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Data-Driven Machine Learning Techniques for Metal Resource Estimation at Quiulacocha Tailings Deposit, Peru

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Abstract

The Quiulacocha tailings deposit in central Peru, containing 70 Mt of historical mine waste, presents both environmental risks and opportunities for secondary metal recovery. This study applies data-driven machine learning techniques to estimate the remaining silver resources using 927 one-meter composites from 40 vertical drillholes. Three supervised learning models—Random Forest (RF), k-Nearest Neighbors (KNN), and Extreme Gradient Boosting (XGBoost)—were trained using spatial coordinates (X, Y, Z) as the sole input features. Model validation was performed using leave-one-out cross-validation (LOOCV), and results were benchmarked against ordinary kriging (OK). Among the models, RF delivered the highest predictive performance (mean error = 0.53 g/t, RMSE = 7.21 g/t, R = 0.82), outperforming OK (R = 0.63, RMSE = 10.47 g/t). Block model predictions indicated higher silver content from machine learning models: 1,532.86 t (RF), 1,542.16 t (XGBoost), and 1,492.09 t (KNN), compared to 1,463.73 t from OK. Additionally, XGBoost maintained superior grade-tonnage relationships under elevated cutoff thresholds, highlighting its potential to delineate high-grade subdomains within the deposit. These findings confirm the value of machine learning in resource estimation under conditions of low spatial continuity, such as tailings, where material mixing and irregular deposition patterns limit correlation across space.

1. Introduction

The reprocessing of mining tailings has gained strategic importance as these materials, historically considered waste, are now recognized as secondary sources of critical and economically valuable metals that were previously unrecovered due to technical or economic limitations [1, 2]. The increasing global demand for raw materials driven by the energy transition and green technologies has exerted additional pressure on resource supply chains, making the valorization of tailings a key component of sustainable mineral development. Within this context, this study aims to evaluate the effectiveness of machine learning (ML) models in estimating residual metal resources in legacy tailings deposits, with particular focus on low spatial continuity settings. We assess the performance of three supervised ML algorithms—Random Forest, k-Nearest Neighbors, and Extreme Gradient Boosting against conventional geostatistical methods, using a dataset derived from vertical drilling in a Peruvian tailings facility.

Interest in tailings reprocessing is growing worldwide and is not limited to specific jurisdictions. For example, over 5,000 tailings ponds covering nearly 1,900 km² have been documented in China alone [3], highlighting widespread environmental and land-use concerns. In Europe, the Raw Materials Initiative of the European Commission [4] identified critical raw materials (CRMs) such as cobalt (Co), silver (Ag), gold (Au), copper (Cu), and nickel (Ni) as essential for technological sovereignty. In response, policies

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such as European Directive 2006/21/EC [5] mandate regular evaluation of abandoned or inactive waste facilities, promoting reuse and rehabilitation in line with circular economy principles [6–8].

From a regulatory and economic standpoint, tailings are increasingly considered recoverable stocks rather than liabilities. National strategies, such as Finland's Mineral Strategy, align with this paradigm shift by advocating the reuse of extractive residues [9]. However, tailings also pose long-term environmental risks due to the presence of residual sulfides and heavy metals [10], which can oxidize and generate acid mine drainage [11, 12]. In addition to geochemical hazards, structural instability of tailings dams remains a critical concern, particularly in abandoned facilities with limited oversight [13, 14]. Integrated characterization combining geophysical and geochemical methods is thus essential for guiding both remediation and resource recovery [15].

Comprehensive characterization of tailings is a necessary prerequisite for assessing their potential for resource recovery [16–19]. Simultaneously, declining ore grades and increasing tailings volumes—projected to exceed 69 billion m^3 globally by 2025 [20]—have renewed interest in reprocessing strategies that serve both economic and environmental objectives. These strategies include the production of alternative materials such as ceramics, cements, and bricks [21–26], as well as the recovery of strategic metals [27–29]. Technological advances in flotation efficiency [30, 31] and resource optimization [32] reinforce the technical feasibility of tailings valorization, supported by plant-scale evidence demonstrating economic viability [33].

Accurate resource estimation is a critical step in evaluating reprocessing potential. However, tailings deposits often exhibit poor spatial continuity due to operational history, material mixing, and deposition dynamics. These factors challenge the validity of classical assumptions such as stationarity [34, 35], rendering traditional geostatistical models less reliable. Although drilling campaigns provide essential compositional data [36, 17, 19], modeling efforts still rely heavily on interpolation techniques like inverse distance weighting (IDW) and ordinary kriging [37–40], despite recognized limitations in spatial accuracy and resolution [41].

Efforts to improve these estimates have included cokriging, sequential Gaussian simulation [42], and transitive kriging [35], with some incorporating economic analysis [27, 43]. Nonetheless, the use of machine learning regression models for resource estimation in tailings remains limited, especially for datasets derived solely from vertical boreholes. Similar comparative studies have demonstrated that machine learning models can outperform traditional estimators in borehole-based grade prediction when using geophysical and geospatial features [44]. This includes the development of intelligent borehole simulation tools in Python, which have shown accurate results with similar input configurations [45]. Other studies have also compared multiple metaheuristic and neural network approaches for grade estimation, emphasizing the importance of benchmarking ML performance under diverse geological conditions [46]. This gap is surprising given the success of ML models in related applications, such as predicting mechanical properties [47–49], fines content [50], or metal grades using geochemical and remote sensing data [51–53]. Notably, silver grade prediction using advanced algorithms such as Cuckoo Search has shown promising results when integrated with geophysical datasets [54].

Recent reviews by Cotrina-Teatino and Marquina-Araujo [55] have highlighted the expanding role of ML in tailings modeling and the need for further exploration of its capabilities in spatial estimation. In this study, we address this gap by posing the question: Can supervised machine learning models accurately and reliably estimate remaining metal resources in a tailings deposit characterized by low spatial continuity and limited sampling density?

To answer this, we apply three ML models—Random Forest (RF), k-Nearest Neighbors (KNN), and Extreme Gradient Boosting (XGBoost)—to a dataset of 927 composited samples from vertical drillholes in the Quiulacocha tailings deposit in central Peru. We compare their predictive performance with ordinary kriging through rigorous cross-validation and provide a 3D spatial modeling framework for resource estimation under challenging geostatistical conditions.

The structure of the paper is as follows: Section 2 describes the location, geology, and mineralogy of the Quiulacocha tailings deposit; Section 3 details the methodology and modeling framework; Section 4 presents the results; and Section 5 offers the conclusions.

2. Location, geology, and mineralogy of the Quiulacocha tailings deposit

This study draws on a geochemical–geospatial survey of the Quiulacocha tailings deposit, situated in the Pasco Department of central Peru (Figure 1). The site lies at >4,300 m a.s.l. on the Eastern Cordillera of the central Peruvian Andes, within the Cerro de Pasco mining district, one of the most important polymetallic provinces of the Central Andes.

