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Artificial intelligence and machine learning to enhance critical mineral deposit discovery

Rhys S. Davies[a,*], McLean Trott[b,c], Jaakko Georgi[d], Alexander Farrar[e,f]

[a] Business School, The University of Western Australia, Crawley, WA 6009, Australia
[b] Department of Geological Sciences and Geological Engineering, Queen's University, Ontario, K7L 3N6, Canada
[c] ALS Geoanalytics, 2103 Dollarton Hwy, North Vancouver, British Columbia V7H 0A7, Canada
[d] Mineral Economy Solutions, Geological Survey of Finland, Kokkola, Finland
[e] Centre for Ore Deposits and Earth Sciences (CODES), University of Tasmania, Tasmania 7001, Australia
[f] First Quantum Minerals, Level 2, 32 Parliament Place, West Perth, Australia

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ABSTRACT

The application of machine learning (ML) in mineral exploration has garnered significant attention and investment, yet greenfield mineral deposit discovery rates remain unchanged. This limited success stems from challenges such as low data quality outside existing mines, inconsistent sampling, limited interdisciplinary collaboration, and the unique complexity of geoscientific problems. Unlike traditional ML applications, mineral exploration demands a focus on subtle variations within finite search spaces, requiring an exploratory rather than accuracy-driven approach. Effective implementation necessitates collaboration between data scientists and geoscientists, leveraging ML as a tool to test hypotheses and analyse diverse datasets. However, reliance solely on ML overlooks the critical role of human creativity in generating and evaluating novel search strategies. Broader adoption of statistical methods, integrated spatial models, and innovative data preparation techniques can address the inconsistencies in exploration datasets. Furthermore, subjective modelling approaches, such as Delphi methods, can complement ML by incorporating expert judgment to overcome predictive limitations. By combining technological advancements with human expertise, the mineral exploration industry can enhance discovery success and achieve long-term sustainability. There is an important short-term requirement to secure the supply of critical metal resources, as their supply from existing mines and brownfield exploration is finite and commercial recycling of critical metals is still in its infancy.

1. Introduction

Critical metals are defined as metals that are essential for modern life and have a high risk of experiencing supply shortages (Lederer et al., 2024). Supply bottlenecks might occur at any stage of the value chain, from exploration, mining and refining, component and subsystem manufacturing, and even recycling (Sykes et al., 2016; Valero et al., 2018; McNulty and Jowitt, 2021). These bottlenecks may result from a combination of factors such as material availability, equipment availability, workforce availability and quality, logistics, regulatory frameworks, and market conditions (Bauer et al., 2023). Although many jurisdictions have issued independent reports defining a range of their respective critical metals, the following are regularly included: rare earth elements (REE's), battery metals such as cobalt (Co) and lithium (Li), platinum group elements (PGE's), gallium (Ga), and base metals required for electrification, such as; copper (Cu), nickel (Ni), and aluminium (Al) (e.g., Moss et al., 2013; Butu et al., 2023). These metals have a wide range of applications, although most are necessary for a global energy transition away from fossil fuel reliance and, by definition, are not available in abundances that are required for this transition to be inevitably successful (Løvik et al., 2018; Calderon et al., 2024; Guj and Schodde, 2025).

Globally, the combined value of newly discovered critical metals deposits has been decreasing since the early 2000's, with the last two decades of exploration bordering between break-even and a wealth-destructive activity (Schodde, 2023; Fig. 1). This is likely due to a number of factors, including increasing average discovery costs, lower quality (and therefore value) discoveries, and a focus on brownfields exploration due to perceived widespread ground maturity and extensive post-mineralisation cover (e.g., McCuaig and Hronsky, 2014; Davies et al., 2018; Farrar et al., 2023).

* Corresponding author.
E-mail address: rhyssamuel.davies@research.uwa.edu.au (R.S. Davies).

