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Localizing the Base Learner weights in Ensemble Methods to Improve the Grade Modeling Accuracy

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Abstract

Machine learning (ML) has significantly transformed multiple disciplines, including mineral resource evaluation in mining engineering, by facilitating more accurate and efficient estimation methods. Ensemble methods, as a fundamental component of modern machine learning, have emerged as powerful tools that robust techniques that integrate multiple predictive models to improve performance beyond that of any individual learner. This study proposes a novel ensemble method for estimating ore grades by localizing the base learner weights in ensemble method. Ordinary kriging, inverse distance weighting, k-nearest neighbors, support vector regression, and artificial neural networks have been used as the base learners of the algorithm. In ML base learners, coordinates (easting, northing and elevation) of samples have been defined as input nodes and grade has been defined as target. The proposed method has been validated for predicting the copper grade (Cu%) in Darehzar porphyry deposit. The performance of proposed method has been by individual base learners and famous ensemble methods. This comparison shows that performance of proposed method is better than other ones. The findings highlight the necessity of adapting ensemble methods to address spatial variability in geological data, thereby establishing a robust framework for ore grade estimation.

1. Introduction

Grade estimation is one of the most complex and crucial stages of mining engineering. The complexity of grade estimation, like many engineering challenges, arises from lack of data, uncertainty and the necessity of human decision-making [1]. Given that the accuracy of estimation is a key factor in decision-making for feasibility studies, production planning, and scheduling, grade estimation methods have evolved significantly in tandem with technological developments [2-3]. A study of global standardized reserve evaluation reports revealed that approximately 54% of cases utilized the Kriging method, as a geostatistical estimation technique, while 29.6% employed the distance weighting method for mineral grade estimation. The use of other methods was less than 10% [4]. The popularity of the Kriging method is largely due to its ability to minimize estimation variance and present Kriging variance as a criterion for assessing the uncertainty of estimates [5] . Although Kriging is a powerful estimation tool, it requires accurate assumptions about stationarity and statistical distribution, as well as sufficient knowledge and computational resources for proper application [5]. Recent advancements in machine learning algorithms (MLAs) have introduced new approaches to solving grade estimation problems [3,6-9]. Among these intelligent methods, artificial neural networks (ANNs) are the most widely used [10-12]. In an ANN, with a large number of samples, the output appears to be closer to the average value [13].

The first application of a hybrid method in grade estimation dates back to the development of the Neural Network estimation of the drift and Residuals Kriging (NNRK) system. The NNRK system combined ANNs with geostatistical

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methods. In this approach, the spatial variable of the deposit was considered as a combination of a long spatial trend component and a fixed regional component. Consequently, NNRK utilized ANN to model the large-scale structure (trend) and geostatistical methods to estimate the residual values. Next, Burnett [14] and Kapageridis [2] developed the GEMNet and GEMNet II neural networks by using neighboring information from samples as input parameters [2,14]. Dutta et al. [15] introduced another hybrid system for grade estimation by combining a kriging model with multiple ANN learners based on the Ensemble methods. They applied this system to estimate Al2O3% and SiO2% in a bauxite deposit, comparing its results with those of kriging and found that the performance of the hybrid system was not superior to Kriging [15]. Dutta et al. [8] developed another hybrid system that combined multilayer perceptron, support vector regression (SVR), and ordinary kriging models. In the literature, only basic (averaging) and generalized (weighted averaging) ensemble methods are used as combiners for base learners [16,17]. Application of these methods in grade estimation have the following basic limitations: 1) The efficiency of estimators is assumed to be constant across all regions, and 2) In deposits with varying zones, there is no change in weights even when the zone changes, which can be problematic. In parallel with the development of ensemble methods, studies have also been conducted in the field of application of metaheuristic optimizers to improve grade estimation, such as hybridizing the ML algorithms [12,18,19]. For example, Extreme Learning algorithm is hybridized with particle swarm optimizer to estimate the iron ore grade [18]. It is important to note that efforts have been undertaken in the field of integrating fractal methods with ML estimators to detect anomalies [1,13]. For example, such methods are used for soil geochemical anomaly detection in Sediment-Hosted Irankuh Pb-Zn Deposit [13].

In this study, we aim to investigate the impact of localized weight allocation across different sections on the composition of the base learners. Considering the suitability of averaging to combine base learners in the ensemble method, different estimators may exhibit varying performance across different regions, influenced by the spatial distribution of the samples. Consequently, applying uniform weights for all learners across all blocks is not suitable. To address this, each sample has been estimated using all estimators or base learners, and then all the blocks in the geological block model has been estimated using all learners. In the next step, the samples in each neighborhood within a specified radius have been identified, and based on the actual values of the samples in the neighborhood and the values estimated by all estimation methods, the weights for the base learners for each block have been determined. Finally, the estimated value for each block has been calculated. To validate the proposed method, it has been validated for grade estimation on a porphyry copper deposit.

2. Materials and Methods:

2.1. ANN

ANNs, which consist of a computational structure [20], are inspired by biological neural processing and incorporate some of the brain's capabilities such as pattern recognition and prediction. Similar to how the brain processes information in parallel through a network of "neurons", neural networks possess abilities that extend beyond traditional algorithmic programming and make them highly effective for nonlinear input-output data [21]. This characteristic of handling nonlinear data is what makes neural networks particularly appealing for estimating ore grades [8].