Regionally, stratigraphy comprises a carbonate platform of the Pucara Group (Upper Triassic–Lower Jurassic limestones), overlain by volcanic and intrusive rocks emplaced during the late Oligocene to early Miocene. The magmatic–hydrothermal evolution includes dacitic domes and porphyritic intrusions that generated Cordilleran-type epithermal systems (Figure 2).

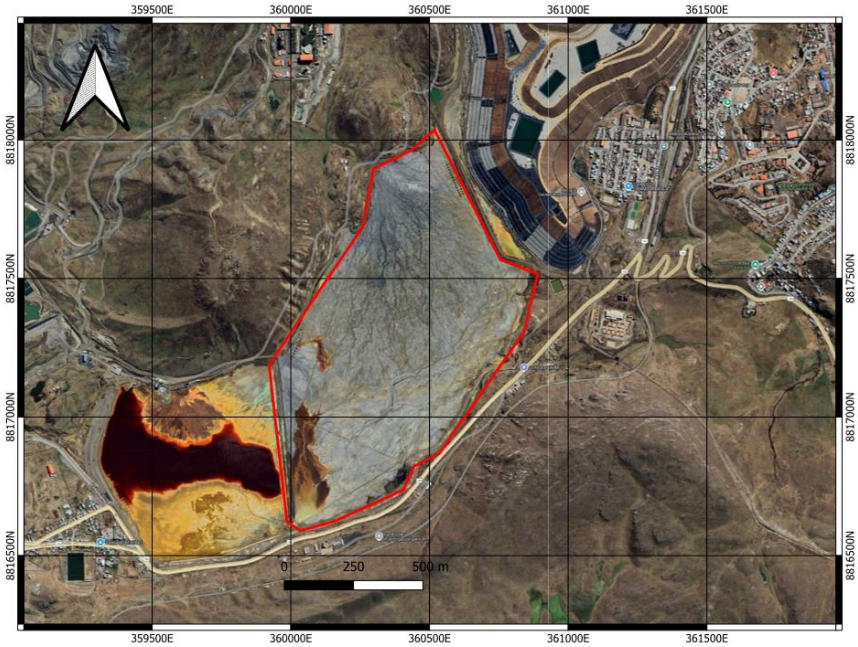

Figure 1. Location map of the Quiulacocha tailings deposit within the Cerro de Pasco district (central Peru).

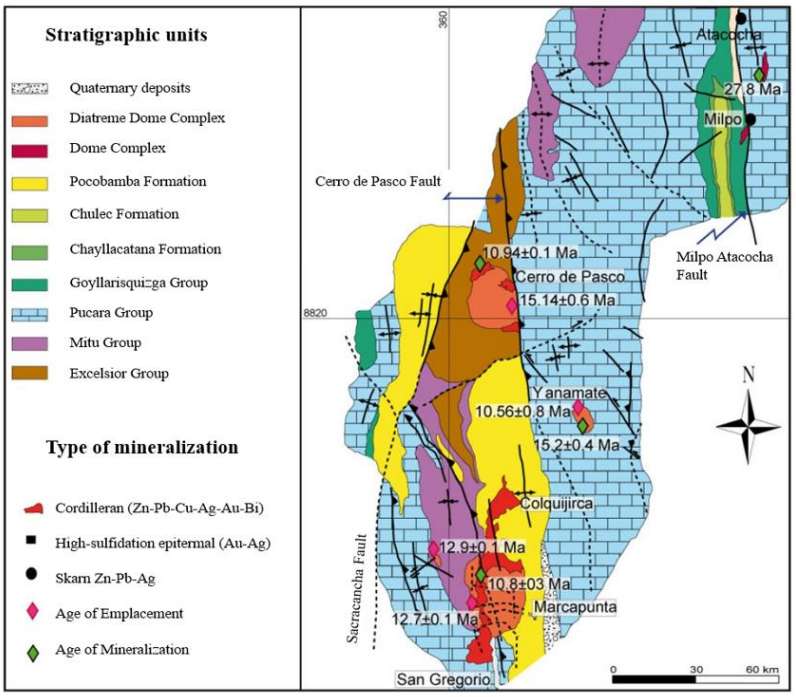

Figure 2. Regional geological and metallogenic framework of the Cerro de Pasco area, highlighting major stratigraphic units, fault systems, and mineralization types.

The Cerro de Pasco deposit is a polymetallic epithermal system genetically linked to porphyry intrusions. Mineralization occurs in veins, replacements, and stratiform mantos, with assemblages dominated by pyrite, sphalerite, galena, and enargite, commonly enriched in Ag and Cu, and locally accompanied by Bi, As, and Sb. A characteristic proximal–distal metallogenic zonation is observed, with Cu-rich cores grading outward into Pb–Zn–Ag domains.

The Quiulacocha facility contains approximately 70 Mt of historical tailings distributed over approximately 115 ha. Deposition began with early exploitation of the Cerro de Pasco mine (initially intermittent since the 17th century) and continued continuously from the early 20th century. Early tailings derived from Cu–Ag–Au processing reportedly contained up to 10% Cu, 4 g/t Au, and >300 g/t Ag; later deposition reflected Zn–Pb–Ag ore bodies with average grades near 7.41% Zn, 2.77% Pb, and 90.33 g/t Ag. A more recent estimate (2012) reported approximately 2.9 Mt grading 1.43% Zn, 0.79% Pb, 43.1 g/t Ag, and 0.04% Cu.

This complex mineralogical and geochemical heterogeneity, inherited from shifting ore sources and processing circuits, makes Quiulacocha an apt natural laboratory for data-driven modeling. It supports delineation of geochemical domains relevant to environmental assessment and to evaluating the potential for resource recovery.

3. Methodology

The aim of this study is to estimate the remaining metal resources within a tailings deposit in central Peru by leveraging geochemical data obtained from systematic drilling. The workflow begins with an exploratory analysis of borehole samples to clean the dataset, identify outliers, and assess the statistical distribution of key variables. Two modeling strategies are employed: a traditional geostatistical approach and a machine learning-based framework. For the geostatistical method, a variogram is constructed and fitted following the guidelines described in Chilès and Delfiner [56], and a three-dimensional block model is generated using ordinary kriging (OK) to interpolate silver grades across the deposit. In parallel, supervised machine learning models—Random Forest, k-Nearest Neighbors, and Extreme Gradient Boosting—are trained to predict silver concentrations based on spatial coordinates and, where applicable, spatial continuity metrics. Model hyperparameters are tuned to optimize performance, and outputs are used to construct a 3D resource block model analogous to that produced via kriging. The predictive performance of each model is evaluated using leave-one-out cross-validation (LOOCV), enabling a rigorous comparison of estimation accuracy, precision, and overall fit. This comparative assessment encompasses both quantitative error metrics and qualitative aspects related to grade continuity, distribution, and high-value zone identification.

