# **Machine learning-driven skarn deposit classification with SHAP-enhanced garnet geochemistry analysis**

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Tables S3 to S6 present the optimal training parameters for the models.

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The corresponding references for the training data

**Introduction**

This supplementary material provides the optimal training parameters and training results for the models used in this study. Tables S3 to S6 present the optimal training parameters for the KNN, RF, SVM, and XGBoost models, respectively. Tables S7 to S13 present the training results, including accuracy and F1-score, for each deposit type under the optimal parameters. The corresponding references for the training data are also provided. Supplementary materials Table S1-S2, as well as the program used in the study, are available on **GitHub**.

## **Tables S3 to S6 present the optimal training parameters for the models**

Table S3 lists the optimal parameters for the KNN model, Table S4 for the RF model, Table S5 for the SVM model, and Table S6 for the XGBoost model. The parameters are associated with various skarn deposit types, such as Fe, Au, and Cu.

**Table S3. KNN**

|  |  |  |  |
| --- | --- | --- | --- |
|  | metric | n\_neighbors | weights |
| Fe | manhattan | 7 | distance |
| Au | manhattan | 7 | distance |
| Cu | manhattan | 4 | distance |
| Zn | manhattan | 4 | distance |
| W | manhattan | 4 | distance |
| Mo | manhattan | 4 | distance |
| Sn | manhattan | 1 | distance |

**Table S4. RF**

|  |  |  |  |
| --- | --- | --- | --- |
|  | max\_depth | min\_samples\_split | n\_estimators |
| Fe | 17 | 5 | 300 |
| Au | 17 | 5 | 400 |
| Cu | 17 | 5 | 400 |
| Zn | 17 | 5 | 400 |
| W | 17 | 5 | 400 |
| Mo | 17 | 5 | 400 |
| Sn | 17 | 5 | 400 |

**Table S5. SVM**

|  |  |  |  |
| --- | --- | --- | --- |
|  | C | gamma | kernel |
| Fe | 10 | scale | ploy |
| Au | 10 | scale | rbf |
| Cu | 10 | scale | ploy |
| Zn | 10 | scale | ploy |
| W | 10 | scale | ploy |
| Mo | 10 | scale | ploy |
| Sn | 10 | scale | ploy |

**Table S6. XGBoost**

|  |  |  |  |
| --- | --- | --- | --- |
|  | learning\_rate | max\_depth | n\_estimators |
| Fe | 0.1 | 9 | 400 |
| Au | 0.2 | 15 | 400 |
| Cu | 0.2 | 11 | 200 |
| Zn | 0.2 | 9 | 250 |
| W | 0.1 | 15 | 400 |
| Mo | 0.2 | 17 | 400 |
| Sn | 0.1 | 17 | 400 |

## **Tables S7 to S13 present the model training results.**

Tables S7 to S13 provide the accuracy and F1-score for each deposit type under the optimal parameters. To address the issue of imbalanced data labels during the training process, we employed the SMOTE method, aiming to improve the F1-score.

**Table S7. Fe**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.774 | 0.891 | 0.903 | 0.916 |
|  | F1-Score | 0.773 | 0.767 | 0.901 | 0.915 |
| Fold 2 | Accuracy | 0.796 | 0.895 | 0.905 | 0.924 |
|  | F1-Score | 0.795 | 0.779 | 0.904 | 0.923 |
| Fold 3 | Accuracy | 0.766 | 0.891 | 0.950 | 0.957 |
|  | F1-Score | 0.770 | 0.764 | 0.951 | 0.958 |
| Fold 4 | Accuracy | 0.824 | 0.889 | 0.952 | 0.961 |
|  | F1-Score | 0.822 | 0.752 | 0.954 | 0.961 |
| Fold 5 | Accuracy | 0.807 | 0.890 | 0.947 | 0.961 |
|  | F1-Score | 0.809 | 0.767 | 0.949 | 0.962 |
| Test | Accuracy | 0.779 | 0.907 | 0.917 | 0.925 |
|  | F1-Score | 0.611 | 0.785 | 0.826 | 0.843 |

**Table S8. Au**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.751 | 0.894 | 0.912 | 0.923 |
|  | F1-Score | 0.772 | 0.606 | 0.909 | 0.921 |
| Fold 2 | Accuracy | 0.746 | 0.915 | 0.947 | 0.959 |
|  | F1-Score | 0.770 | 0.706 | 0.948 | 0.960 |
| Fold 3 | Accuracy | 0.764 | 0.908 | 0.964 | 0.964 |
|  | F1-Score | 0.785 | 0.672 | 0.965 | 0.965 |
| Fold 4 | Accuracy | 0.756 | 0.889 | 0.962 | 0.966 |
|  | F1-Score | 0.774 | 0.613 | 0.962 | 0.966 |
| Fold 5 | Accuracy | 0.765 | 0.905 | 0.954 | 0.962 |
|  | F1-Score | 0.785 | 0.661 | 0.955 | 0.962 |
| Test | Accuracy | 0.713 | 0.911 | 0.931 | 0.944 |
|  | F1-Score | 0.501 | 0.700 | 0.773 | 0.820 |

