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Simulation-based mineral prospectivity modeling and Gray Wolf optimization algorithm for delimiting exploration targets

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ABSTRACT

Exploration targeting is a multi-step process concerned with delimiting progressively smaller areas that are prospective for the targeted mineral deposit type, capable of hosting a potentially economic deposit and deserving of exploration funds. In mineral prospectivity modeling (MPM), target delineation represents the final stage of a procedure designed to identify discrete, explorable areas of high discovery potential within a much larger area of interest, typically covering entire camps, districts or provinces. However, defining unbiased thresholds for discriminating between high, moderate and low priority exploration targets is not a straightforward task. To avoid human bias in this thresholding process, a more structured, automated approach is needed. This study presents a simulation-based approach to MPM that adapts the Grey Wolf Optimizer (GWO) algorithm, a swarm intelligence method capable of objectively delineating exploration targets from MPM results. Our approach aims to reduce bias by applying Monte Carlo Simulation to the assignment of robust weights to the predictor maps at the core of the MPM procedure. The GWO algorithm facilitates the classification and prioritization and enhances the accuracy and reliability of the resulting targets. The proposed procedure is demonstrated here using a porphyry copper (Cu) example from the Chahargonbad district, SE Iran. The results show that the GWO-based framework not only identifies high-priority exploration zones but also reduces the uncertainty inherent in traditional manual selection methods. As such, this novel approach contributes to both theoretical and practical advancements in the field of mineral exploration, offering a scalable solution that can be adapted to various geological settings.

1. Introduction

Given the significant decline in mineral discoveries over the last decade (Schodde, 2023) and low base-rate of discovery success (McCuaig et al., 2010; Yousefi et al., 2024a,b), effective management of risk and expenditure is critical in mineral exploration. Mineral prospectivity modeling (MPM) has emerged as a crucial tool in this endeavor, particularly in the early stages of camp- to regional-scale exploration activities (Carranza, 2008; Esmaeiloghli et al., 2019; McCuaig et al., 2010; Yousefi et al., 2019, Yousefi et al., 2021). MPM leverages predictive technologies to significantly reduce the exploration search space, thereby optimizing resource allocation. However, traditional approaches to MPM often involve manual intervention, which can introduce bias and reduce model reliability. This study aims to mitigate these issues via the Grey Wolf Optimizer (GWO) algorithm, a novel swarm intelligence method suitable for automating the task of optimizing the definition of MPM-derived exploration targets. The reason for having adopted a GWO approach lies in its success in overcoming complex optimization problems across different scientific fields, including engineering and geosciences. Unlike conventional methods such as logistic regression and weights of evidence (WoE), GWO offers a balance between exploration and mining, ensuring that a thorough search of the solution space is conducted while avoiding local optima. Overall, this study aims to demonstrate the effectiveness of GWO in improving the accuracy of mineral quantitative predictions, thereby providing a more robust framework for MPM. Several alternative

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algorithms and methods have been trialed in the context of MPM, including machine learning techniques and other swarm intelligence algorithms like Particle Swarm Optimization (PSO) and Ant Colony Optimization (ACO) (Zuo, 2020; Qin et al., 2021; Zuo and Carranza, 2023; Zuo et al., 2023; Shi et al., 2023; Mirzabozorg et al.2024). However, GWO was selected here as the method of choice due to its adaptability, simplicity of implementation, and its proven track record in achieving high optimization performance with fewer parameters to tune (Mirjalili et al., 2016). Our study, built around the strengths of GWO, explores the potential of this method to significantly improve the reliability of exploration targets generated in MPM.

Geological knowledge and mathematical frameworks are the cornerstones of MPM. The former is required for translating the critical ore-forming processes into mappable targeting criteria, which can be captured in predictor maps. These maps can then be weighted and combined in a mathematical framework for generating predictive maps of mineral prospectivity (Carranza, 2008; Joly et al.2012; Chen, 2015; Chen and Wu, 2016; Hagemann et al., 2016a,b; Yousefi et al., 2019, 2021, Yousefi et al., 2024a,b; Lou and Liu, 2023; Esmaeiloghli et al., 2024). Two general types of mathematical frameworks are employed in MPM: data- and knowledge-driven. The former approach lends itself well to brownfields environments, which contain numerous mineral deposits and occurrences and are data rich. The latter approach, on the other hand, is best suited to greenfields environments, which have few known mineral deposits and occurrences, or none, and are typically data poor (McCuaig et al., 2010).

Amongst the broad range of knowledge-driven mathematical frameworks available for MPM (Bonham-Carter 1994; Dubois et al. 2000; Porwal et al. 2003), fuzzy logic accounts for both the fuzziness and uncertain nature of geological features (Sadeghi and Cohen, 2023). Hence, it has been a method of choice in MPM (e.g., Sekandari and Beiranvand Pour, 2021; Mirzabozorg and Abedi, 2023). The effectiveness of fuzzy-logic-based MPM can be assessed as follows (Lisitsin 2015; Ghasemzadeh et al., 2019; Barak et al.,2023; Yousefi et al., 2024a,b): (i) how well does the model perform in terms of reducing the search space (i.e., the area occupied by exploration targets, A); and (ii) how well does the model predict and fit the known mineralization (i.e., the proportion of known mineralization matching the prospectivity model, F), where the effectiveness index, E, is measured by F/A (Kreuzer et al., 2010; Pirajno, 2010; Korsch and Doublier, 2016; Chen and Wu, 2017; Ghasemzadeh et al., 2019; Echogdali et al., 2021; Liu et al., 2023a,b).

Whilst MPM can help reduce the search radius in greenfields and brownfields terrains to a great extent, MPM results still require optimization as to reduce exploration uncertainties (Kreuzer et al., 2007; Harris et al., 2015; Liu et al., 2023a,b; Saremi et al.,2024; Hajihosseinlou et al.,2024; Wang et al., 2024). Swarm intelligence algorithms could be considered ideal to reach this purpose (Lin et al., 2021; Mostafaei et al., 2024). Many studies have been centered on optimizing fuzzy logic-based prospectivity models have been optimized by improving the effectiveness index (e.g., Nykänen et al., 2017). However, these studies have not used optimization algorithms. Our work is based on the premise that optimization algorithms can help to significantly improve the effectiveness index of fuzzy logic-based prospectivity models and, therefore, the modelling results.