3.1. Database description

This study utilizes data from an exploration campaign at the Quiulacocha tailings impoundment in the Pasco region of the central Peruvian highlands. The facility covers approximately 115 hectares and contains about 70 million tonnes of historical tailings derived from open-pit and underground operations at Cerro de Pasco. Early 20th-century deposition occurred during Cu–Ag–Au processing, with reported grades up to 10% Cu, 4 g/t Au, and over 300 g/t Ag; subsequent phases reflected Zn–Pb–Ag ore processing, averaging 7.41% Zn, 2.77% Pb, and 90.33 g/t Ag. A 2012 assessment (BO Consulting) reported approximately 2.9 million tonnes at 1.43% Zn, 0.79% Pb, 43.1 g/t Ag, and 0.04% Cu. The tailings materials are dominated by sulfides with arsenic-bearing phases, iron oxides, lead, and other residual compounds from historical processing.

Deposit characterization was carried out with 40 vertical drillholes on a near-regular grid of ~100 m spacing (Figure 3a). In total, 927 one-meter composites were collected from collar to the basal layer, capturing the full vertical extent of the column, with a maximum drilled thickness of 36 m (Figure 3b). The surveyed footprint spans approximately 589 m in the east–west direction and 1,035 m north–south.

Each composite includes multi-element geochemistry. For the present analysis, silver (Ag) grade is the target variable. Associated attributes include easting, northing, depth relative to the collar, and a unique borehole identifier. Although data for Zn, Pb, Cu, Au, Ga, In, Fe, and other elements are available, they are not considered here. The distribution of Ag grades (Figure 4) is right-skewed with a long upper tail, indicative of high-grade outliers. Across the 927 samples, the mean is 51.62 g/t (range 4.75–168.00 g/t), with a standard deviation of 12.63 g/t (variance 159.64), consistent with moderate dispersion.

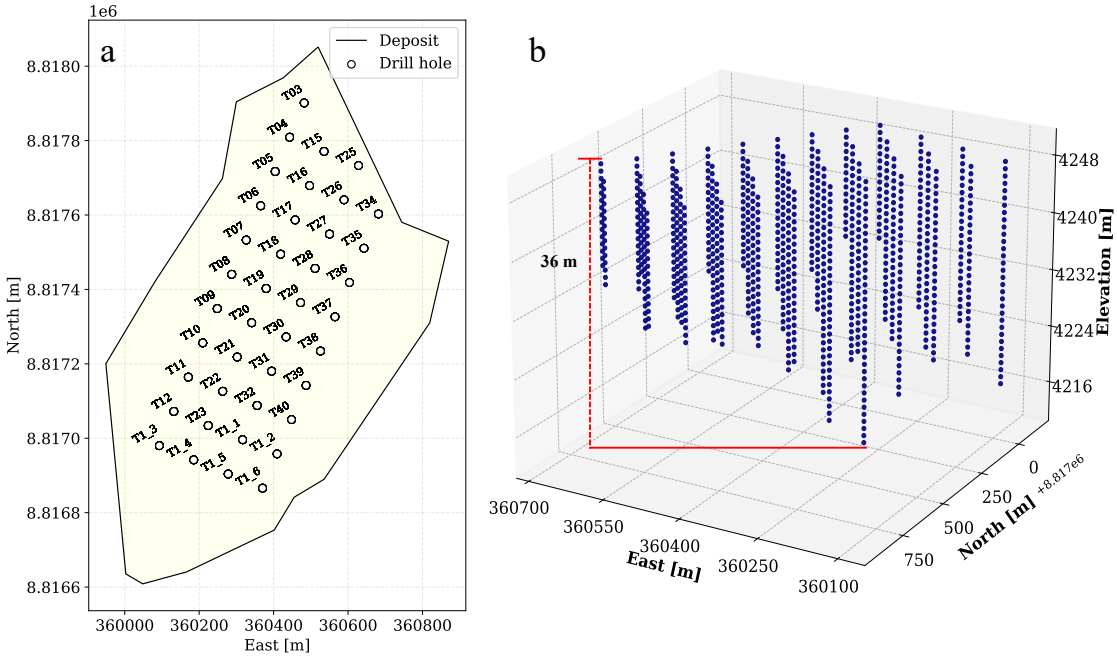

Figure 3. Geometry of the Quiulacocha tailings deposit with associated drillholes. (a) 2D view. (b) 3D view

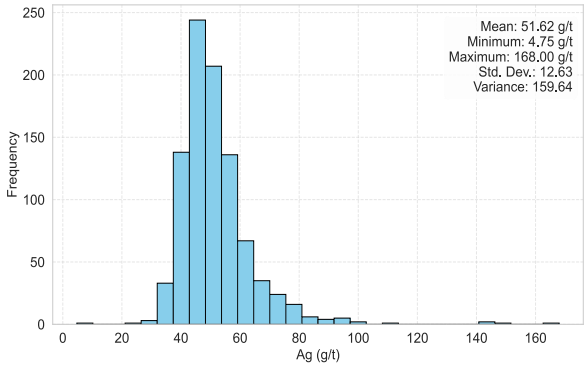

Figure 4. Histogram of composited Ag grades in the Quiulacocha tailings deposit

3.2. Machine learning models employed

To predict silver grades based on geochemical drillhole data, three supervised machine learning algorithms were implemented: Random Forest, k-Nearest Neighbors, and Extreme Gradient Boosting. These non-parametric regression models are well established in geosciences for their capacity to capture non-linear spatial patterns and manage datasets with complex structures and skewed distributions [57-63]. The models were selected based on three primary criteria: (1) their robustness against overfitting in high-variance datasets, (2) their flexibility in modeling spatial dependencies without relying on parametric assumptions, and (3) their proven efficacy in geological applications involving sparse or irregular sampling. The input features used in all machine learning models consisted exclusively of the spatial coordinates X, Y, and Z, corresponding to the easting, northing, and depth of each sample. The response variable was the silver concentration in grams per ton (Ag, g/t).

Prior to training, the predictor variables (X, Y, Z) were standardized using z-score normalization to ensure numerical stability and improve training convergence, particularly for distance-based models such as k-Nearest Neighbors. The silver grade was used as the target variable in raw form for tree-based models (Random Forest and XGBoost), while a normal score transformation was also tested to evaluate its impact on model behavior. Models were trained using leave-one-out cross-validation (LOOCV), a rigorous validation approach in which each sample is sequentially excluded from the training set and predicted as a test case. Model performance was evaluated using a comprehensive set of metrics: mean error (ME) to assess bias, standard deviation of residuals (SD) for precision, root mean squared error (RMSE) to capture both variance and magnitude of prediction errors, mean absolute error (MAE) as a robust measure of average deviation, and the Pearson correlation coefficient (R) to evaluate goodness-of-fit between observed and predicted values.

