Geochemical Perspectives Letters

Zircon as a pathfinder to REE deposits

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Supplementary Information

The Supplementary Information includes:

- Instructions for Supplementary Information
- Detailed Methods for Statistical Analysis
- Tables S-1 to S-3
- Jupyter Notebook
- Supplementary Information References

Instructions for Supplementary Information

The supplementary information contains detailed descriptions of the statistical analysis, summary statistics of this analysis (Table S-1 and Table S-2), complete datasets of zircon geochemistry used in this study (Table S-3), and a Jupyter Notebook containing material for training and classification.

Detailed Methods for Statistical Analysis

This section details the steps employed to classify zircon based on their trace element compositions. The analysis involved training and evaluating six distinct classification models. This used the following packages pandas v. 2.1.1 (McKinney, 2010), NumPy v.1.26.0 (Harris *et al*., 2020), matplotlib v. 3.8.0 (Hunter, 2007), scikit-learn v. 1.3.2 (Pedregosa *et al*., 2011), and seaborn v. 0.13.0 (Waskom, 2021).

Data Compilation

The zircon trace element dataset was compiled from previously published peer reviewed papers. Only zircon grains that the original studies interpreted as autocrystic (magmatic), based on petrologic, grain-scale imaging (cathodoluminescence or backscattered electrons), composition, and/or geochronologic information were included. The compilation followed the interpretations made in the original studies, rather than geochemical data alone, because of the original studies' access to a greater suite of information, to maintain consistency across the compiled dataset, and to remove potential bias imposed by the use of either too narrow or too broad of a geochemical-only filter. Data were only compiled by studies using in-situ techniques (laser ablation-inductively coupled-plasma mass spectrometry; LA-ICP-MS) and secondary ion mass spectrometry (SIMS). The analytical method is captured in the compiled dataset and no systematic biases across elements were observed when comparing the data by method. Individual samples were classified into three categories based on literature estimates of the host rock fertility. Classification fields drew upon the compilations of Berger *et al.* (2009) and Simandl and Paradis (2018) with additional information drawn from Beard *et al.* (2023) and the individual studies compiled for zircon data, and references therein.

Data Preparation and Preprocessing

The training dataset contained geochemical data including log-transformed ratios and elemental concentrations (log10_LuHf, log10_ThU, log10_GdYb, log10_UNb, log10_UYb, log10_ThNb, log10_NbYb, log10_SmYb, log10_Eu, log10_ThYb, log10_SumHREE, log10_CeU) as features (*X*) and a categorical variable representing the mineralization potential (*y*) as the target.

Feature and Target Definition

The geochemical features were selected based on their established relevance in petrogenesis and ore deposit studies. The classification target represented whether the zircon analysis was from an REE-enriched, Nb ± REE-enriched , or barren rock, was derived from independent geological observations (Berger *et al.*, 2009; Ford *et al.*, 2023; Fortier *et al.*, 2019; Verplanck *et al.*, 2016).

Data Partitioning

The dataset was split into training (80%) and testing (20%) sets using a stratified random split. The `train_test_split` function from the `scikit-learn` library (version 1.3.2) was used with `test_size=0.2`, and `random_state=42` for reproducibility. Stratification ensures that the class distribution in the training and testing sets mirrors the distribution in the original dataset, which is crucial for robust model evaluation, especially with imbalanced classes.

Feature Scaling

Prior to training, the numerical features in both the training and testing sets were standardized using `StandardScaler` from the `scikit-learn` library. This involved subtracting the mean and dividing by the standard deviation for each feature. Mathematically, for a feature x, the standardized value z is calculated as: $z = (x - \mu) / \sigma$ where μ is the mean of x, and σ is the standard deviation of x. This scaling step is essential for algorithms sensitive to the magnitude of input features, such as SVM and KNN, ensuring that all features contribute equally to the model training process and preventing features with larger values from dominating the distance calculations. The `fit_transform` method of `StandardScaler` was applied to the training data, and the `transform` method was used on the testing data to prevent data leakage, maintaining the independence of the test set.

Model Training and Evaluation

Six classification models were initialized and trained on the preprocessed training data. The model parameters were set to their default values. For SVM, the scaled training data (*X_train_scaled*) were used, while the original training data (*X_train*) was used for the tree-based models (Decision Tree, Random Forest, Gradient Boosting) and Naive Bayes. A brief description of each model is provided below:

Naïve Bayes: A probabilistic classifier based on Bayes' theorem, assuming feature independence. The `GaussianNB` class from the `scikit-learn` library was used for continuous features.

Decision Tree: A tree-like structure where each internal node represents a feature, each branch represents a decision rule, and each leaf node represents a class label. The `DecisionTreeClassifier` class from the `scikit-learn` library was used.

Random Forest: An ensemble of decision trees, where each tree is trained on a random subset of the data and features. The final prediction is made by aggregating the predictions of all trees. The `RandomForestClassifier` class from the `scikit-learn` library was used.