2.2. SVM

SVMs are divided into two groups [22]: Support Vector Classification (SVC) and Support Vector Regression (SVR). SVC is used to address classification problems [23] while SVR is employed for regression tasks. The SVM method, commonly referred to as Support Vector Regression due to its regression capabilities, is based on statistical learning theory (SLT) [24-26] and performs structural risk minimization (SRM).[27], SVR has a solid mathematical foundation and is robust against noise in measurements [28].

2.3. Ensemble Method

Unlike traditional learning methods that train a single model, ensemble methods involve training and combining multiple learning models. The individual models in ensemble methods are referred to as base learners. The performance of an ensemble model is significantly stronger than that of its base models. In fact, the appeal of ensemble models lies in their ability to enhance the performance of weaker learning models. Generally, the ensemble method consists of two steps: generating base learning models and

combining them to create a robust ensemble model. An ensemble model is particularly advantageous when there is disagreement among the predictions of individual members in the ensemble, meaning that the errors among these members are less correlated. Conversely, combining multiple models in an ensemble approach will yield little benefit if the prediction errors are highly correlated [15].Various methods have been proposed for combining base learning models. The most common of these is weighted averaging [29,30]. Other methods include non-linear approaches such as voting [31], which utilizes ranking information [32] , and the super Bayesian method [33].

Most methods developed in the literature of ensemble modeling combine base learners using averaging methods and weighted averaging methods. However, they have the following fundamental limitation:

1. The performance of estimators is assumed to be uniform across all regions, and even in the weighted averaging method, the weight assigned to a learner is a constant value.

2. When it comes to deposits with varying mineral zones, weights remain unchanged even when the zone shifts, which can pose significant challenges.

2.4. Base Ensemble Method (BEM)

This method offers a straightforward approach to combine the outputs of base learning models, where the ensemble output is simply the average of each component model's output. The output of the base group is defined as follows:

$$BEM(x)= \left(\frac{1}{N}\right) \sum_{i=1}^{N} f_i(\mathrm{x}) \quad (1)$$

where N is the number of base learning models in the ensemble, and f_i is the output of each ith base learning model. Although this approach does not consider the differences in performance among the underlying learning models, it remains easy to understand and implement.

2.5. Generalized Ensemble Method (GEM)

This method generalizes the BEM by assigning weights to each output of the base learning models to minimize the ensemble's mean squared error (MSE) as follows:

$$\mathrm{GEM(x)}= \sum_{i=1}^{n} w_i f_i(\mathrm{x}) \quad \text{Subject to: } \sum_{i=1}^{n} w_i = 1 \quad (2)$$

$$w_i = \frac{\sum_{j=1}^{n} c_{ij}^{-1}}{\sum_{k=1}^{n}\sum_{j=1}^{n} c_{kj}^{-1}}$$

$$e_i(x) = f(x) - f_i(x)$$

where c_{ij} is the correlation matrix=expected value of $[e_i(x)e_j(x)]$, $e_i(x)$ represents the network error, and $f(x)$ is measured value. The overall performance of the network using this method is superior to that of the BEM. In practice, errors tend to be highly correlated.

The rows of C in the matrix (equation (2)) are nearly linearly dependent, thus inverting C can lead to serious round-off errors.

2.6. Localized ensemble methods (LEM):

Most methods in ensemble modeling have utilized averaging (BEM) and weighted averaging (GEM) to combine base learners, which come with several fundamental limitations:

1. The spatial relation of the samples has not been considered. Given the nature of geological problems and the anisotropic characteristics of most deposits, this oversight can lead to errors.

2. In different areas of the region, various estimators may exhibit different levels of performance depending on the location of the samples.

In this research, LEM has been developed to solve these limitations. After training the base learners based on the training subset, the estimation error has been calculated using cross-validation and a correlation coefficient matrix. Then, the N nearest training data points to the target point has been detected and the weight of learners have been determined based on their performance in estimation of the N nearest training data. In other words, the ensemble weights have been determined based on the local variability of the estimates in the neighborhood of the estimation point. (Figures 1.a and b)

This method generalizes the GEM approach, differing in that the weights of the base learners for each block are determined based on the number of samples closest to the estimation block, for which the base learners exhibit the least estimation error. In the GEM method, all samples are assigned different weights during the estimation of each block based on their estimation errors. In contrast, the LEM considers the number of samples near each block, which can vary and is determined by the lowest estimation error of the base learner.