Before implementing the models, the data was transformed into a structured training table, where each observation is represented by a vector $x_i \in \mathbb{R}^d$ containing spatial coordinates (X, Y, Z) and additional variables, and a corresponding output $y_i \in \mathbb{R}$ representing the silver grade. No logarithmic transformations or normalization were applied to the dependent variable, as ensemble and

tree-based models can handle raw values as part of the exploratory analysis. Formally, the dataset is defined as:

$$D = \{(x_i, y_i)\}_{i=1}^{n}, \quad (1)$$

and the objective is to find a predictive function $\hat{f}$ that minimizes the mean squared prediction error:

$$\hat{f} = \underset{f}{arg\,min} \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 \quad (2)$$

Random Forest: An ensemble model that combines multiple decision trees built on random subsets of data and variables [53]. The prediction is obtained by averaging the outputs of the trees:

$$\hat{f}_{RF}(x) = \frac{1}{T}\sum_{t=1}^{T} f_t(x) \quad (3)$$

k-Nearest Neighbors: A similarity-based model in which the value of an unknown observation is estimated as the average of the k closest observations [63]:

$$\hat{f}_{KNN}(x_0) = \frac{1}{k}\sum_{j \in N_k(x_o)} y_j \quad (4)$$

Extreme Gradient Boosting: A sequential boosting method that builds trees additively by optimizing a regularized objective function [59]:

$$\mathcal{L} = \sum_{i=1}^{n} l(y_i, \hat{f}(x_i)) + \sum_{k=1}^{K} \Omega(f_k) \quad (5)$$

To enhance the predictive capability of the models, spatial continuity of the deposit was incorporated through an additional variable derived from the fitted variogram model. Specifically, a function $\Gamma(x_i)$ was defined to represent the local spatial structure around each point:

$$\Gamma(x_i) = \gamma(\|x_i - x_j\|, j \in \aleph_1(x_i)) \quad (6)$$

where $\gamma(h)$ is the fitted variogram function, and x_j is the nearest sampling point to x_i. This variable was included as an additional feature in the extended input vector.

For all estimation methods, predictions were extended to a three-dimensional block model with a resolution of 10 × 10 × 2 meters. Predictions were made for the centroid of each block using the final fitted models. For models trained in normal-score space, predictions were back-transformed using quantile mapping to recover values in the original Ag grade scale. The final block model includes estimated silver concentrations for each of the three machine learning models and for ordinary kriging, allowing direct comparison across methods.

4. Results and discussions

Spatial estimation was performed using both ordinary kriging and machine learning models, with silver grade as the target variable. This section presents the results in three parts: kriging-based estimation, machine learning predictions, and a comparative assessment based on cross-validation metrics.

4.1. Ordinary kriging prediction

The spatial continuity of silver concentrations was analyzed through variogram modeling using the gstools package in Python 3.11.11. An omnidirectional experimental variogram was constructed with a lag interval of 50 meters, 15 lags, and an angular tolerance of 25°, reflecting the spatial configuration and anisotropy assumptions of the composited dataset. The best-fitting theoretical model was exponential, with parameters: nugget = 0.05, sill = 1.10, and range = 400 meters (Figure 5). While the fitted model presents a relatively low nugget effect, this was supported by the dense vertical sampling interval (1 m composites) and the observed continuity of Ag grades in the drillhole data. The decision to adopt a low-nugget configuration was further validated through sensitivity testing, where models with larger nugget terms led to underestimation of high-grade zones and decreased interpolation performance. As such, the selected variogram prioritizes model fidelity to empirical variance while maintaining geostatistical consistency.

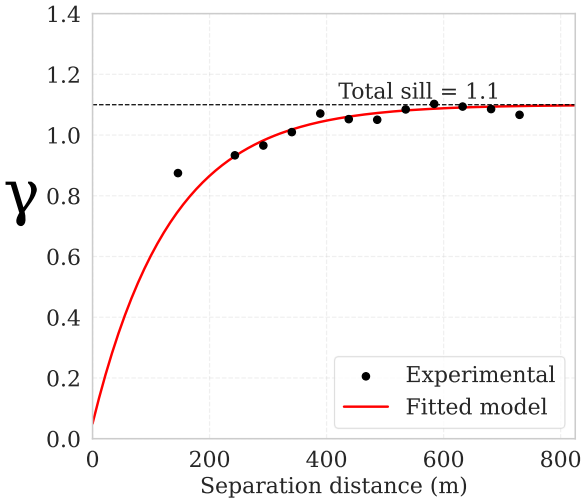

Figure 5. Variogram of silver grade used for estimation with ordinary kriging.

To verify the assumption of isotropy, directional variograms were computed in normal-score space along multiple azimuths (0°, 45°, 90°) and in the vertical direction. All directions yielded identical parameters (nugget = 48.368, sill = 1.74, range = 0), confirming the absence of anisotropy. Given the limited lateral support of the borehole dataset and the consistent behavior across all directions, the use of an omnidirectional variogram was deemed statistically and geologically appropriate.

4.2. Prediction using machine learning models

All models were trained and validated using a total of 927 composite samples, each corresponding to a 1-meter interval obtained from vertical drilling. Instead of employing a conventional training/testing split, we used leave-one-out cross-validation to assess model performance. This approach ensures that each individual sample is excluded once from the training set and used as a test case, providing a robust and unbiased estimate of predictive capability. LOOCV is particularly well suited for datasets of moderate size, where maximizing data utilization for training is crucial. The same LOOCV protocol was consistently applied across all machine learning models to ensure a fair comparison.

To estimate silver grades, machine learning models were implemented using standard hyperparameter configurations: RF ($n\_estimators = 100$), KNN ($n\_neighbors = 8, weights = \text{“}distance\text{”}$), and XGB ($n\_estimators = 100, max\_depth = 6, learning\_rate = 0.1$). Spatial continuity was incorporated by using only the spatial coordinates (X, Y, Z) as predictor variables, allowing each model to account for spatial structure according to its internal logic: via random partitioning (RF), metric proximity (KNN), or nonlinear feature interactions (XGB). See Table 1 for further details.

Table 1. Hyperparameters configuration of the machine learning model used

Model	Hyperparameters	Value	Spatial continuity consideration
RF	n_estimators	100	Incorporated implicitly through tree-based random partitioning of spatial data
	random_state	42	
KNN	n_neighbors	8	Incorporated via the distance metric used to define neighborhood
	weights	“distance”	
XGB	n_estimators	100	Incorporated as input variables and captured via nonlinear interactions by boosted trees
	max_depth	6	
	learning_rate	0.1	
	random_state	42	

4.3. Method comparison

The predictive performance of the models was evaluated using leave-one-out cross-validation, employing five key metrics: mean error (bias), standard deviation of the error (precision), root mean square error (RMSE), mean absolute error (MAE), and Pearson correlation coefficient (R). These metrics provide a comprehensive assessment of model accuracy, variability, and overall fit. As shown in Table 2, the Random Forest (RF) model achieved the best overall performance, yielding the lowest bias (0.53), the lowest RMSE (7.21), the lowest MAE (3.85), and the highest correlation with observed values (R = 0.82). This indicates that RF not only delivers the most accurate point predictions but also minimizes large deviations in modeling heterogeneous variables such as ore grades. While KNN and XGBoost also demonstrate good performance, they exhibit higher dispersion.