This paper intends to bridge this knowledge gap by applying a metaheuristic algorithm known as GWO. The latter belongs to the family of swarm intelligence algorithms (Roshanravan et al., 2019; Lin et al., 2021; Mostafaei et al., 2024) whose origin lies in the strategies that living beings use to fulfill their needs like hunting, nesting, etc. Such algorithms are applied to solve complicated problems by providing rapid and rational solutions (Derrac et al., 2011; Cui and Gao, 2012). Swarm intelligence algorithms deal with high-value properties consisting of self-organization, parallel, distributive, flexibility, and robustness, and have been applied for problem-solving in various domains of science, in particular engineering problems (Parpinelli and Lopes 2011; Leboucher et al., 2012; Zhang et al., 2013). GWO has been widely used in a broad range of applications relevant to optimal power dispatch (Sulaiman et al., 2015), geoelectrical data inversion (Li et al., 2018), engineering design (Nadimi-Shahraki et al., 2021), network anomaly detection (Wang et al., 2023, Yang et al.,2023), wind speed prediction and reconstruction (Zhu et al., 2024) and estimation of battery charge and capacity (Lei et al., 2024).

In this study, we adapted the GWO algorithm to recognize and delimit porphyry copper (Cu) exploration targets using a set of independent mineral exploration variables derived from geochemical, geological, and structural data of the Chahargonbad district, Urumieh-Dokhtar Volcanic Belt, Iran. For comparative purpose, we also generated a logistic regression prospectivity model.

2. Study area, exploration criteria, and input data

The Chahargonbad district, located within the central Urumieh-Dokhtar Volcanic Belt of Iran, spans an area of approximately 2600 km^2. This NW-SE-trending Cenozoic magmatic arc is a key geological feature formed due to the subduction of the Arabian plate beneath central Iran during the Alpine orogeny (Derakhshani and Farhoudi, 2005; Moinevaziri et al., 2015; Azizi et al., 2019; Rezaei et al., 2022). The region is characterized by extensive Oligocene to Miocene dioritic to granodioritic intrusions, which are temporally and spatially associated with the formation of significant porphyry Cu deposits (Hezarkhani, 2006). These intrusions serve as both the heat and metal sources necessary for mineralization, driving hydrothermal fluid flow and subsequent Cu deposition within the surrounding volcanic rocks.

The mineralization model for the Chahargonbad district is underpinned by the interaction between these intrusive bodies and the surrounding volcanic units, which create favorable conditions for Cu deposition. Detailed structural analysis indicates that faults and fractures within the volcanic belt acted as conduits for ore-bearing hydrothermal fluids, further concentrating mineralization along these structures.

The study area hosts 18 monzonite-quartz monzonite porphyry Cu deposits (Fig. 1) with the age of Middle Eocene (Hezarkhani, 2006; Kianpouryan et al., 2015). This study applies a selective approach in choosing exploration data based on the specific mineralization model of the region. The geological features, including lithological contacts, fault systems, and alteration zones, are mapped and used as input layers in the MPM. By focusing on these key geological indicators, the research ensures that the GWO algorithm optimizes exploration targets in alignment with the actual mineralization processes occurring in the Chahargonbad district. This targeted approach not only enhances the accuracy of the predictions but also increases the potential for discovering new, economically viable mineral deposits.

In the porphyry Cu mineral system, intrusive bodies can act as heat and metal source to form mineralization as focused fluid flux within the intrusive and surrounding volcanic rocks and also in carbonates/skarns (Kreuzer et al., 2008; Porwal et al., 2015; Kreuzer et al., 2015; Zhang et al., 2017; Yousefi and Hronsky, 2023). In the study area, the intrusive bodies and their surrounded volcanic rocks are potential traps for porphyry Cu deposition (Lindsay et al., 2014; Yang and Zuo, 2024; Yang et al., 2024). The intrusive contacts can be used as a geological indicator feature (Yousefi and Hronsky, 2023) to create an exploration evidence map.

Fault-fracture systems and other structural features play a key role in transporting ore-bearing hydrothermal fluids in porphyry systems (Zhao et al.,2015; Chudasama et al.,2018; Mami Khalifani et al., 2019; Hronsky, 2020; Yousefi et al., 2024a,b).

Several alteration types, such as potassic, propylitic, phyllic, argillic and gossanous (i.e., iron oxide) alteration assemblages, can be found in and around porphyry Cu deposits (Sillitoe, 2010). Porphyry Cu mineralization is generally surrounded by argillic and iron oxide alteration, which can be detected by remote sensing if outcropping (Ranjbar et al., 2011). Depending on erosion level and exposure, the phyllic alteration

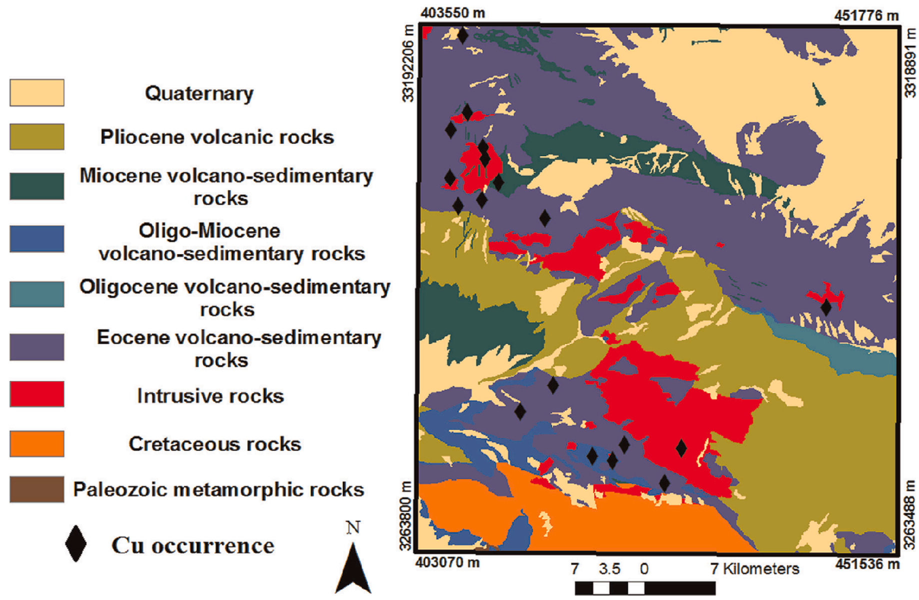

Fig. 1. Simplified geological map of the study area (Khan Nazer et al., 1995). Also shown are the locations of the known porphyry Cu deposits.

zone is typically found in the upper structural levels of porphyry Cu systems and represents one of the most important areas of exploration (Sillitoe, 2010).

Geochemical signatures are used as evidence layers (also referred to as predictor maps) in MPM, however, a key issue in geochemistry for mineral exploration is the determination of a significant multi-element signature for this type of deposits (Carranza and Hale, 1997; Yilmaz et al., 2019; Chen et al., 2019; Lou and Liu, 2023; Liu et al., 2023a,b; Wang et al., 2024; Esmaeiloghli et al., 2024). In the analysis of geochemical data, factor analysis is usually performed, factor scores are calculated, and, subsequently, geochemical maps are produced based on the scores that showing the probability of mineralization upstream of each sample. The Geochemical Mineralization Prospectivity Index (GMPI) was used to generate geochemical predictor maps using stream sediment data (Yousefi et al., 2012). The GMPI method is the application of the logistic function on the factor scores obtained from stepwise factor analysis, which is referred to as fuzzy weight. Therefore, the GMPI map is a weighted geochemical evidence map for porphyry Cu MPM.