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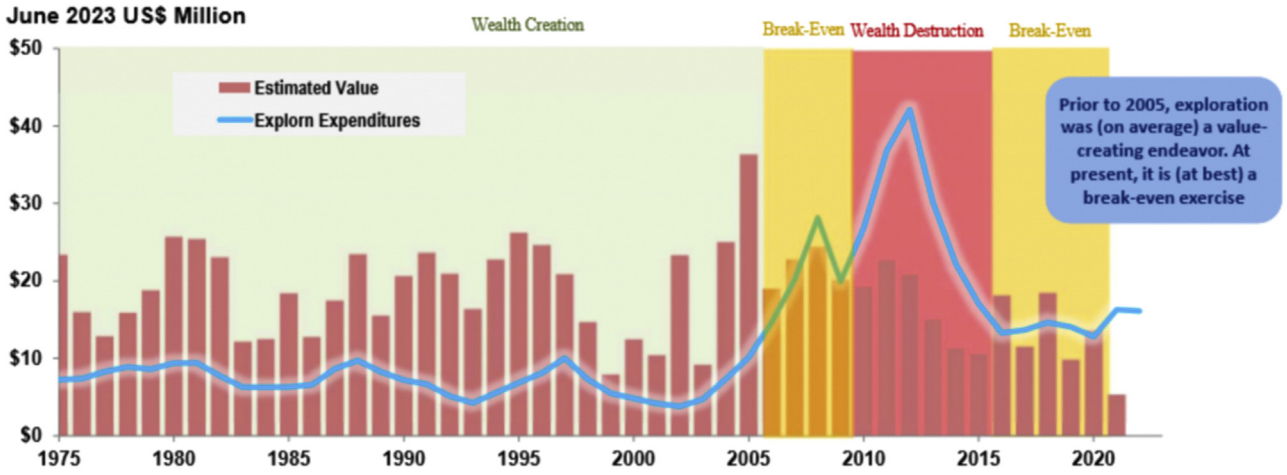

Fig. 1. Global exploration spend and estimated values of discoveries from 1957 to 2021, showing a wealth-destructive period of exploration between circa. 2010–2015 and a continued break-even period post-2015 (Schodde, 2023).

Further high-quality discoveries are required to secure a free supply of critical metals into the mid- and long-term future. Such an increase in exploration success would likely be supported by the application of new techniques and technologies to less-mature search spaces (Hronsky and Groves, 2008; Davies et al., 2020a). New technologies such as artificial intelligence (AI) and its sub-discipline of machine learning (ML) are expected to help drive future exploration success, with potential to increase discovery rates through enhanced conceptual targeting, and reduce costs/maximise value to provide meaningful efficiency gains (Davies et al., 2020b).

2. Artificial intelligence and machine learning

AI is a branch of computer science, falling under the more general discipline of data analytics, that has existed as an area of academic research since the 1950's. However, recent breakthroughs in computing power and data availability have led to increased global interest and practical application (Woodhead and Landry, 2021). Conceptually, AI was developed to emulate human learning, although it's important to note that this paradigm has not been fully realised. A long-term goal of AI research is to develop artificial general intelligence (AGI), which would instil machines with the ability to think, reason, and create. Many researchers agree that this remains a distant goal (e.g., Fjelland, 2020; Macey-Dare, 2023) and is unlikely to affect the short–term practical application of AI. For a comprehensive history of AI, please refer to Wooldridge (2021).

Conventionally, computer programming has involved numerical or physical modelling to simulate real-world processes. For ML, a sub-discipline of AI, the aim is to predict the behaviour of complex systems that often cannot be explicitly modelled using conventional modelling approaches. The goal of an ML model is to train using known data, so as to define generalised patterns that can then be applied to new data in order to make predictions, or to identify data-supported groupings in unknown data. Problems that are suited to the application of ML usually involve complex, non-linear relationships between large numbers of interacting variables (Jooshaki et al., 2021). This can encompass specific dependent variables, and also changes in the broader geological environment and its evolution over time.