Table 2. Cross-validation statistics for silver grade estimation using ordinary kriging and machine learning

Metric	OK	RF	KNN	XGB
Mean Error (Bias)	1.78	0.53	1.04	0.68
Standard Deviation of Error	10.32	7.20	7.80	8.45
Standardized Mean Error	0.17	0.07	0.13	0.08
Root Mean Squared Error (RMSE)	10.47	7.21	7.87	8.48
Mean Absolute Error (MAE)	6.34	3.85	4.17	4.56
Correlation (R)	0.63	0.82	0.80	0.75

Figure 6 shows the relationship between observed and predicted values. The RF model aligns more closely with the bisector line, indicating low bias and good calibration. KNN and XGBoost also demonstrate reasonable fits, although with greater dispersion at higher values.

Finally, one-way F-tests for variance were performed at a 5% significance level, confirming that the differences observed among the models are statistically significant. Overall, the results suggest that machine learning models, particularly Random Forest, offer a substantial improvement in metal grade estimation under conditions of low spatial continuity (see Table 3).

4.4. Remaining resources prediction

Based on the constructed models, a three-dimensional block model was generated with a resolution of 10 × 10 × 2 meters to estimate silver grades in the deposit, assuming an average density of 1.6 t/m³. The spatial distributions (Figure 7) show consistent patterns across methods, with greater local differentiation in the machine learning models, particularly XGBoost, which captures sharper grade contrasts in high-gradient areas.

To provide a clearer understanding of spatial trends and continuity, Figure 8 presents a three-dimensional visualization of the estimated silver grade block models for each method. The ML-based models demonstrate greater resolution in the vertical and lateral differentiation of grades compared with OK, highlighting their usefulness for delineating economically viable sub-domains within the tailings deposit.

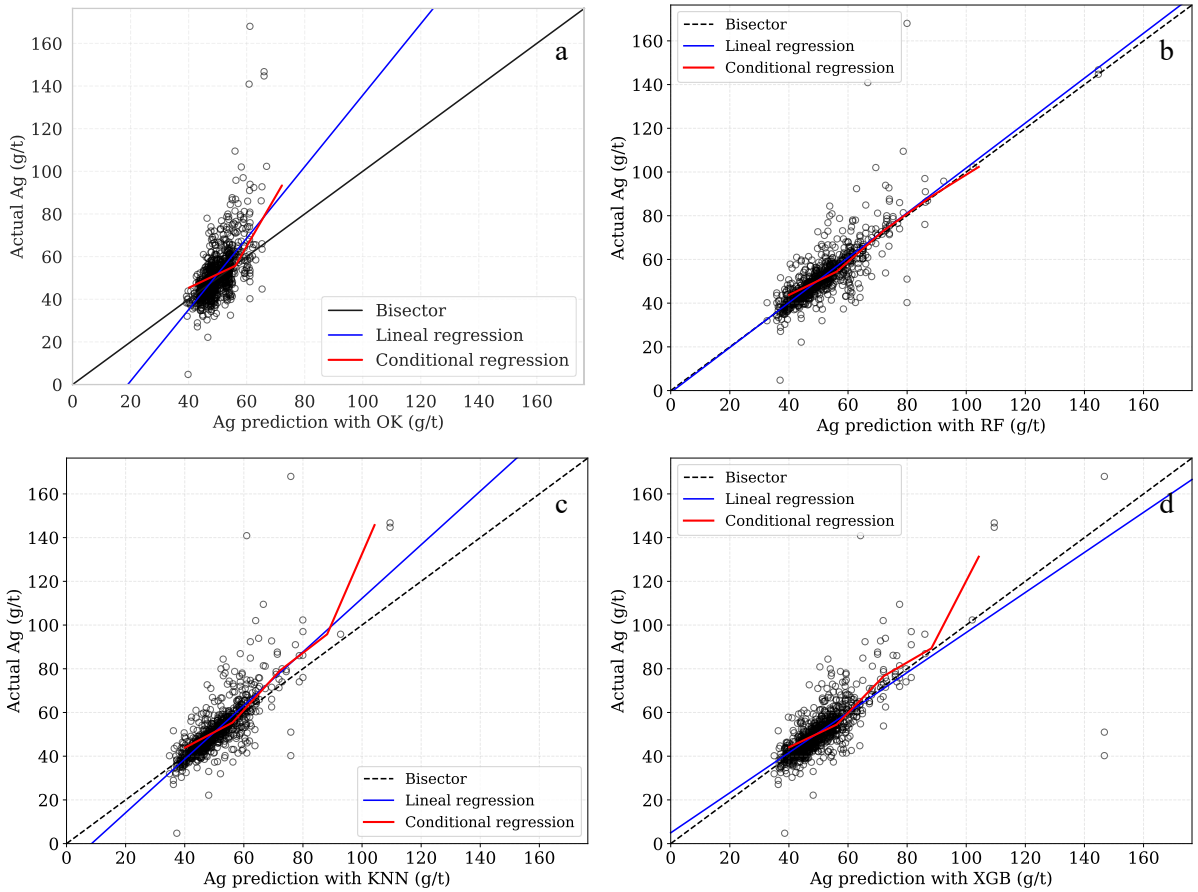

Figure 6. LOOCV validation of silver grade estimation using OK and machine learning models.

Table 3. Comparison of cross-validation error variances using one-way Fisher's F-test at a 0.05 significance level

Variable	Method	Error variance	F	F-critical	Significant difference?
Ag	OK	106.53	2.06	1.11	Yes
	RF	51.83			
	OK	106.53	1.75	1.11	Yes
	KNN	60.90			
	OK	106.53	1.49	1.11	Yes
	XGB	71.59			