Mineral system components can be classified into sub-systems of ore-forming processes (Hagemann et al., 2016a,b; Hronsky and Kreuzer, 2019), which act at different scales and times (McCuaig et al., 2010; Champion and Huston, 2016). Yousefi et al., (2019) have divided the process of ore formation into pre-, syn, and post-mineralization sub-systems, meaning controlling geological processes of mineralization occur at different stages regarding to the scales and times. Categorizing the controlling geological processes by respecting the order of the events results in effective and more reliable prospectivity models.

This division is based on the available data, e.g., in the geochemical evidence, stream sediment data are related to post-mineralization but litho-geochemical data are related to *syn*-mineralization. Iron oxides and argillic are classified as post-mineralization in alterations evidence. The host-rock is placed in the pre-mineralization group.

In this study, we used a set of exploration data comprising stream sediment geochemistry, lithology, and structure (sourced from the Geological Survey of Iran), and maps of argillic, iron oxide and phyllic alterations that were identified from ASTER and ETM + data previously processed by National Iranian Copper Industries (NICICO). The most effective mappable expressions of ore formation processes are divided into pre-mineralization, *syn*-mineralization, and post-mineralization sub-systems (Table 1).

Table 1
Components of porphyry Cu mineralization system applied for the study area of this paper.

Ore formation subsystem	Corresponding Factor
Pre-mineralization	Intrusive bodies, Fault density
Syn-mineralization	Fault density, phyllic alteration
Post-mineralization	GMPI, argillic and iron oxide alteration

3. Methods

3.1. Monte Carlo simulation

The Monte Carlos simulation (MCS) method is a statistical technique used to model and analyze complex systems or processes that involve uncertainty and randomness (Metropolis and Ulam, 1949). It relies on generating a large number of random samples to simulate possible outcomes and uses statistical analysis to estimate the probabilities of different results. This method is widely used in fields such as finance, engineering, physics, and risk management to solve problems that are difficult or impossible to calculate analytically (Metropolis and Ulam, 1949; Binder, 2005). By running multiple iterations with varying input parameters, MCS provide insights into the range of potential outcomes, helping decision-makers assess risk, optimize strategies, and make informed choices (Kroese et al., 2014). MSC has been applied across various geoscience disciplines such (Ballesio et al., 2019; Scalzo et al., 2019; Amaya et al., 2021).

3.2. Logistic regression

Logistic regression is a statistical method used for modeling the relationship between a dependent variable and one or more independent variables when the dependent variable is categorical (Kleinbaum et al., 2002). It is particularly useful for binary classification problems, where the outcome variable has two possible categories, such as success/failure ore yes/no. (Hosmer et al., 2013). Logistic regression estimates the probability of an event occurring by applying a logistic function to a linear combination of the input variables. Unlike linear regression, it outputs probabilities bounded between 0 and 1, making it suitable for classification tasks. This method is widely used in fields like medicine, social sciences, and machine learning for tasks such as predicting disease presence, customer churn, or voting behavior (Hosmer et al., 2013; Kleinbaum et al., 2010) as well as in MPM (e.g., Agterberg et al., 1990; Agterberg, 1992; Harris and Pan, 1999; Carranza and Hale, 2001; Porwal et al., 2010; Carranza, 2011; Xiao et al., 2021; Chen et al., 2022).

3.3. GWO algorithm

GWO algorithm, inspired by the social hierarchy and cooperative hunting strategies of grey wolves, is applied in this study to optimize the outputs of Mineral Prospectivity Modeling (MPM). The GWO algorithm mimics the leadership hierarchy within a wolf pack, which consists of alpha (α), beta (β), delta (δ), and omega (ω) wolves. This hierarchy is used to guide the search for optimal solutions, with the alpha wolf representing the best solution at any given time.

Social levels-The social life of wolves is displayed in Fig. 2. Accordingly, at the highest point of this pyramid, alpha wolves behave as leaders of the pack and are responsible for making daily decisions. In the second place, beta wolves obey the alpha's orders and thoughts, deltas are ready to receive their duty from the upper classes and finally, omegas are controlled by three other major groups and contribute to making balance in the social structure (Ahmadi et al., 2021).

GWO Algorithm Principles: Gray wolves use an interesting strategy to chasing their prey. It is composed of three main steps: decreasing the distance to their prey as much as possible, compelling their prey to stop moving, and attacking their prey once the previous two strategies have been achieved.

The GWO algorithm operates by iteratively adjusting the positions of wolves in the search space based on their distance from the prey (the optimal solution). The following equations are used to update the position of each wolf:

$$\mathrm{D}=\left|C.x_p(t)-x(t)\right| \quad (1)$$

$$x(t+1)=x_p(t)-A.D \quad (2)$$

where D is the distance between the wolf and the prey,$x_p(t)$ is the prey's position (optimal solution), and $x(t)$ is the current position of the wolf. The coefficients A and C are vectors that control the influence of the alpha, beta, and delta wolves on the search direction. These coefficients are adjusted dynamically over the course of the iterations to balance exploration and exploitation.

$$A=2a.r_1-a \quad (3)$$

$$C=2r_2 \quad (4)$$

where a is linearly reduced in [0, 2], and r_1 and r_2 involve random vectors with a measure of [0, 1].

In this algorithm, the prey is considered as the best solution and the alpha has maximum merit to follow the prey. Omegas modified their location with the help of the other three main groups led to finding the best solution. The following equation has been proposed by (Mirjalili et al., 2014; Safaldin et al., 2021) to explain the process of updating location:

$$D_\alpha=|C_1x_\alpha(t)-x(t)| \quad (5)$$

$$D_\beta=\left|C_2x_\beta(t)-x(t)\right| \quad (6)$$

$$D_\partial=|C_3x_\partial(t)-x(t)| \quad (7)$$

where $C_i=2^*r_{i1}$, r_{i1} is a random vector in [0, 1], and $i=1.2.3$

$$X_1=|X_\alpha(t)-A_1.D_\alpha| \quad (8)$$

$$X_2=\left|X_\beta(t)-A_2.D_\beta\right| \quad (9)$$

$$X_3=|X_\partial(t)-A_3.D_\partial| \quad (10)$$

$$X=(X_1+X_2+X_3)/3 \quad (11)$$

where

$A_i=2a.r_{i2}-a$where r_{i2} involves a random vector in [0, 1] and $X_\alpha(t)$,$X_\beta(t)$ and $X_\partial(t)$ imply to position of alpha, beta, and delta at the t irritation (Kumar et al., 2017). Fig. 3 shows a flowchart of where the above methods are used.