ML algorithms fall into three broad categories: supervised, unsupervised, and self-supervised/reinforcement learning (Fig. 2). Supervised and unsupervised models represent two end-members; where the former relies on empirical evidence of labelled training data to determine relationships between variables, and the latter is used to tease out patterns in unlabelled data, without the use of any posteriori evidence. Self-supervised and reinforcement learning models are extensions of these; defining classes within unlabelled data sets and interacting directly with the environment to receive feedback and update training data. For classification algorithms, labels can be categorical; assigning a specific class to each sample, or numerical; using a regression model to assign each sample a numerical value (Sharifani and Amini, 2023).

ML models have been used within a broad range of disciplines, including computer science and software development (Malhotra, 2015; Handelman et al., 2019), websites, email, search engines and online advertising (Jabeen et al., 2023), banking (Amini and Rahmani, 2023), economics (Mosavi et al., 2020), healthcare (Palaniappan et al., 2013; Senders et al., 2018), energy (Mosavi et al., 2019; Taheri et al., 2021), environment (Bellinger et al., 2017), services (Portugal et al., 2018) and manufacturing (Zhou et al., 2019), for speech recognition, language processing and translation (Spasic and Nenadic, 2020), machine vision/image recognition (Chai et al., 2021), medical diagnosis (Richens et al., 2020), self-driving vehicles and robots (Carrio et al., 2017), traffic prediction, power demand and climate forecasting (Jooshaki et al., 2014; Mozaffari et al., 2020), computer games, filtering emails, malware and online fraud (Amini and Rahmani, 2023), product recommendations, and virtual assistants (Sharifani and Amini, 2023). ML models are in many cases utilised on a daily basis, and perhaps unwittingly, by the average internet user, for tasks like recommending song, television, or movie choices based on prior selections in streaming services, or identifying plant species in a garden based on an online image library.

Although there are many examples of ML being applied successfully in other industries, mineral exploration and mining have been slower on the uptake (Woodhead and Landry, 2021), particularly regarding deployment of models to solve practical industry challenges and provide insights that result in the discovery of new orebodies. Uptake has improved recently: Jung and Choi (2021) and Jooshaki et al. (2021) conducted comprehensive reviews of published academic articles and found that ML studies have been actively and widely conducted in the minerals industry since at least 2018, covering practically every aspect of the mining life cycle. For specific examples in resource development please refer to Choi and Yi (2020), and for mineral processing refer to McCoy and Auret (2019). Those relating to mineral exploration, particularly efforts to discover new ore bodies containing critical metals, are discussed in detail in the following section.