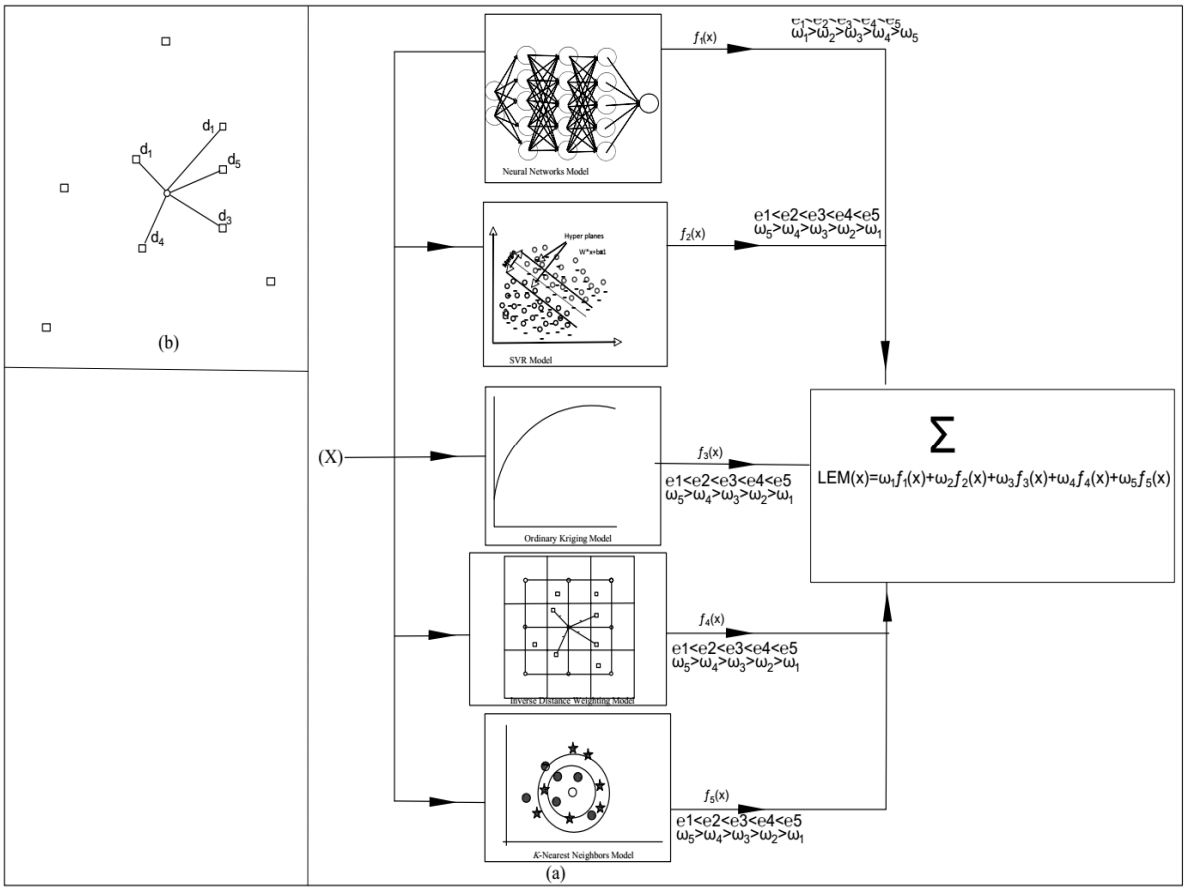

Figure 1. a) Basic framework of an ensemble model, and b) N nearest training data points to the target point (b).

3. Dataset

The developed ensemble model has been validated in Darehzar porphyry deposit. The deposit is located in the northeast of Sirjan in Kerman Province in Iran. Based on the 1:100,000 geological map of Pariz. The Darehzar porphyry copper deposit, along with the Sar Cheshmeh porphyry deposit and possibly the Nochun, Galleh Ghoochi, and other porphyry deposits, is situated within the Tertiary magmatic zone of Urmia-Dokhtar. The formation of the deposit is attributed to hydrothermal alteration associated with the intrusion of the Darehzar quartz monzonitic-granodioritic porphyry stock into mafic volcanic rocks. The hydrothermal alteration and Cu-Mo mineralization processes are concentrated within the Darehzar porphyry pluton, which dates back to the Miocene period, and extends to the surrounding basaltic country rocks [34-37]. Colored mélange and pre-Tertiary rocks are visible in the southern regions, situated at a considerable distance from the deposit. The Eocene-age formations, predominantly composed of volcanic-sedimentary rocks, are distributed throughout the northeastern areas [34,38,39] Most of the deposit has been formed in this porphyry stock, while some limited mineralization has also been seen in microdiorite to diorite and granodiorite dikes. A geological map of the area is presented in Fig. 2. Minerals in the deposit can be divided into sulfides, including pyrite, molybdenite, chalcopyrite, bornite, chalcocite, covellite, cubanite, chalcanthite and oxides containing malachite, azurite, tenorite, chrysocolla and goethite [34,38,39].