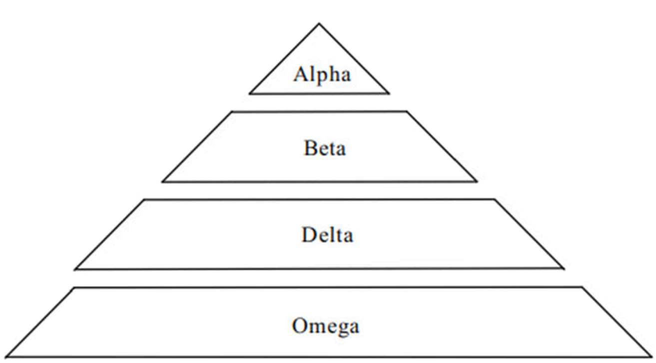

Fig. 2. Social hierarchy classification of gray wolf (Mirjalili et al., 2014).

4. Results

4.1. Generating continuous weighted evidence maps

According to previous works and investigations on the Chahargonbad area (Yousefi and Carranza, 2015), six individual evidence maps, which are suitable for detecting porphyry Cu deposits, were selected and plotted. These layers involve (i) proximity to intrusive contact, (ii) fault density (FD), (iii) multi–element geochemical signature presented as GMPI (Yousefi et al., 2012, Yousefi et al., 2024a,b), (iv) proximity to iron oxide alteration, (v) proximity to argillic alteration, (vi) proximity to phyllic alteration, and are presented in Fig. 4a,4b,4c,4d,4e,4f respectively.

Through the process of preparing the aforementioned layers, we used logistic function to lie these spatial distributions in the [0, 1] range for the purpose of mitigating the problem of the systematic error caused by the discretization of continuous maps in knowledge-driven models (Yousefi and Carranza, 2015).

4.2. Integration using MCS

There have been various strategies to integrate the evidence layers aiming to make an ensemble model (Yousefi et al., 2019; Yousefi et al., 2021). To avoid the subjectivity accompanied by geologists assigning weights to ore formation contributing factors (source, transport, and deposition criteria), it is recommended to apply a set of stochastically simulated weights (Hsu and pan, 2009). MCS as a solution to respond to this need, has been applied to generate such set weights to model evidence layers (Pakyuz-Charrier et al., 2018; Athens and Caers, 2019; Fouedjio and Talebi, 2022). Through the MCS as a proper method to produce criteria weights, a normal distribution with the mean and standard deviation of 0.5 and 0.2 were selected and the simulation process continued for 100 iterations. Considering the derived weights and converting them into relative weights, they were prepared for building models. Accordingly, one hundred models were made by a linear sum of criteria in each raster location for every weight set value. Finally, to generate the desired exploration targeting score, an arithmetic mean of these models was calculated and presented in Fig. 5.

4.3. Selection of exploration targets

In MPM, predictor maps are integrated using various mathematical

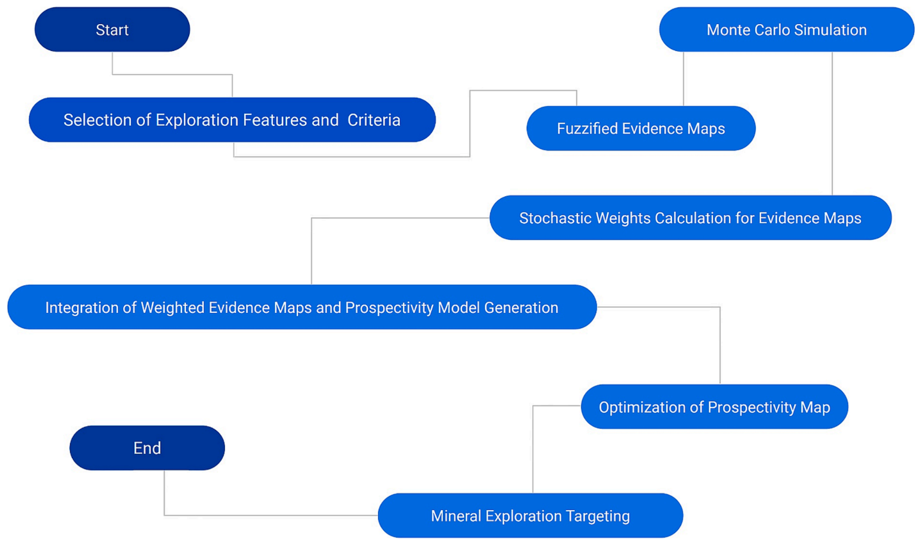

Fig. 3. Flowchart illustrating the process used to research.

methods with appropriate method selection typically determined by the targeted deposits and available data. However, the delineation of exploration targets from the resulting prospectivity models presents a challenge (Yousefi et al., 2024a), namely with regards to a) determining appropriate delineation thresholds, and b) delineating target boundaries. Several methods are being used to achieve the above, each of which with its own advantages and disadvantages.

4.3.1. Percentile-based selection of exploration targets

After preparing the exploration targeting score map, we need to determine the best areas to continue exploration. The selection criterion for these areas is the main challenge of mineral prospective mapping studies. Traditionally, the mean percentage of exploration targeting score map is used to select anomaly areas. In regional exploration studies, 90 % and 95 % of the mean values are generally used to determine desirable areas (Bonham-Carter, 1994; Carranza, 2008; Yousefi et al., 2012). The exploration targeting score map based on the 90 % and 95 % mean values was prepared and presented in Fig. 6, also the desired areas have been identified.

Besides these results, we here introduce a novel framework that consists of applying GWO on the mean raster model and deriving the optimized value. In other words, zones having greater optimized value should be considered as desired zones.

4.3.2. Logistic Regression-based generation of exploration targets

The data that were processed to build a logistic regression model are the same that used in the MCS model. Thirty-four samples including 17 mineralized and 17 unmineralized were applied in logistic regression MPM procedure. The dataset then got divided into three subsets: training (60 %), validation (20 %), and test (20 %). The training set was used to train the logistic regression model, while the validation set was used to tune hyperparameters and make decisions about the model's architecture. The test set, which the model had not seen during training, was used to evaluate the model's performance. This approach helps ensure that the model generalizes well to new, unseen data. The logistic regression model was then trained using the training set. The coefficients derived from the model (Table 2) indicated the impact of each feature on the prediction of the target variable. For instance, features like Intrusive Proximity and Iron Oxide Alteration had higher coefficients, suggesting a stronger influence on the likelihood of a sample being mineralized. The classification report (Table3) provided detailed metrics for both the validation and test sets, including precision, recall, F1-score, and support for each class (mineralized and unmineralized). In the validation set, the model shows a perfect precision of 1.00 for mineralized samples, meaning all predicted mineralized samples are actually mineralized. However, the recall for mineralized samples is 0.67, indicating that the model missed some actual mineralized samples. The F1-score, which balances precision and recall, is 0.80 for mineralized samples. For unmineralized samples, the model achieved a precision of 0.80, a recall of 1.00, and an F1-score of 0.89. These metrics suggest that the model performed well on the validation set, particularly in identifying unmineralized samples. On the test set, the model's performance was slightly lower. The precision for mineralized samples is 0.67, and the recall is 0.50, resulting in an F1-score of 0.57. For unmineralized samples, the precision, the recall, and the F1-score are 0.50, 0.67, and 0.57, respectively. These results indicate that while the model is able to identify some mineralized and unmineralized samples correctly, there is space for improvement, particularly in balancing precision and recall. Then, the derived model was applied on the location of all cells within the study area to determine whether they are placed within mineralized or unmineralized classes. Fig. 7 illustrates the mineral prospecting map using logistic regression approach.