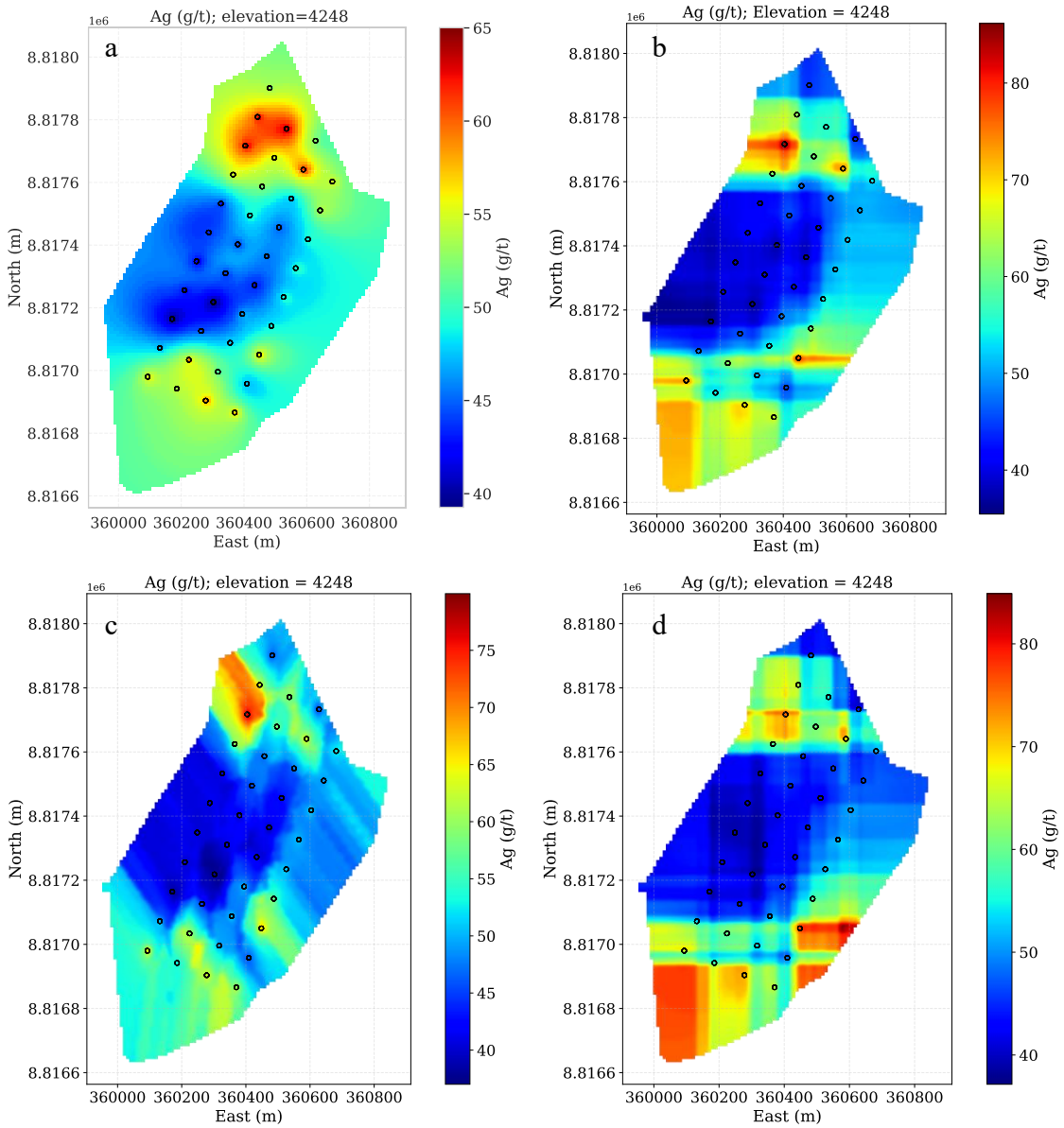

Figure 7. Silver grade estimation using OK and machine learning models. (a) OK, (b) RF, (c) KNN, (d) XGBoost

In volumetric terms, total resource estimates (Table 4) indicate that all machine learning models exceed the traditional approach in estimated metal content, with XGBoost reaching the highest value (1,542.16 t), followed by RF (1,532.86 t) and KNN (1,492.09 t). These differences reflect the higher sensitivity of non-parametric models in identifying high-grade zones. This is further supported by the frequency distributions (Figure 9), where the histograms for RF, KNN, and XGBoost display longer tails toward higher Ag values compared to the more centralized distribution produced by the traditional method.

Finally, tonnage versus average grade plots by cutoff value (Figure 10) show that the machine learning models maintain higher average grades across the full range of cutoffs without significantly compromising volume. XGBoost stands out for providing the best trade-off between grade and tonnage under stricter cutoff scenarios, positioning it as the most efficient model for identifying economically valuable zones within the deposit.

Table 4. Summary statistics of total predicted Ag resources for the Quiulacocha tailings deposit.

Resource	OK	RF	KNN	XGB
Mean (g/t)	49.55	51.89	50.51	52.50
Metal (t)	1,463.73	1,532.86	1,492.09	1,542.16
Difference (t)	-	69.13	28.36	78.43

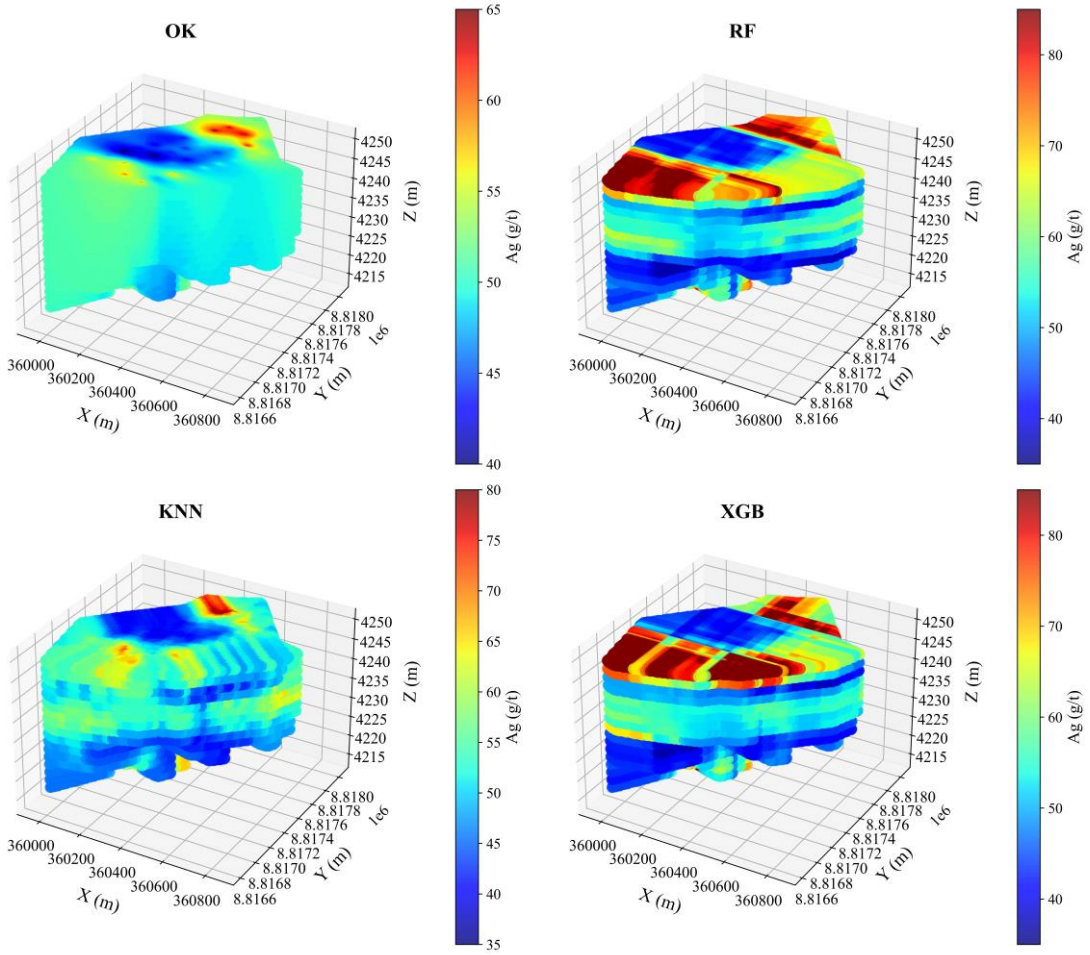

Figure 8. Three-dimensional visualization of the block models of silver grade (Ag, g/t) estimated using OK, RF, KNN, and XGB