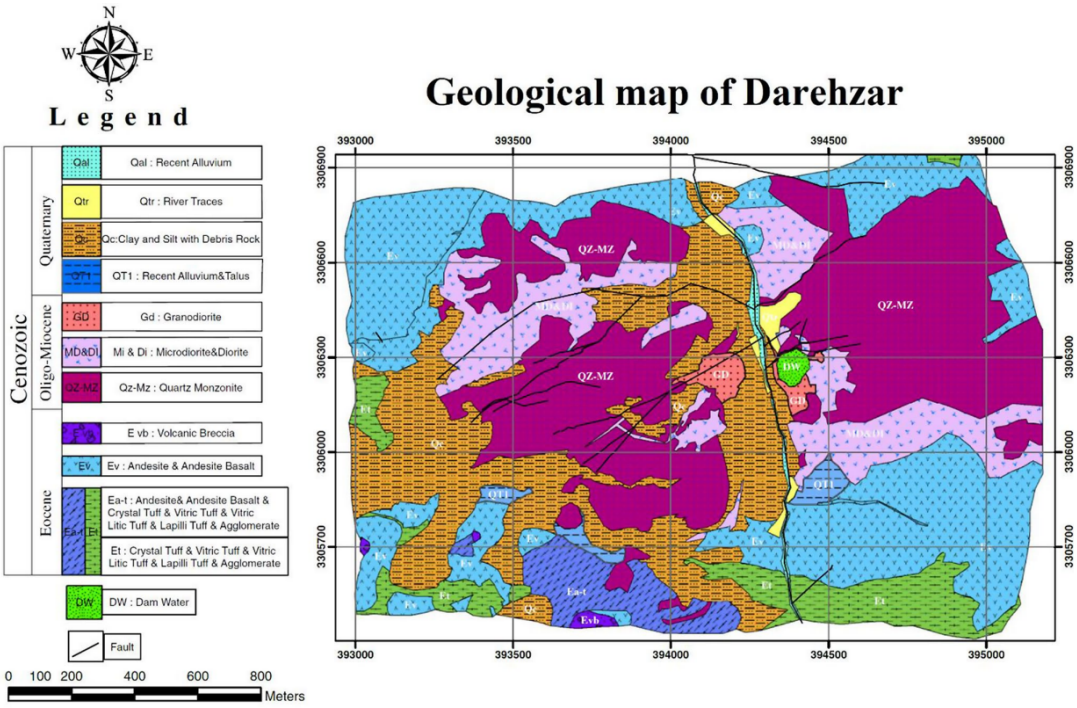

Figure 2. Geological map of the Darehzar porphyry copper deposit [39]

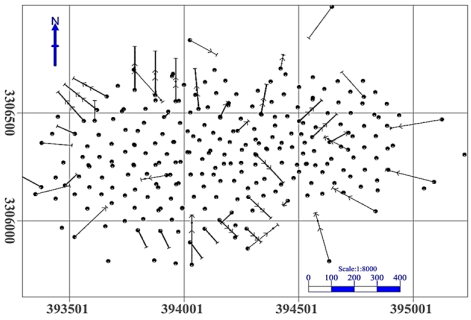

Figure 3. The pattern of exploratory boreholes in the Darehzar porphyry copper deposit

The dataset utilized in this study consisted of assayed samples taken from 168 exploratory boreholes drilled in the Darehzar deposit (Figure. 3). The data were collected in terms of easting (x), northing (y), and elevation (Z) coordinates, along with the percentage of copper (Cu%) for each drill hole. Since over 86% of the data belongs to the hypogene zone, this article focuses solely on modeling the grade within the hypogene zone. A detailed preliminary statistical analysis was conducted, including frequency distribution through histogram plots of the composited datasets. Summary statistics indicated that the mean and standard deviation values for Cu% were 0.23 and 0.23, respectively (table1). A visual examination of the histogram plots indicates that the Cu% data could be more accurately represented by a positive skewed distribution (figure 4). The dataset has been divided into training and validation subsets. Out of the 17,231 available data, 13,391 (75%) were used for training, and 3840 (25%) for validation. A detailed preliminary statistical analysis was conducted, including frequency distribution through histogram plots of the training, and validation composite datasets (Figure 4).

Table 1. descriptive statistics of Cu grade in Darezar deposit.

	Dataset	Train Subset	Test Dataset
Mean	0.23	0.23	0.23
Median	0.16	0.16	0.16
Mode	0.03	0.04	0.05
Standard Deviation	0.23	0.24	0.22
Range	2.08	2.08	2.08
Minimum	0.00	0.00	0.00
Maximum	2.08	2.08	2.08
Sum	3977.038	3109.46	867.57
Count	17229	13391	3838