4.3.3. GWO-based classification of exploration targets

In this study, the GWO algorithm is integrated into a simulation-based framework for MPM. The first step involves generating evidence layers from geological, geochemical, and structural data collected from the Chahargonbad district. These evidence layers are then fuzzified and normalized to ensure they fall within a [0, 1] range, which is suitable for integration into the GWO model.

MCS is employed to stochastically generate weights for each evidence layer, reducing the subjectivity associated with manual weight assignments. The GWO algorithm is then applied to these weighted evidence layers to identify optimal exploration targets. The algorithm's objective function minimizes the discrepancy between the predicted and known mineralization zones, ensuring that the identified targets are geologically plausible.

Although the average prospectivity map provides a primary interpretation of zones with high potential for copper mineralization, it includes a spectrum that varies between 0.023 and 0.90. So, it is required that this model endures optimization. There are numerous algorithms that are applied to reach this goal. In this particular study, we used GWO algorithm to optimize the mean map. A GWO algorithm with a maximum iteration of 100 and a pack including 50 wolves was designed in which the following function was considered as the cost function.

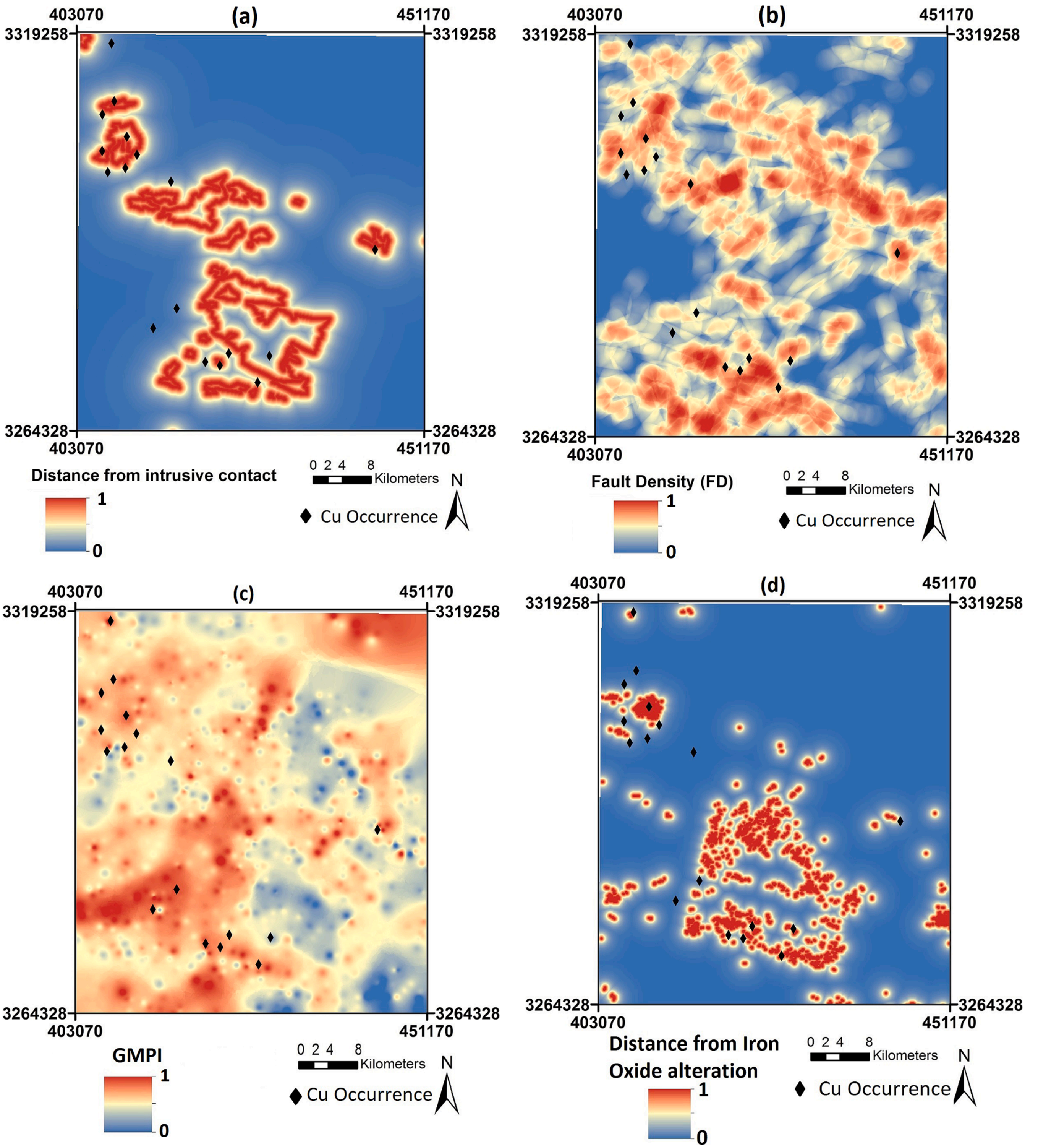

Fig. 4. Fuzzified maps of a) proximity to intrusive contact, b) fault density, c) GMPI, d) proximity to iron oxide alteration, e) proximity to argillic alteration, f) proximity to phyllic alteration.

$$f(x) = \sum_{i=1}^{n} |x - x_i| \quad (12)$$

in this context, (x) is the optimized value that the GWO algorithm is trying to find. This value is important because it minimizes the overall difference between itself and the mineral prospectivity mapping values of previously explored deposits. Specifically, x_i represents the mineral prospectivity mapping value at the (i)-th previously explored deposit, which is derived from spatial data showing geological features or mineralization indicators. The variable (n) is the total number of copper porphyry deposits in the study area. The GWO algorithm's goal is to find the value of (x) that minimizes the sum of the absolute differences between (x) and each $(, x_i)$. This ensures that (x) closely matches the mineral prospectivity mapping values of the previously discovered deposits, thereby accurately representing the exploration targets.