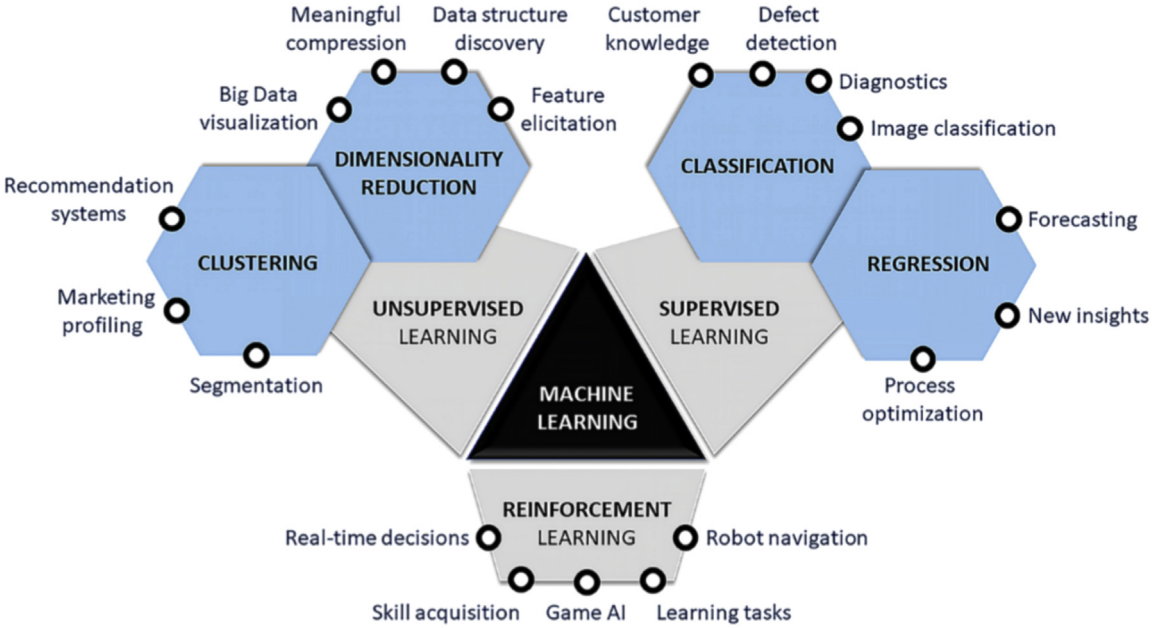

Fig. 2. ML algorithms fall into three broad categories; supervised, unsupervised, and self-supervised/reinforcement learning (Woodhead and Landry, 2021).

3. Application of machine learning to critical mineral exploration: Current status

The most significant benefit of implementing ML in mineral exploration is to support geoscientists in the analysis and interpretation of data (Woodhead and Landry, 2021; Yang et al., 2024). Much like its parent-discipline of statistics, ML tools can be applied to any stage of the exploration process in which data are generated (numeric, categorical, or text), from regional-scale targeting right through to resource definition. ML techniques can be employed to support a myriad of sub-steps in this process, and although it has a propensity for dealing with complex data, it is arguably best employed in solving relatively well-defined problems (Davies et al., 2021).

There have been a number of recent efforts to employ AI in the minerals industry, with a particular prevalence of ML models applied to support mineral exploration (Woodhead and Landry, 2021). In the vast majority of ML studies applied to mineral exploration, practitioners make use of large and complex geoscientific datasets that contain multiple interacting parameters (Jooshaki et al., 2021). Examples of these datasets include; text documents (Holden et al., 2019), lithogeochemical (Chen et al., 2018; Maepa et al., 2021), spatial (Maepa et al., 2021; McMillan et al., 2021), geochemical (Chen et al., 2018; Wang et al., 2019a; Luo et al., 2020), geophysical (Cracknell and Reading, 2014; Singh et al., 2024), geological (Maepa and Smith, 2018), remote sensing and hyperspectral (Schneider et al., 2011; Gloaguen et al., 2020), and core photography (Trott et al., 2022, 2023) data. Some examples of ML applied to the analysis of these datasets include; generating mineral prospectivity maps (Rodriguez-Galiano et al., 2015; Yeomans et al., 2020; Hafezi et al., 2024), mapping geological structures (Montsion et al., 2021; Kwan et al., 2025), identifying geochemical anomalies (Zuo and Xiong, 2018; Wang et al., 2019b), mapping regolith and lithology (Metelka et al., 2018; Lhissou et al., 2020), mapping drill-core (Acosta et al., 2020; Barker et al., 2021), and determining mineral, alteration or rock type and abundance (Carr et al., 2009; Schneider, et al., 2014; Hood et al., 2018; Koch et al., 2019; Van Duijvenbode et al., 2020).

Ninety percent of the studies reviewed by Jooshaki et al. (2021) applied ML classification models, whereas the other ten percent applied regression models to predict numerical outputs. These studies employed a wide range of ML techniques, predominantly conventional, but also some deep learning methods. The efficacy of these models were typically evaluated using Root Mean Square Error and Coefficient of Determination. Despite a significant increase in the availability of multi-parameter datasets in the minerals industry during the last decade, these datasets rarely fulfil the requirements to be defined as 'big data,' defined as "information assets characterised by such a high volume, velocity and variety to require specific technology and analytical methods for its transformation into value" (De Mauro et al., 2015). Based on their literature review, Jung and Choi (2021) demonstrated that generally fewer than 10 % of ML studies within the geoscience literature have made use of 'big data' techniques.