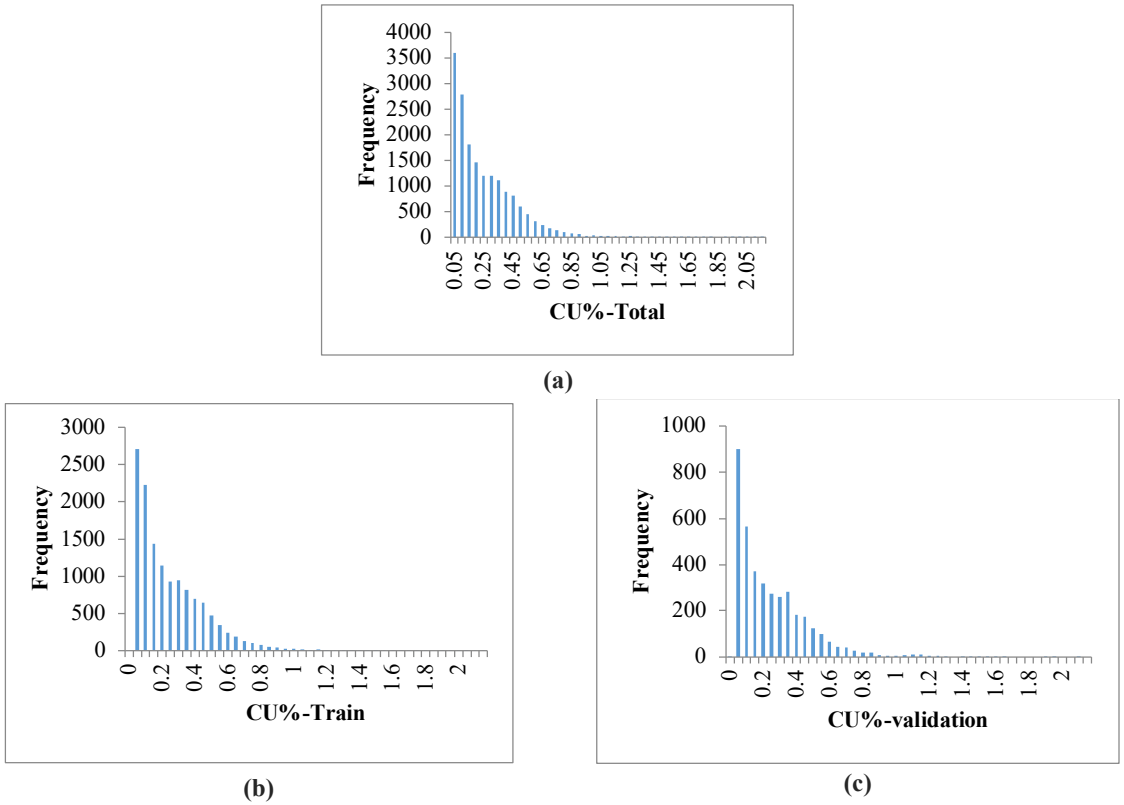

Figure 4. Histogram of Cu% grade in the dataset (a), train subset (b) and test subset (c).

3. Results and Dissections

Base learners (BPANN, SVR, OK, Inverse distance weighting (IDW) and *k*-nearest neighbors (KNN)), for the ensemble model were initially trained based on the training subset, which consisted of 13,391 samples. To generalize training procedure, 5-fold cross-validation was employed. For the ANN modeling, the hidden layer consists of five neurons. The selection of this number of hidden neurons was based on achieving the minimum generalization errors across trial-and-error method. The Levenberg-Marquardt backpropagation (LMBP) learning algorithm was utilized for the NN modeling. The remaining parameters of ANN architecture are presented in Table 2.

Among the available options for a kernel function of SVR, the Radial Basis Function (RBF) kernel was chosen. Also, the data was scaled under the assumption of a uniform distribution. In other words, the scaled value of each feature was calculated using the maximum and minimum values of that feature. Hyperparameters of SVR are ε, C, and σ. The optimal values for ε, C, and σ for this case study were determined using the grid search method, resulting in values of 0.002, 19483.96937, and 8, respectively.

One of the key inputs of OK is the variogram model. Accordingly, the experimental variogram of the data was calculated and a suitable model was fitted to it (Figure 5). As shown in Figure 5, a two-structure model has been fitted to this variogram. The nugget effect of this model was 0.12, sill of the first and second structures were 0.017 and 0.024, respectively. Also, the range of the first and second structures were 109 and 378 m, respectively. It should be mentioned that the power parameter in the IDW and K parameter in the KNN selected as 2 and 1, respectively.

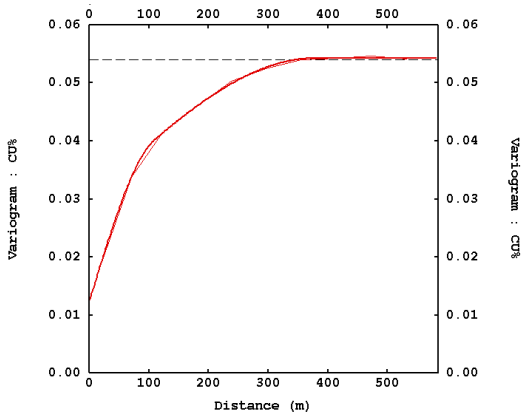

Figure 5. Experimental variogram of Cu% and fitted model to it.

After training the base learners (Figure 6), their performances have been evaluated based on the test subset (Figure 7 and Table 3). Table 3 shows that performances of these learners in estimation of Cu are weak, their *R* parameters are in the range of 45-62%. Also, their MSE and RMES are in the range of ~0.04-0.08 and ~0.17-0.28. The weakest learner is KNN and the best performance is related to ANN.

Table 2. Architecture of neural network model Cu

	Inputs	Number of hidden layers	Number of nodes; activation function hidden layer (1)	Number of nodes; activation function hidden layer (2)	Number of nodes; activation function hidden layer (3)
Model NN	x, y, z	3	5, tanh	5, tanh	5, tanh