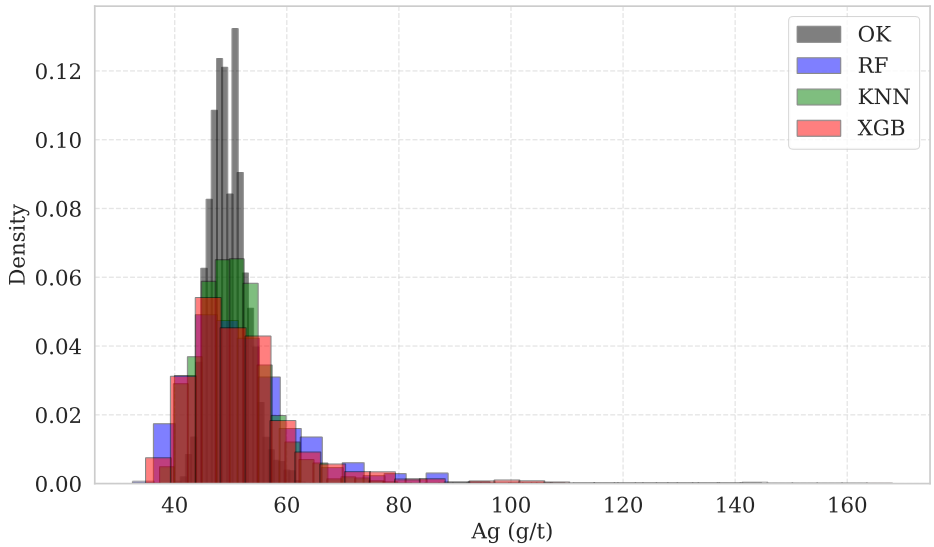

Figure 9. Summary statistics of total predicted Ag resources for the Quiulacocha tailings deposit

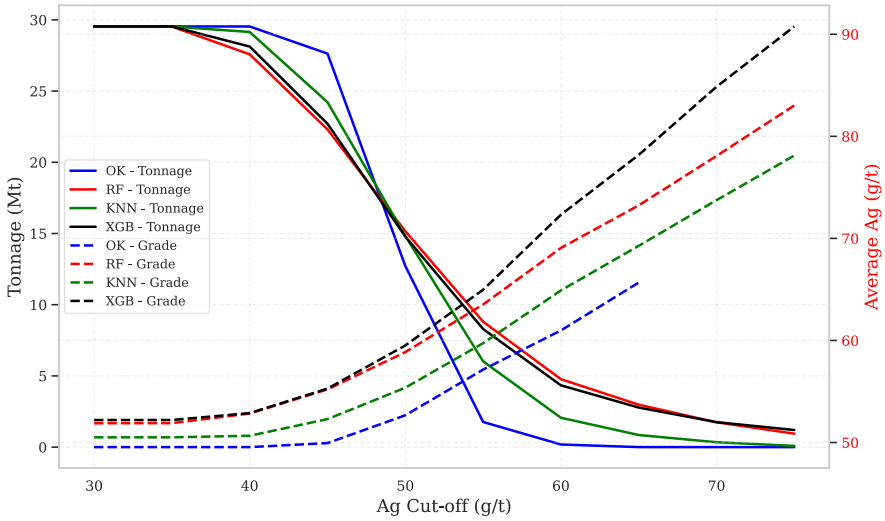

Figure 10. Tonnage vs. average grade by cutoff value for OK and machine learning models

4.5. Discussion

The cross-validation results demonstrate that supervised machine learning models can consistently outperform traditional geostatistical interpolation under the low spatial continuity conditions typical of tailings deposits. In this study, all three ML algorithms (RF, KNN, and XGBoost) yielded lower error variances and higher correlation coefficients than ordinary kriging, with Random Forest emerging as the best overall estimator. Under leave-one-out cross-validation (LOOCV), RF achieved the lowest RMSE (7.21 g/t), the lowest MAE (3.85 g/t), and the highest correlation with observed grades (R = 0.82), compared with RMSE = 10.47 g/t and R = 0.63 for OK. The standardized mean errors remained close to zero for all methods, indicating the absence of systematic bias, but the markedly lower dispersion of residuals for RF (error variance 51.83 versus 106.53 for OK) confirms a substantial gain in precision. These findings are consistent with recent comparative studies, where ensemble tree models and gradient boosting have matched or exceeded kriging in ore-grade prediction under complex spatial patterns [61-63, 64].

From a geostatistical perspective, the superiority of ML models in this setting can be linked to the nature of tailings deposits. As highlighted in previous works on tailings modelling, the combination of heterogeneous feed sources, changes in processing circuits, and hydraulic deposition processes often yields weak lateral continuity, high nugget effects, and vertically stratified structures that are difficult to represent with simple variogram models [35, 41]. In Quiulacocha, the omnidirectional exponential variogram and the low nugget adopted for OK provided a reasonable global fit, but the LOOCV results and the F-test statistics show that this model still fails to capture part of the short-scale spatial variability, particularly in high-grade intervals. By contrast, RF, KNN, and XGBoost learn non-parametric relationships between spatial coordinates and grade and can approximate complex spatial trends without enforcing strict second-order stationarity or linearity. This flexibility is particularly advantageous when data geometry (here, 40 vertical drillholes on a ~100 m grid) limits the robustness of classical variogram inference, as also reported for other tailings facilities and narrow, irregular deposits [35, 41].

The comparative behaviour of the three ML algorithms is also consistent with their theoretical properties and with previous applications in mineral resource estimation. RF yielded the most stable and accurate predictions, which can be attributed to its bagging-based ensemble structure and its ability to average over many decorrelated trees, thereby reducing variance while preserving non-linear relationships. XGBoost, in turn, achieved slightly higher metal forecasts and superior performance under strict cutoff conditions, reflecting its boosting strategy that iteratively focuses on hard-to-predict samples and can better resolve sharp local contrasts. Similar behaviour has been documented in Fe and Cu deposits, where XGBoost often produces higher-range grade estimates than kriging while maintaining acceptable smoothing and error statistics [61, 65]. KNN, as a purely distance-based method, showed competitive but slightly inferior results relative to RF and XGBoost, which is consistent with its sensitivity to sampling density

and local clustering: in a drilling configuration dominated by vertical profiles and relatively sparse lateral support, the definition of neighborhoods is strongly constrained by drill spacing and may lead to local over- or under-representation of high-grade composites.