Four examples of ML models applied to specific stages of critical metal exploration are expanded upon in the following section.

3.1. Rock, mineral and alteration classification

Although application of ML tools to early-stage exploration for critical metals is often constrained by data availability, advanced stage exploration projects (pre-feasibility stage or later) often acquire so much data that it becomes difficult to parse without using 'big data' ML tools and techniques. Hyperspectral core scanning, RGB (red–green–blue) image, and multi-element geochemical data are commonly collected for these projects, and quickly become voluminous as more drilling is carried out. A parallel problem that emerges during large drilling campaigns, or integration of new and historic drilling datasets, is internal consistency. This is particularly true for categorical parameters like lithology or alteration, where individual loggers are influenced by many subjective factors (Davies et al., 2020c). 3D modelling of geological parameters like this can have a significant impact on exploration decision-making and the geometallurgical considerations for advanced stage critical metal projects.

Application of ML workflows to empirical data can allow these data to be parsed to constrain meaningful, data-supported geological units and domains, assisting the manual logging process and resulting in more cohesive 3D models. Ultimately, the desired im-

pact is better exploration and mining outcomes, and the inherent improvement in project economics.

3.1.1. Predictive algorithms

Unsurprisingly, ML-assisted workflows for integration of drillhole datasets and prediction of geological parameters are becoming of increasing interest to academia and industry. These workflows tend to test a variety of supervised algorithms, ranging from convolutional neural network (CNN), multi-layer perceptron (MLP), random forest (RF), linear discriminant analysis (LDA), quadratic discriminant analysis (QDA) and support vector machine (SVM) (e.g., Ordonez-Calderon and Gelcich, 2018; Bressan et al., 2020; Alférez et al., 2021; Alzubaidi et al., 2021). Outcomes between algorithms tend to be similar but favour Random Forests or related forest methods for most geological problems.

Random Forests are an ensemble learning method that combines multiple decision trees to improve predictive performance. Each decision tree in the ensemble is built using a subset of the training data, selected through a process called bootstrap aggregation, or bagging (Breiman, 1996, 2001). That means that each tree is trained on a random sample of the data, with replacement, resulting in approximately two-thirds of the data being used for training (bag samples) and the remaining one-third for validation (out-of-bag (OOB) samples).

The decision trees in a Random Forest can be either classification trees (for predicting categorical variables) or regression trees (for predicting numerical variables). At each node in a decision tree, a random subset of predictor variables is chosen to determine the best split. The final prediction of the Random Forest is obtained by averaging the predictions of all the individual trees.

To run the analysis of the decision trees, recursive splitting and multiple classifications or regressions are carried out from the dataset (for details, e.g., flowchart of Random Forest, see Rodriquez-Galiano et al., 2014). In other words, the Random Forest algorithm starts by splitting the target variable, or the parent node (root), into binary pieces, where the child nodes are 'purer' than the parent node. Through this process, the decision trees search through all candidate splits to find the optimal split that maximizes the 'purity' of the resulting tree. Whereas regression trees can be grown or pruned according to a specific condition, decision trees in Random Forest can be grown to maximum 'purity'. The Random Forest algorithm uses the Gini impurity index (Breiman et al., 2017) to calculate the information purity of child nodes compared to that of their parent node. Split thresholds are determined from the maximum reduction in purity (Breiman, 2001). From the root (parent) node, the data splitting process in each internal node of a restriction or condition of the tree is repeated until a pre-specified stop condition is reached.