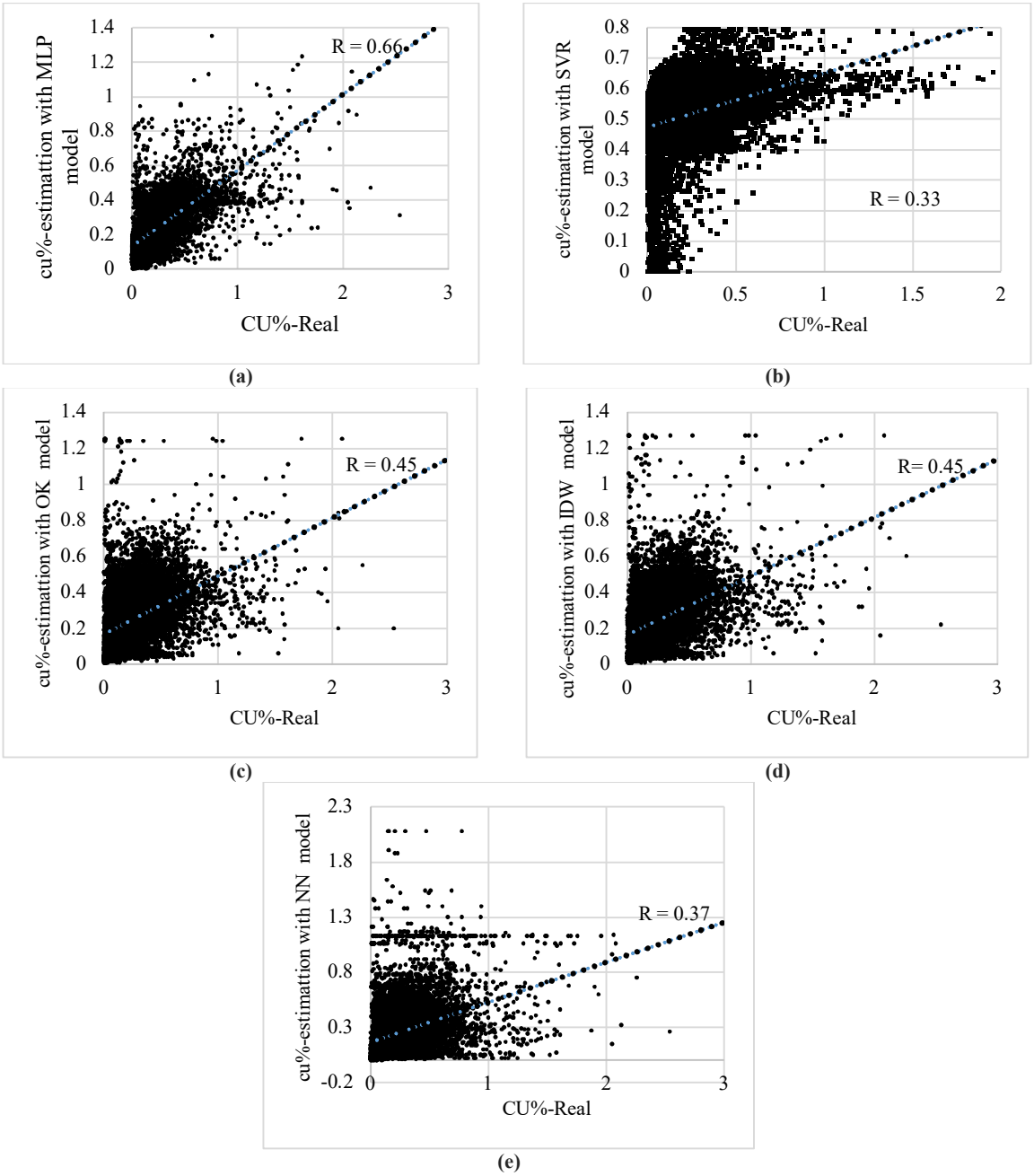

Figure 6. The ANN (a), SVR (b), OK (c), IDW (d) and KNN (e) model performance to predict the Cu grade in train subset.