**Table S9. Cu**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.723 | 0.837 | 0.878 | 0.896 |
|  | F1-Score | 0.716 | 0.767 | 0.875 | 0.893 |
| Fold 2 | Accuracy | 0.753 | 0.839 | 0.882 | 0.893 |
|  | F1-Score | 0.750 | 0.782 | 0.879 | 0.891 |
| Fold 3 | Accuracy | 0.734 | 0.853 | 0.885 | 0.896 |
|  | F1-Score | 0.718 | 0.796 | 0.883 | 0.894 |
| Fold 4 | Accuracy | 0.733 | 0.847 | 0.928 | 0.926 |
|  | F1-Score | 0.722 | 0.788 | 0.930 | 0.928 |
| Fold 5 | Accuracy | 0.772 | 0.839 | 0.919 | 0.930 |
|  | F1-Score | 0.764 | 0.772 | 0.923 | 0.933 |
| Test | Accuracy | 0.754 | 0.864 | 0.883 | 0.883 |
|  | F1-Score | 0.682 | 0.810 | 0.839 | 0.840 |

**Table S10. Zn**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.724 | 0.915 | 0.935 | 0.942 |
|  | F1-Score | 0.722 | 0.838 | 0.933 | 0.942 |
| Fold 2 | Accuracy | 0.754 | 0.909 | 0.944 | 0.950 |
|  | F1-Score | 0.749 | 0.827 | 0.943 | 0.950 |
| Fold 3 | Accuracy | 0.746 | 0.920 | 0.956 | 0.962 |
|  | F1-Score | 0.744 | 0.853 | 0.956 | 0.962 |
| Fold 4 | Accuracy | 0.754 | 0.898 | 0.965 | 0.966 |
|  | F1-Score | 0.752 | 0.799 | 0.965 | 0.967 |
| Fold 5 | Accuracy | 0.751 | 0.895 | 0.957 | 0.954 |
|  | F1-Score | 0.742 | 0.806 | 0.957 | 0.955 |
| Test | Accuracy | 0.764 | 0.915 | 0.935 | 0.930 |
|  | F1-Score | 0.641 | 0.851 | 0.883 | 0.878 |

**Table S11. W**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.725 | 0.891 | 0.899 | 0.921 |
|  | F1-Score | 0.717 | 0.694 | 0.896 | 0.919 |
| Fold 2 | Accuracy | 0.733 | 0.888 | 0.936 | 0.941 |
|  | F1-Score | 0.719 | 0.691 | 0.936 | 0.942 |
| Fold 3 | Accuracy | 0.729 | 0.898 | 0.951 | 0.962 |
|  | F1-Score | 0.725 | 0.716 | 0.952 | 0.963 |
| Fold 4 | Accuracy | 0.714 | 0.898 | 0.952 | 0.955 |
|  | F1-Score | 0.704 | 0.710 | 0.952 | 0.956 |
| Fold 5 | Accuracy | 0.744 | 0.887 | 0.951 | 0.954 |
|  | F1-Score | 0.738 | 0.693 | 0.952 | 0.955 |
| Test | Accuracy | 0.776 | 0.893 | 0.907 | 0.912 |
|  | F1-Score | 0.556 | 0.703 | 0.762 | 0.780 |

**Table S12. Mo**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.719 | 0.859 | 0.899 | 0.921 |
|  | F1-Score | 0.705 | 0.691 | 0.893 | 0.919 |
| Fold 2 | Accuracy | 0.743 | 0.871 | 0.917 | 0.920 |
|  | F1-Score | 0.728 | 0.734 | 0.915 | 0.918 |
| Fold 3 | Accuracy | 0.763 | 0.876 | 0.959 | 0.961 |
|  | F1-Score | 0.749 | 0.741 | 0.960 | 0.962 |
| Fold 4 | Accuracy | 0.726 | 0.877 | 0.950 | 0.951 |
|  | F1-Score | 0.707 | 0.746 | 0.951 | 0.952 |
| Fold 5 | Accuracy | 0.724 | 0.865 | 0.947 | 0.944 |
|  | F1-Score | 0.696 | 0.709 | 0.949 | 0.946 |
| Test | Accuracy | 0.754 | 0.892 | 0.904 | 0.913 |
|  | F1-Score | 0.590 | 0.788 | 0.814 | 0.833 |

**Table S13. Sn**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | SVM | KNN | RF | XGB |
| Fold 1 | Accuracy | 0.769 | 0.860 | 0.906 | 0.915 |
|  | F1-Score | 0.788 | 0.808 | 0.907 | 0.915 |
| Fold 2 | Accuracy | 0.782 | 0.863 | 0.903 | 0.923 |
|  | F1-Score | 0.798 | 0.812 | 0.904 | 0.923 |
| Fold 3 | Accuracy | 0.790 | 0.876 | 0.922 | 0.939 |
|  | F1-Score | 0.805 | 0.829 | 0.922 | 0.939 |
| Fold 4 | Accuracy | 0.772 | 0.859 | 0.915 | 0.929 |
|  | F1-Score | 0.794 | 0.812 | 0.919 | 0.931 |
| Fold 5 | Accuracy | 0.784 | 0.847 | 0.926 | 0.930 |
|  | F1-Score | 0.803 | 0.791 | 0.930 | 0.933 |
| Test | Accuracy | 0.731 | 0.862 | 0.891 | 0.905 |
|  | F1-Score | 0.682 | 0.814 | 0.851 | 0.868 |

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