Support Vector Machine (SVM): A model that finds the optimal hyperplane that best separates data points of different classes. A radial basis function (RBF) kernel was used. The `SVC` class from the `scikit-learn` library was used.

k-Nearest Neighbors (KNN): A non-parametric method that classifies a data point based on the majority class of its *k* nearest neighbors in the feature space. The `KNeighborsClassifier` class from the `scikit-learn` library was used.

Gradient Boosting: An ensemble of weak prediction models, typically decision trees, that are trained sequentially, with each model correcting the errors of the previous ones. The `GradientBoostingClassifier` class from the `scikit-learn` library was used.

The performance of each trained model was evaluated on the held-out test set. Accuracy, precision, recall, and F1-score were calculated using `accuracy_score` and `classification_report` from the `scikit-learn` library to assess the classification performance for each category. The predicted probabilities for each class were also obtained using the `predict_proba` method to serve as confidence scores for the predictions. The classification report (Tables S-1 and S-2) provides a detailed breakdown of the performance of each model for each class, including:

Precision: The proportion of positive identifications that were actually correct.
Recall: The proportion of actual positives that were identified correctly.
F1-score: The harmonic mean of precision and recall, providing a balanced measure of a model's accuracy.
Support: The number of occurrences of each class in the test set.

The overall accuracy (Table S-1) represents the proportion of correctly classified samples out of the total number of samples in the test set. A complete report of individual scores by model and class is provided in Table S-2.

Feature Importance

For the tree-based models (Decision Tree, Random Forest, and Gradient Boosting), feature importance scores were calculated. Feature importance measures the contribution of each feature to the model's predictive power. Gini importance (mean decrease in impurity) was used. The importance scores are normalized such that they sum to 1. The `feature_importances_` attribute of the trained models was used to obtain these scores.

Classification of Unknown Zircons

After training and validating the machine learning models, the same models were used to predict the classification type for new, unknown samples from the detrital zircon database of Roberts *et al.* (2024). This process involved the following steps:

First, the Roberts *et al.* (2024) dataset was loaded using a pandas DataFrame. Then the data were filtered to remove any rows containing missing or non-numeric values in the feature columns, ensuring the integrity of the input data. The cleaned unknown data was then scaled using the same StandardScaler instance that was fitted on the original training data. This is a critical step to ensure that the unknown data are in the same feature space as the data the models were trained on. The transform method of the scaler was used for this purpose.

For each of the six trained models, the predict method was called on the scaled unknown data to obtain the predicted rock type. The 'predict_proba' method was also used to get the confidence scores for each prediction, providing a measure of the model's certainty for its classification of each zircon grain.

The predictions and confidence scores from all models were compiled into a single pandas DataFrame, alongside the original 'Best Age' and 'Reference' columns from the input data. This final DataFrame, saved to a .csv file, summarizes the classification results for each unknown sample.

Supplementary Tables and Jupyter Notebook

Table S-1 Overall Model Accuracy on the Test Dataset.

Supervised machine learning model type	Overall accuracy score (percent)
Naïve Bayes	86
Decision Tree	96
Random Forest	97
Support Vector Machine	97
k-Nearest Neighbors	97
Gradient Boosting	96

Table S-2 Classification Reports for Each Model.

Model	Class	Precision	Recall	F1-Score	Support
Naïve Bayes	Barren	0.98	0.85	0.91	372
	REE	0.31	0.79	0.45	19
	Nb ± REE	0.64	0.93	0.76	40
	Macro average	0.64	0.86	0.88	431
Decision Tree	Barren	0.98	0.97	0.98	372
	REE	0.79	0.79	0.79	19
	Nb ± REE	0.83	0.88	0.85	40
	Macro average	0.87	0.88	0.87	431
Random Forest	Barren	0.98	0.98	0.98	372
	REE	1.00	0.79	0.88	19
	Nb ± REE	0.85	0.88	0.86	40
	Macro average	0.94	0.88	0.91	431
Support Vector Machines	Barren	0.98	0.98	0.98	372
	REE	1.00	0.84	0.91	19
	Nb ± REE	0.85	0.85	0.85	40
	Macro average	0.94	0.89	0.91	431
K-Nearest Neighbor	Barren	0.99	0.98	0.98	372
	REE	1.00	0.84	0.91	19
	Nb ± REE	0.84	0.95	0.89	40
	Macro average	0.94	0.92	0.89	431
Gradient Boost	Barren	0.97	0.98	0.98	372
	REE	1.00	0.84	0.91	19
	Nb ± REE	0.80	0.82	0.81	40
	Macro average	0.96	0.87	0.91	431

Table S-3 The zircon igneous geochemical dataset and classified detrital zircons.

Notebook Jupyter notebook "ZirconREENbClassifier.ipynb" for analysing and classifying zircon compositions.

Table S-3 (.xlsx) and the Jupyter notebook (.ipynb) are available for download from the online version of this article at https://doi.org/10.7185/geochemlet.2540.

Note

Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

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