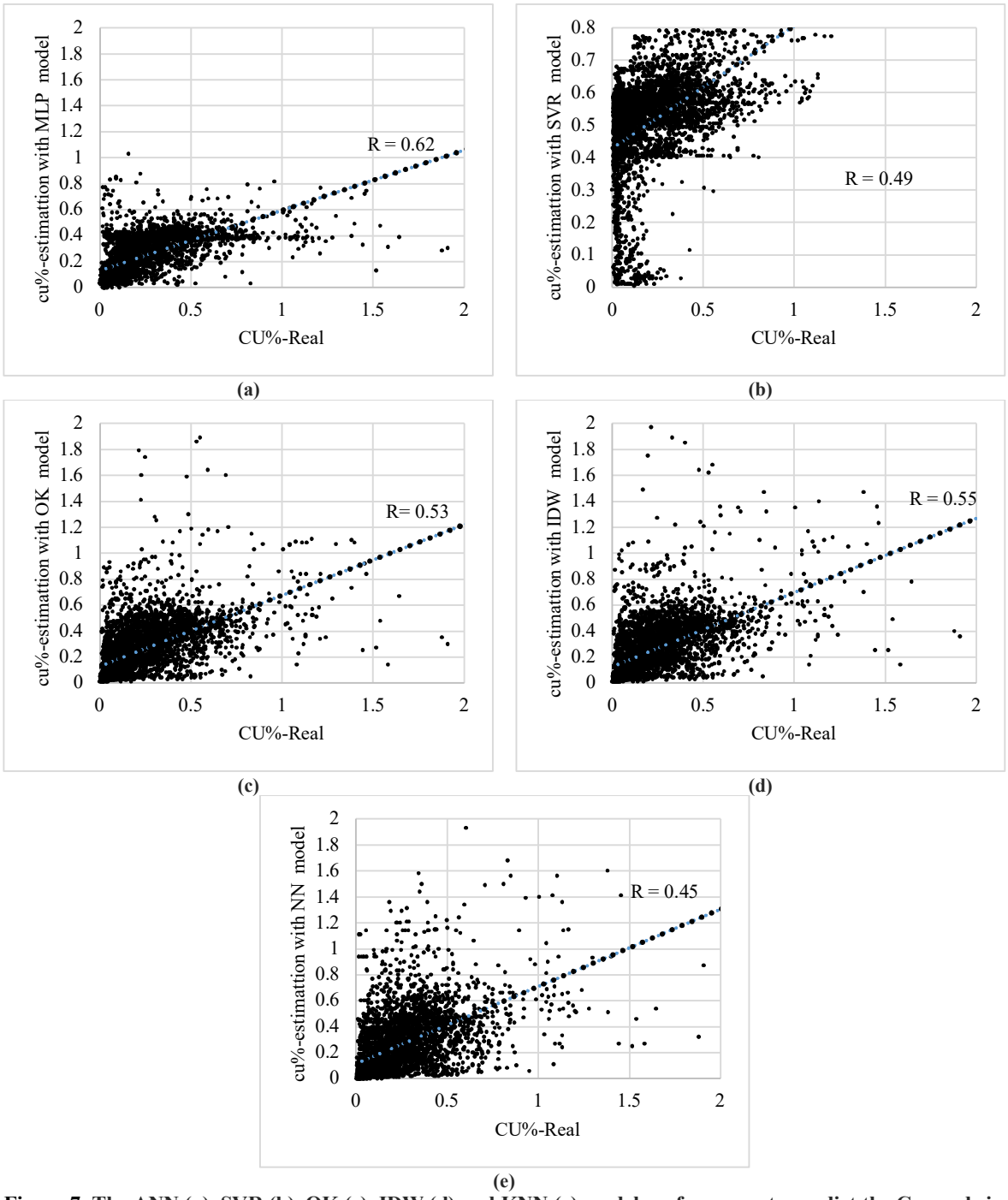

Figure 7. The ANN (a), SVR (b), OK (c), IDW (d) and KNN (e) model performance to predict the Cu grade in test subset.

Table 3. *RMSE* and *MSE* and *R* for test CU%

Base Learner	*MSE*	*RMSE*	*R*
KNN	0.076	0.276	0.45
IDW	0.048	0.219	0.55
OK	0.048	0.219	0.53
SVR	0.124	0.352	0.49
ANN	0.040	0.176	0.62

BEM ensemble of base learners developed based on equation 1. Similarly, its performance has been evaluated based on the test datasets (Figure 8.a and table 4). As can be seen, the performance of BEM is better than that of 4 of the base learners and has a 3% difference compared to ANN (as the best learner). Next, the ensemble network's error was assessed using three-dimensional validation

subset, that consist of 3,838 samples of boreholes. Following the estimation error derived from cross-validation and the correlation coefficient matrix, each validation point was estimated by combining the weights of the base learners. This was done using the ten training data points closest to the target validation point. Given that the true values of the validation data are known, the ensemble network's error was calculated and compared to the individual errors of each base learner. Then, the weights of base learners have been calculated based on the equation 2, and GEM ensemble model has been developed. The performance of GEM (Figure 8.b and table 4) is 4% more than BEM. Then, a .m Matlab script has been developed to calculate the LEM weights and LEM model has been calculated. The performance of LEM is summarized in Table 4. Also, the scatter plot of real and predicted values by LEM is presented in Figure 8.b. As can be seen, the performance of LEM has been better than that of individual base learners as well as BEM, and it could be concluded that localizing the base learners weights in ensemble method has yielded better results than each of the individual learners, BEM and GEM ensemble methods.