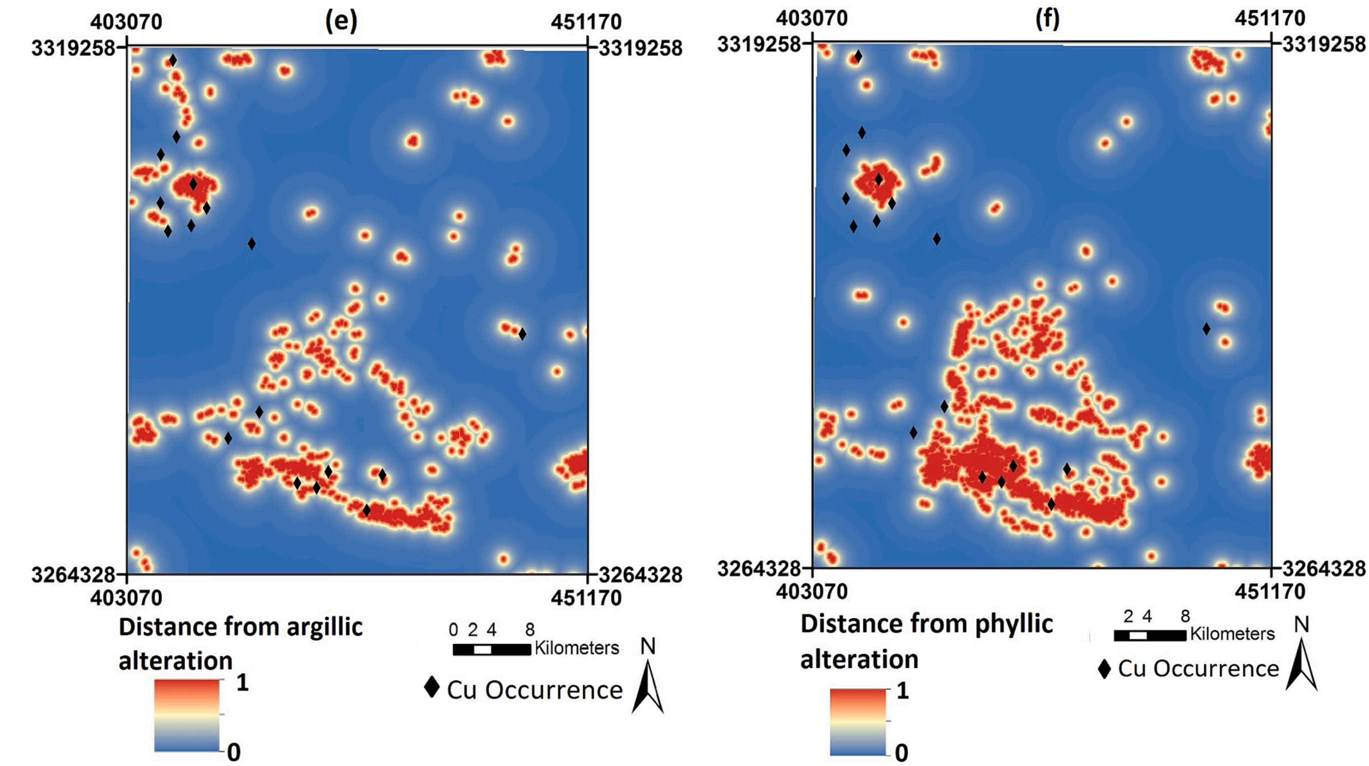

Fig. 4. (*continued*).

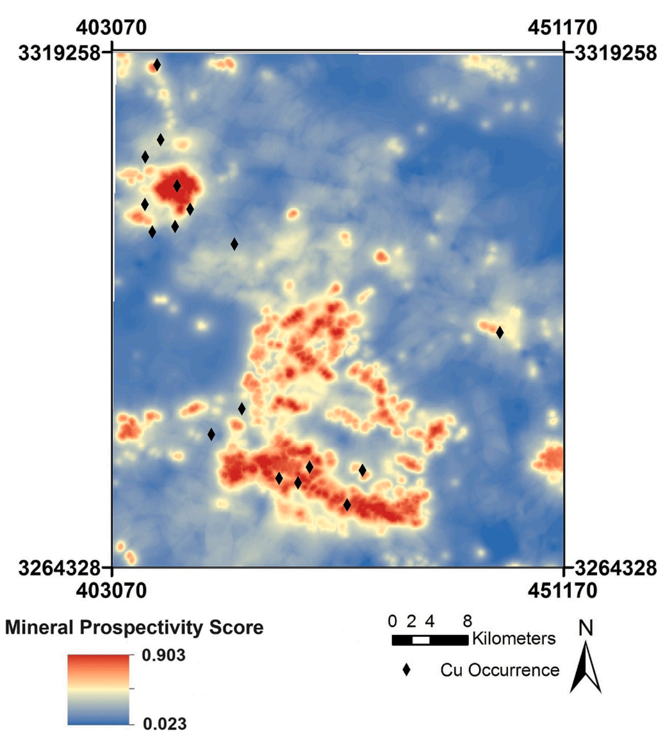

Fig. 5. Simulation-based model of mineral prospectivity.

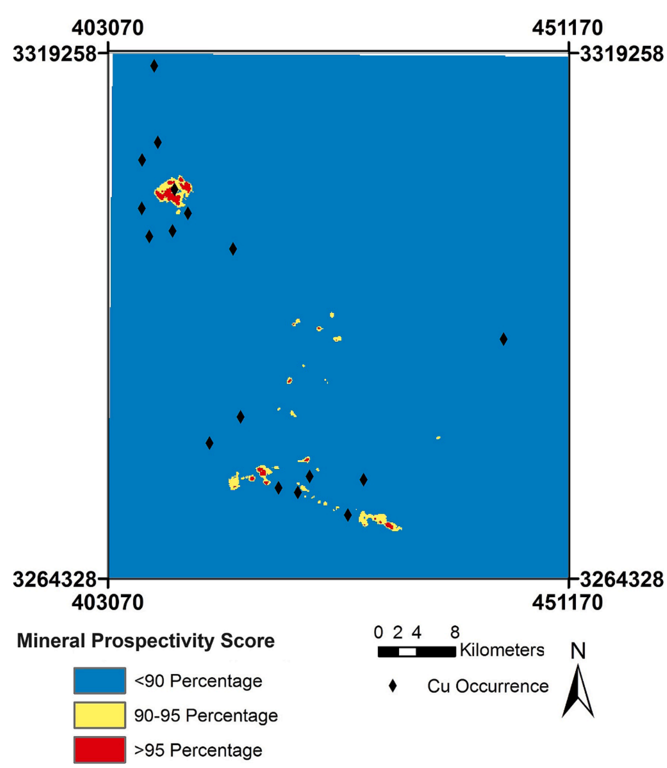

Fig. 6. Classified map of prospectivity value based on the percentile maps.

