracy requirements. In practical operations, we also find it difficult to obtain reliable coordination information regarding high coordination shells.

Additionally, this study observed that Bagging significantly amplifies importance differences between features in feature importance distribution maps, whereas feature importance distribution in Random Forest models is relatively more balanced. This phenomenon may be related to Bagging' s tendency toward overfitting. Specifically, Bagging removes only one feature per iteration for optimization, causing features with higher importance to be further amplified across multiple iterations. In contrast, the Random Forest model used in this study simultaneously screens 14 features per iteration for optimization, thereby avoiding excessive enhancement of single feature importance and effectively improving model generalization capability. This finding indicates that Random Forest models can better balance feature importance and reduce overfitting risks when handling high-dimensional data, providing a more robust solution for EXAFS spectral analysis.

This study successfully developed and validated a machine learning method for predicting coordination numbers of fourth-period transition metal elements from EXAFS spectra. By collecting large-scale EXAFS data from the Materials Project database and combining neural networks with decision tree algorithms, our models achieved approximately 70% average prediction accuracy in coordination number classification tasks. Notably, neural network models performed exceptionally well on certain elements (such as V), with accuracy reaching 81.74%, demonstrating their powerful potential for processing complex spectral data.

The results indicate that Random Forest models not only achieve prediction performance comparable to neural networks but also reveal key information in EXAFS spectra through feature importance analysis. Specifically, intensity information from data points at $R < 3.0$ Å in R-space after Fourier transformation is crucial for coordination number prediction. This discovery aligns with the EXAFS theoretical perspective that short-range atomic interactions domi-

nate spectral features, providing theoretical support and interpretability for the model' s decision-making process.

However, the study also found that model prediction accuracy exhibits significant element dependence. For example, Co showed lower accuracy (67.39%), possibly related to the diversity of coordination number distributions in the database. Furthermore, feature importance analysis revealed that for certain elements (such as Co), the importance of peak position and intensity parameters was lower than expected, suggesting that potentially useful spectral features remain underutilized. This phenomenon indicates that current feature extraction methods still have room for improvement.

Future research directions should include optimizing feature engineering, exploring more sophisticated spectral feature extraction techniques, and attempting other advanced machine learning algorithms to improve prediction accuracy and generalization capability across different elements. Additionally, hybrid approaches combining physical models with machine learning warrant further investigation to enhance the efficiency and reliability of EXAFS spectral analysis. The results of this study provide new tools and ideas for rapid analysis of local material structures, holding significant scientific importance and application value.

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