The block-model results provide additional insight into how these methodological differences translate into resource estimates. At the 10 × 10 × 2 m resolution adopted here, all three ML models predict higher contained metal than OK, with increases of approximately 2–5% in total silver content (from 1,463.73 t for OK to 1,492.09–1,542.16 t for KNN and XGBoost). This uplift is not purely an artifact of global bias; mean errors remain small but are instead associated with the ability of RF and XGBoost to better preserve upper-tail behaviour observed in the composite data. The histograms of estimated grades show longer upper tails for the ML models, indicating a more faithful reproduction of localized enrichment zones that are partially smoothed out by OK. This pattern parallels observations in other studies where tree-based models and gradient boosting algorithms have shown greater sensitivity to high-grade clusters than kriging or inverse distance weighting, particularly in heterogeneous deposits with complex grade distributions [64, 66]. In the context of tailings reprocessing, such differences are critical, as project economics are often influenced by relatively small volumes of high-grade material.

The tonnage–grade curves by cutoff further illustrate this point. Across the full cutoff range, ML models maintain higher average grades than OK for similar tonnage, indicating a more favourable grade–tonnage trade-off. XGBoost performs especially well at elevated cutoffs, where it preserves higher grades while still retaining competitive volumes, suggesting its suitability for defining high-value subdomains or pilot reprocessing zones. Similar conclusions have been reported in recent works where boosting-based algorithms are used to delineate “sweet spots” for selective mining or retreatment within larger, heterogeneous systems [61, 65]. For decision-making, this implies that the choice of estimator (OK vs ML) can directly influence cutoff optimization, pit or panel design in tailings retreatment projects, and ultimately the classification of resources versus reserves.

At the same time, the present framework also highlights important methodological considerations and limitations. First, although LOOCV is a rigorous and nearly unbiased estimator of predictive performance, its application to spatially clustered data can still be optimistic because individual left-out samples may have neighboring points at very short distances in the training set. A stricter evaluation could involve blocked or spatial k-fold cross-validation, where clusters of samples (e.g., by drillhole or spatial blocks) are withheld together to better mimic future prediction conditions. Second, the models used here rely exclusively on spatial coordinates (X, Y, Z) and an optional spatial continuity feature derived from the variogram. This minimalist choice was deliberate to test how far coordinate-only ML can go under low continuity, but it ignores potentially informative variables such as Zn, Pb, Cu, Fe grades, mineralogical indicators, or physical properties (e.g., density, grain size, sulphide content), which have proven to be strong predictors in other multivariate grade estimation and tailings characterization studies [67-69]. Incorporating such variables could bring ML models closer to the role of multivariate geostatistical methods (e.g., cokriging or transitive kriging) in leveraging cross-correlations to improve estimates [35].

Another key limitation concerns uncertainty quantification. Conventional OK provides not only an estimate but also a model-based kriging variance that can be propagated into resource classification and risk analysis, whereas the ML models in this study are used in a purely deterministic fashion. Although cross-validation metrics offer an indirect measure of global uncertainty, they do not provide local conditional distributions or exceedance probabilities, which are important for classifying resources in accordance with reporting codes. Recent work has begun to address this gap by combining ML with geostatistical simulation, data augmentation, or ensemble-based prediction intervals in tailings contexts [70]. Extending the present framework to include quantile random forests, Bayesian boosting, or bootstrapped ensembles could provide local uncertainty measures without sacrificing the advantages of non-parametric spatial modelling.

Despite these limitations, the applied implications of the results are significant. In legacy tailings such as Quiulacocha, drilling campaigns are often constrained by cost, accessibility, and safety considerations, leading to sparse grids and limited lateral coverage. Under such constraints, ML offers a way to extract more predictive value from existing data, potentially reducing the need for very dense sampling solely to support variogram inference and kriging. Moreover, the methodology presented here is readily extendable

to other target variables (e.g., Zn, Pb, critical elements) and to integrated geoenvironmental parameters (e.g., acid-generation potential, leachable metals), enabling joint optimization of resource recovery and environmental risk management. This aligns with the emerging view of tailings as dual objects—simultaneously environmental liabilities and secondary resources—and complements recent geochemical and geostatistical studies that emphasize high-resolution characterization as a basis for both remediation and revalorization [41, 71]. Furthermore, recent studies in the Peruvian context have successfully applied machine learning to predict fuel consumption in haul trucks [72] or to optimize production in open-pit operations [73], reinforcing the versatility and operational relevance of ML in mining systems.

Finally, the broader relevance of this work lies in its contribution to sustainable mining and circular economy strategies. By demonstrating that data-driven ML models can provide technically sound, and in many cases superior, estimates of remaining metal resources in a complex tailings deposit, the study illustrates how digital and analytical tools can support the transition from linear "extract–use–dispose" paradigms toward circular reprocessing of mining wastes. This aligns with recent reviews highlighting tailings reprocessing, secondary resource recovery, and enhanced characterization as central pillars of circular economy implementation in the mining sector. In practical terms, coupling the type of ML-based resource models developed here with techno-economic evaluations, metallurgical testing, and risk assessments.

5. Conclusions

This study demonstrated the technical superiority of supervised machine learning models over conventional geostatistical methods for estimating silver grades and resources in a legacy tailings deposit with limited spatial continuity. Using 927 composite samples from 40 vertical drillholes in the Quiulacocha impoundment, models were trained solely with spatial coordinates (X, Y, Z) and evaluated using leave-one-out cross-validation. The Random Forest model achieved the best overall accuracy, with a mean error (bias) of 0.53 g/t, a standard deviation of 7.20 g/t, an RMSE of 7.21 g/t, and a Pearson correlation coefficient of 0.82, significantly outperforming ordinary kriging (RMSE = 10.47 g/t, R = 0.63).

The 3D block model results showed that machine learning models predicted higher total silver content than kriging: 1,532.86 t (RF), 1,542.16 t (XGBoost), and 1,492.09 t (KNN) versus 1,463.73 t (OK), assuming a bulk density of 1.6 t/m³. XGBoost also demonstrated greater efficiency under stricter cutoff grades, maintaining higher average grades across cutoff ranges, thus supporting its use for delineating high-value reprocessing zones.

These findings confirm the applicability of non-parametric machine learning models in complex geospatial settings where traditional variogram-based approaches underperform. The methodology is computationally efficient and extensible to other elements or environmental parameters. Future work should incorporate additional features (Zn, Pb, mineralogy, grain size) and uncertainty quantification techniques (quantile regression forests or ensemble bootstrapping) to improve prediction robustness and align outputs with international reporting standards for mineral resources.

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