During running the algorithm, the Function Evaluation was investigated for 5000 times during running the code. Obviously, the trend of the GWO algorithm to find the optimum value has been illustrated in Fig. 8.

The GWO algorithm was run for 100 iterations with a population size of 50 wolves, a configuration that balances computational efficiency with the thoroughness of the search.

The result of running this code led to the revealing of the optimized cost value of 3.23, which belongs to 0.415 among mean raster values. Fig. 8 illustrates the reduction in Best Cost over 100 iterations, with the final Best Cost achieved being 3.2322, belonging to 0.415 among raster

Table 2
Logistic regression models coefficients.

Phyllic	Iron Oxide	Argillic	Intrusive Proximity	Fault density	GMPI	Intercept
0.54	0.69	0.63	1.23	0.88	0.59	−1.07

values. While the reduction in Best Cost may appear limited, dropping from 3.2328 to 3.2322, this small decrease is significant in the context of the complex, nonlinear search space in which the GWO algorithm operates. The algorithm's ability to achieve even this small improvement demonstrates its precision in fine-tuning the solution. Moreover, this limited reduction indicates that the algorithm has effectively converged, suggesting that further significant improvements are unlikely without risking overfitting.

It is essential to understand that the effectiveness of the GWO algorithm is not solely reflected in the magnitude of the Best Cost reduction. The primary goal of this optimization was to accurately predict and delineate exploration targets, which was successfully achieved as validated by the alignment of predicted targets with known mineralization zones.

In other words, areas that possess higher mean values than the 0.415 fall within optimized locations.

The Fig. 9 displays the optimized region derived by applying the GWO algorithm, in which the green color refers to the potential area, and the well-known deposits have been illustrated by black tetrahedral.

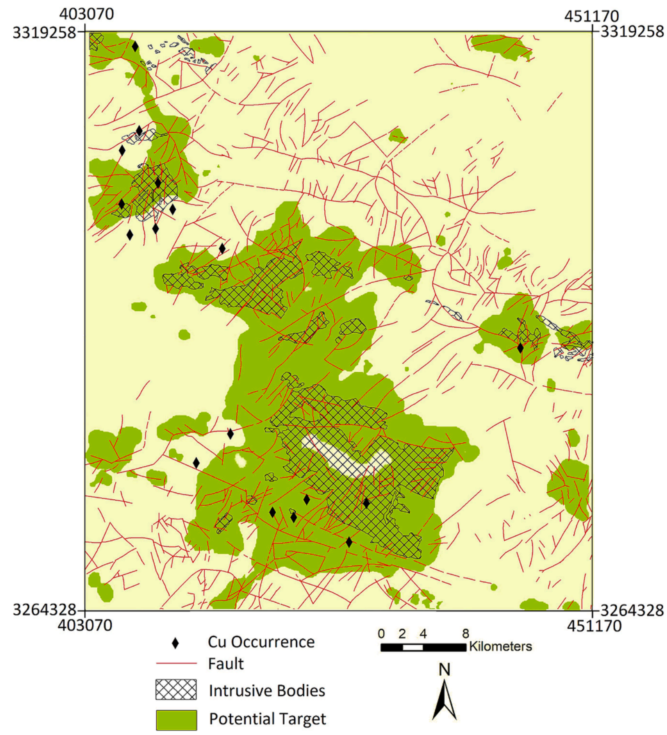

Fig. 7. Classified map of prospectivity value based on the logistic regression.

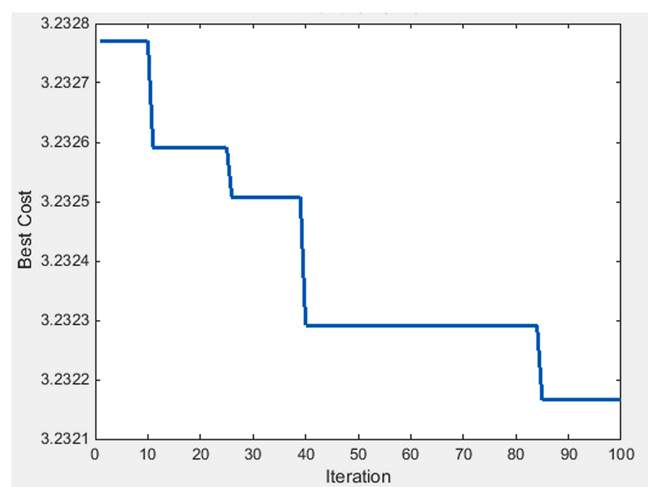

Fig. 8. Trend result of GWO algorithm on exploration targeting score map.

5. Discussion

Delimiting mineral exploration targets derived from MPM is a challenging task (e.g., Yousefi et al., 2024a,b) and, arguably, one that is in need of further research. There are examples in the literature of studies that present their MPM results in a binary manner, solely based on certain mathematical and rational relationships and without consideration of the likely impact of previously discovered deposits on the final MPM model. A classified map based on percentile thresholds (e.g., 90th and 95th: Fig. 6) is a typical approach to presenting MPM results. In this method, any threshold increase will result in greater certainty but fewer and smaller target areas, which, in turn, may result in some deposits not being identified. As exemplified in Fig. 6, the percentile map captures only two out of 17 porphyry Cu deposits in our study area.

In general, knowledge-based MPM methods suffer from bias and uncertainty introduced by expert judgment in that in traditional approaches, continuous spatial data are classified into some arbitrary classes and then the same weight is assigned to all values in each class of evidential features (Ghasemzadeh et al., 2022a,b). In data-driven MPM, bias is caused by accessibility factors and exploration criteria, in particular the use of known mineral occurrences (KMOs) as training sites. Thus, data-driven mineral prospectivity models, for example, supervised models, are influenced by the locations of KMOs. Therefore, supervised methods benefit from the advantages of both training data and pattern recognition. There are various techniques in data-driven modelling. The logistic regression model and the GWO algorithm offer distinct approaches to MPM, each with its own strengths and limitations. Logistic regression, a statistical method, is straightforward and interpretable, making it easier to understand the impact of each feature on the prediction of mineralized areas (Harris and Pan, 1999; Carranza and Hale, 2002). By using regression logistic method 9 out of 17 Cu occurrences were detected (Fig. 7).

Here we tested the validity and performance of the GWO algorithm, presenting a new approach to MPM and target selection. More specifically, we used this algorithm to determine the distribution of such value among the study area to demarcate potential zones and to optimize target selection (Fig. 9). As per Fig. 9, the area of greatest mineral potential is mostly located along the boundary of the fertile intrusive body, a result that illustrates the high efficiency of the GWO approach in that the porphyry Cu mineralization in the study area is associated with the contacts of intrusive bodies.