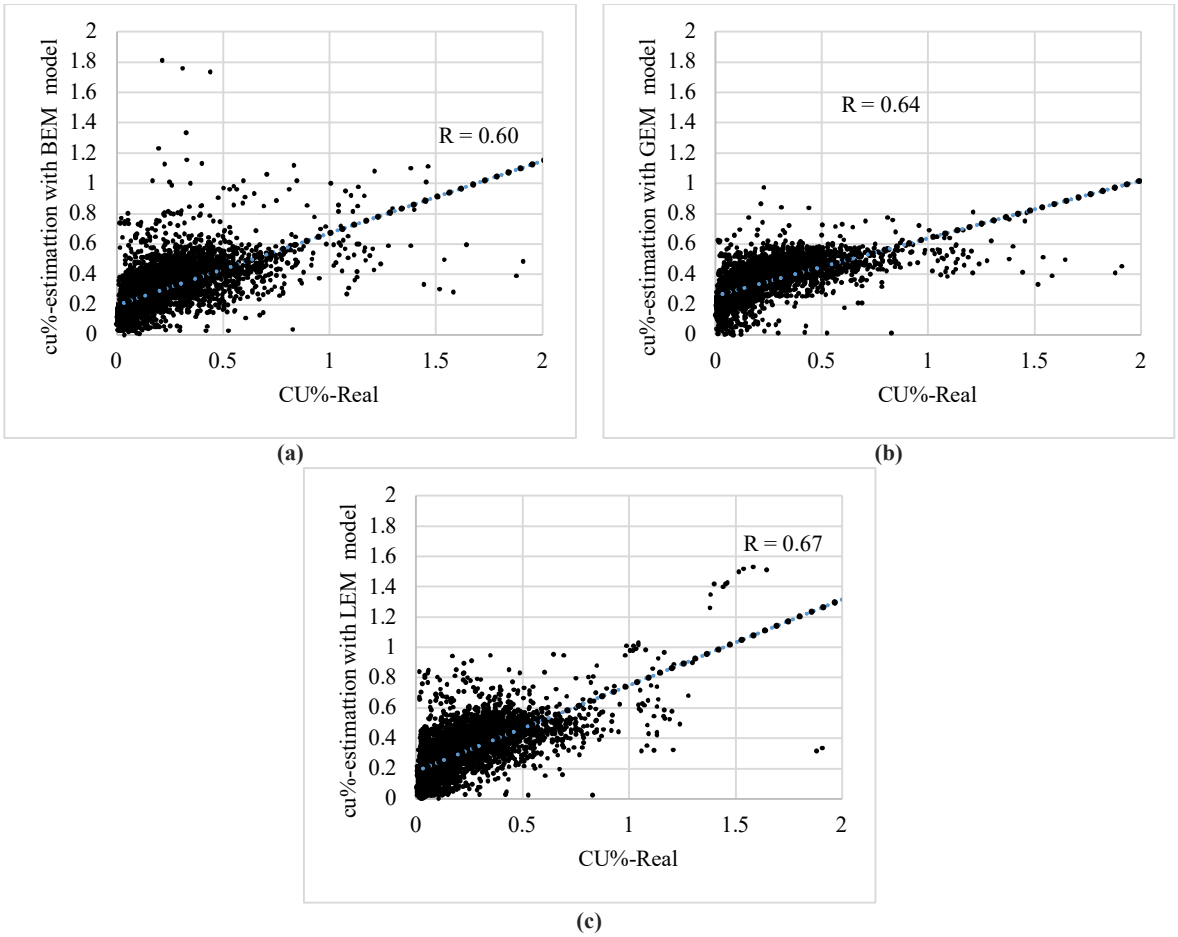

Figure 8. The BEM (a), GEM (b) and LEM(c) model performance to predict the Cu grade in test subset.

Table 4. *RMSE* and *MSE* and *R* for test dataset

	MSE	RMSE	*R*
BEM	*0.040*	*0.199*	*0.60*
GEM	*0.038*	*0.190*	*0.64*
LEM	*0.035*	*0.187*	*0.67*

4. Conclusions

This study demonstrates the significant advancements in ore grade estimation through the development of a novel localized ensemble methodology (LEM) that effectively addresses the limitations of traditional ensemble methods. By integrating various predictive models, including ordinary kriging, inverse distance weighting, k-nearest neighbors, support vector regression, and artificial neural networks, LEM enhances the accuracy of copper grade (Cu%) predictions in porphyry copper deposits.

The innovative aspect of LEM lies in its ability to localize the weights of base learners based on

their performance in the vicinity of the unknown estimation point. This localized approach allows for a more understanding of spatial variability in geological data, which is critical in mining engineering applications. The validation results, showing a correlation coefficient of 67% between estimated and actual grades, underscore the efficacy of this method compared to individual base learners and traditional ensemble techniques.

In general, the evaluation and comparison of the performance of various estimation methods should be based on criteria such as performance metrics and generalization, utilizing techniques like cross-validation. The results of this comparison in the present study indicate that, for this case study, the performance of machine learning-based methods is generally superior to that of classical methods. However, it is important to note that geostatistical methods, although less complex than machine learning approaches, require structural analysis that is often dependent on expert opinion. Consequently, the quality of their output is largely contingent upon the level of expertise of the practitioner.

The findings highlight the importance of adapting ensemble methods to account for the heterogeneity of mineral deposits, reinforcing the notion that a one-size-fits-all approach is insufficient in the context of grade estimation. By localizing weight allocation, LEM not only improves prediction accuracy but also contributes to more informed decision-making in resource evaluation and management. Future research should focus on further refining this methodology and exploring its applicability across diverse geological settings to enhance its robustness and reliability in mineral resource estimation.

It is important to note that one way to improve estimation accuracy is by enhancing the input space configuration. Given the lack of supplementary data for this area, only the coordinates have been used in the input space configuration. It is recommended that future studies investigate the impact of the availability of supplementary data, such as geophysical information, on the accuracy of estimates.

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محلی سازی اوزان محلی سازی ترکیب یادگیرنده‌های پایه در روش‌های انسمبل با هدف بهبود دقت مدل‌سازی عیار

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تخمین عیار
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چکیده

یادگیری ماشین با آسان سازی روش‌های تخمین دقیق‌تر و کارآمدتر، مباحث مختلفی، از جمله ارزیابی ذخیره معدنی، در مهندسی معدن را به طور قابل توجهی متحول کرده است. روش‌های انسمبل، که یکی از مؤلفه‌های اساسی یادگیری ماشینی مدرن هستند، به‌عنوان ابزارهای قدرتمندی، با ادغام چندین مدل تخمین پایه، بهبود عملکرد تخمین‌ها را تقویت می‌بخشند. در این مطالعه یک روش انسمبل جدید برای تخمین عیار کانسنگ با محلی سازی وزن‌های یادگیرنده پایه ارائه شده است. کریجینگ معمولی، وزن دهی معکوس فاصله، k-نزدیکترین همسایه، رگرسیون بردار پشتیبان و شبکه‌های عصبی مصنوعی به عنوان یادگیرندگان پایه این الگوریتم استفاده شده است. در مدل‌های پایه، مختصات (طول جغرافیایی، عرض جغرافیایی و ارتفاع) نمونه‌ها به عنوان ورودی و عیار به عنوان خروجی تعریف شده است. روش پیشنهادی، برای پیش‌بینی عیار مس در کانسار مس پورفیری درمزار، اعتبارسنجی شده است. این مطالعه نشان داد که عملکرد روش پیشنهادی بهتر از سایر روش‌های متداول انسمبل است. یافته‌ها، ضرورت توجه به تغییرپذیری محلی عیار در روش‌های انسمبل را برجسته نموده و مبنایی قوی‌تر برای تخمین عیار کانسنگ فراهم می‌آورند.

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