Table 3
Logistic regression model's evaluations.

	val_precision	val_recall	val_f1-score	val_support	test_precision	test_recall	test_f1-score	test_support
Mineralized	1.00	0.67	0.80	3	0.67	0.50	0.57	4
Unmineralized	0.80	1.00	0.89	4	0.50	0.67	0.57	3

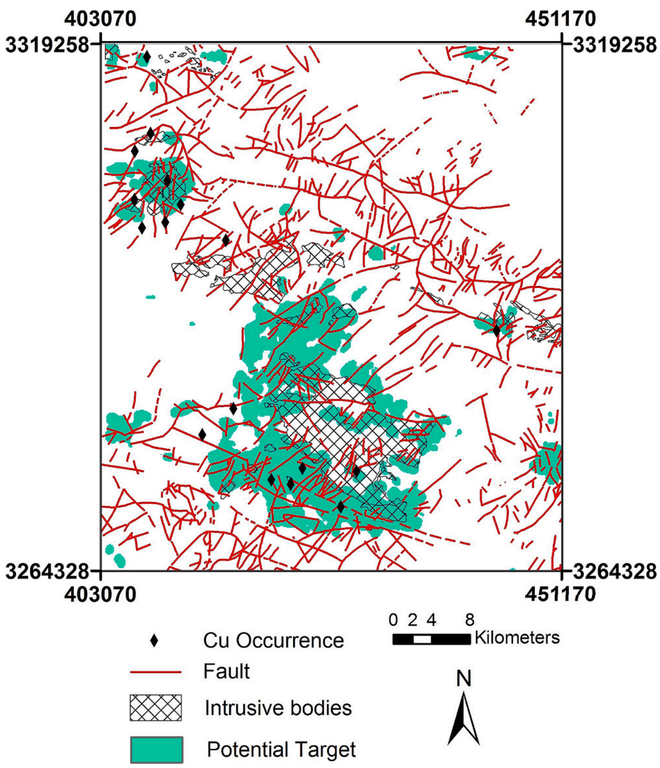

Fig. 9. The map of exploration targets detected by GWO algorithm superimposed by faults and intrusive bodies.

The performance of our approach was assessed in two ways: Firstly, the ability of the model to incorporate Cu deposits within the proposed areas, and, secondly, the percentage of selected areas as an exploratory target to the areas introduced by other formworks. Considering the derived result, the GWO model has been able to include more explored Cu deposits within an area rather than the percentile map (11/17 by GWO versus 2/17 percentile map), and it identified many more locations as potential targets. This difference could be explained as follows: Since approaches like a percentile map, do not take into account how values in MPM models relate to previously discovered deposits within the study area, they are unable to make a proper binary map, especially when such deposits fall within a wide range in the MPM model.

Comparing the results of the logistic regression and GWO methods shows that the logistic regression model covered two less copper occurrences compared to the GWO algorithm and introduced target areas that were almost twice as large. In fact, the combined target areas identified by logistic regression are 43.56 % larger than those delineated by the GWO algorithm. This model also showed susceptibility to overfitting, particularly when dealing with a small dataset, as evidenced by its lower performance on the test set compared to the validation set. The GWO-based approach identified more high-priority exploration zones and covered more known Cu occurrences, demonstrating its robustness and reliability. Additionally, GWO's ability to handle complex, nonlinear search spaces without human bias makes it a powerful tool for MPM. Accordingly, while logistic regression provides a simpler and more interpretable model, the GWO algorithm offers superior performance in terms of precision and reliability, making it a more effective tool for exploration targeting.

As illustrated in Fig. 9, which shows potential targets as identified by the GWO algorithm superimposed on geology, faults and intrusive bodies appear to have played an important role in localizing Cu mineralization given their spatial abundance and proximity relationships. A large part of the detected potential targets is related to faults and intrusive bodies. As mentioned above, the porphyry Cu mineralization in the study area is associated with the contact between intrusive masses and volcanic units. In addition, faults appear to have played a major role, most likely with regards to their control on the migration of mineralizing fluids. Therefore, the intrusive mass boundary and fault density have been introduced as potential areas. Last but not least, it is worth noting that some of the GWO targets are not spatially associated with outcropping intrusive bodies. However, these types of targets are characterized by a strong GMPI and are always located in proximity to intrusive bodies. As such, these targets represent valid areas of interest in which any undiscovered Cu mineralization may be surface blind.

The performance of the GWO algorithm was evaluated by comparing its results with those obtained using a percentile-based classification method. This comparison was chosen for its relevance and practicality in the context of mineral prospectivity modeling. Percentile-based classification is a widely-used baseline method in mineral exploration, making it a suitable benchmark for evaluating the effectiveness of the GWO algorithm. While alternative methods such as logistic regression, WoE, and deep learning classification techniques are recognized for their effectiveness, the focus of this study was to establish the initial efficacy of GWO in optimizing the process of delineating valid exploration targets.

The choice to compare GWO to percentile-based classification was driven by the need for a straightforward, interpretable method that allows for a clear demonstration of GWO's advantages, particularly in handling non-linear search spaces and reducing bias. This initial comparison provides a robust foundation for future studies that may extend the analysis to include more complex methods.

6. Concluding remarks

- The successful application in this study of the Grey Wolf Optimizer (GWO) algorithm has demonstrated its potential as a robust data-driven method for optimizing mineral prospectivity models. By integrating Monte Carlo Simulation (MCS) to generate unbiased weights for the evidence layers, this approach has significantly reduced the subjectivity and bias inherent in traditional MPM methods such as logistic regression.
- The ability of GWO to more accurately delineate high-priority exploration targets, as evidenced by its superior performance in cross-validation tests and ROC curve analysis, underscores its practical value in mineral exploration targeting.
- The theoretical foundation of this research is built on the principles of swarm intelligence and optimization algorithms, which have been rigorously applied to the context of mineral exploration. GWO's unique approach to balancing exploration and mining during the search process has proven effective in navigating the complex geological landscapes of the Chahargonbad district. The results not only validate the algorithm's effectiveness but also highlight the potential for its application to other mineral systems.
- This study contributes to the broader field of geosciences by offering a scalable, automated solution for mineral exploration targeting. Future research could explore the integration of other advanced optimization techniques, such as hybrid algorithms, to further enhance the accuracy and reliability of exploration models. The findings of this research provide a strong theoretical and practical foundation for the continued development and application of GWO in mineral exploration.
- The GWO algorithm automatically discriminates between mineral potential and non-potential areas without the need for human interference and/or expert opinion.
- The GWO modeling results are optimized for targeting as the algorithm detected the largest amount of Cu occurrences and have covered more areas where the risk of losing potential mineralization can be significantly reduced.

- Overall, the results indicate that the GWO algorithm presents a valid tool for delineating exploration search spaces. Moreover, the GWO approach delivers better results than other approaches because it is independent of the statistical level of uncertainty affecting other algorithms.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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