3.1.2. Model metrics

Classification models, including Random Forest, are evaluated using a variety of metrics. These metrics are derived primarily by passing a subset of the labelled data which was not exposed to the training process (referred to as the 'test' set) through the trained model, and examining the proportions of correctly predicted samples and incorrectly predicted samples. Model Accuracy, for example, is the number of correctly predicted samples divided by the total number of samples in the test set. In a fictional test set consisting of 100 rock samples, 80 of which were correctly classified into their rock type, the model accuracy would be 80/100 = 0.8. In other words, assuming that the test set is representative of the training data, the model is likely to be correct 80 % of the time for new data. A variety of other metrics are calculated in similar fashion for distinct purposes, like Precision (intended to minimize false positives), Recall (minimize false negatives), and F1 (harmonic mean of precision and recall). When the labelling (knowns) for a dataset are well established, these metrics are an effective means of quantifying how well an algorithm will perform when it encounters new data. This can become problematic in the geosciences, where labels might be assigned somewhat ambiguously. Two scenarios often lead to ambiguity in labels (logs): 1) subtly distinct rock types might be labelled (logged) as rock type A by geologist X but rock type B by geologist Y; geologists X and Y may have both logged multiple holes in the training set, or 2) a gradational change between units of a geological feature like alteration facies; geologist X may place the boundary between two alteration types several meters above or below where geologist Y would. An additional problem affecting model metrics is mismatch in scale; geologists X and Y may be logging at a bench scale, ignoring minor lithologies within larger intervals. An algorithm trained on 2 m drillhole geochemistry samples, to reproduce geologist X and Y's classification, will produce a label for every 2 m sample, and be very likely to include those minor lithologies that were ignored initially. These restrictions do not invalidate application of machine learning to geological problems; they do, however, confirm that model metrics must be considered with caution and that review of outputs by experts in the deposit or geology in question is absolutely necessary.

3.1.3. Input data

Input drillhole data vary widely between cases, ranging from petrophysical data (Bressan et al., 2020), to image data (Alférez et al., 2021; Alzubaidi et al., 2021) for prediction of rock type, to compositional data (Ordonez-Calderon and Gelcich, 2018) for prediction of alteration type. Recent studies are showing the benefit of integrating multiple input data types to improve predictive outcomes (Houshmand et al., 2022, Trott et al., 2022).

For example, Trott et al. (2023), describe a workflow (Fig. 3), for incorporating textural features extracted from core photographs, compositional data from laboratory geochemistry, and mineralogical information from hyperspectral scanning data to predict alteration for the Josemaria porphyry copper-gold deposit in Argentina. The workflow describes steps taken to: (1) structure data types into a single (wide) table format, (2) refine the logged classifications to end members, (3) generate a predictive model (e.g., random forest), (4) extrapolate this prediction outward, and finally (5) reduce noise and simplify the predictions into scale-relevant domains apt for 3D modelling. The resulting model provides a (model) accuracy of 82.5 % with a standard deviation of 1.8 % (via 10 fold cross validation); an acceptable accuracy considering that this value is influenced significantly by ambiguity in the logged alteration used for validation, and the scale of logging (multiple meters per interval) compared with the scale of inputs (data structured to match the 2 m geochemical sampling interval).

Predicted alteration assemblages, as shown in Fig. 4b, are granular, noisy, and clearly more detailed than the original scale of logging (Fig. 4a). However, each prediction is accompanied by a class membership probability (CMP), plotted in Fig. 4c. CMP is a measure of similarity between a sample and each class, calculated by summing the number of trees predicting that class and dividing it by the total number of trees. In other words, if a Random Forest predicts a sample as 'phyllic' alteration in 150 trees, and 'advanced argillic' in 50 trees, the sample's CMP(phyllic) = 150/200 = 0.75, and CMP(advanced argillic) = 50/200 = 0.25. In this sense, CMP values are useful for determining how well a given sample matches its predicted category (similar alteration types may have similar CMPs, for instance, as seen in 4c around 50 m depth, where the CMP for advanced argillic (pink trace) is only slightly lower than the CMP for sericitic (yellow trace) alteration. This is a useful means of relating results to transitional geological phenomena, and also provides numeric values that permit denoising and domaining

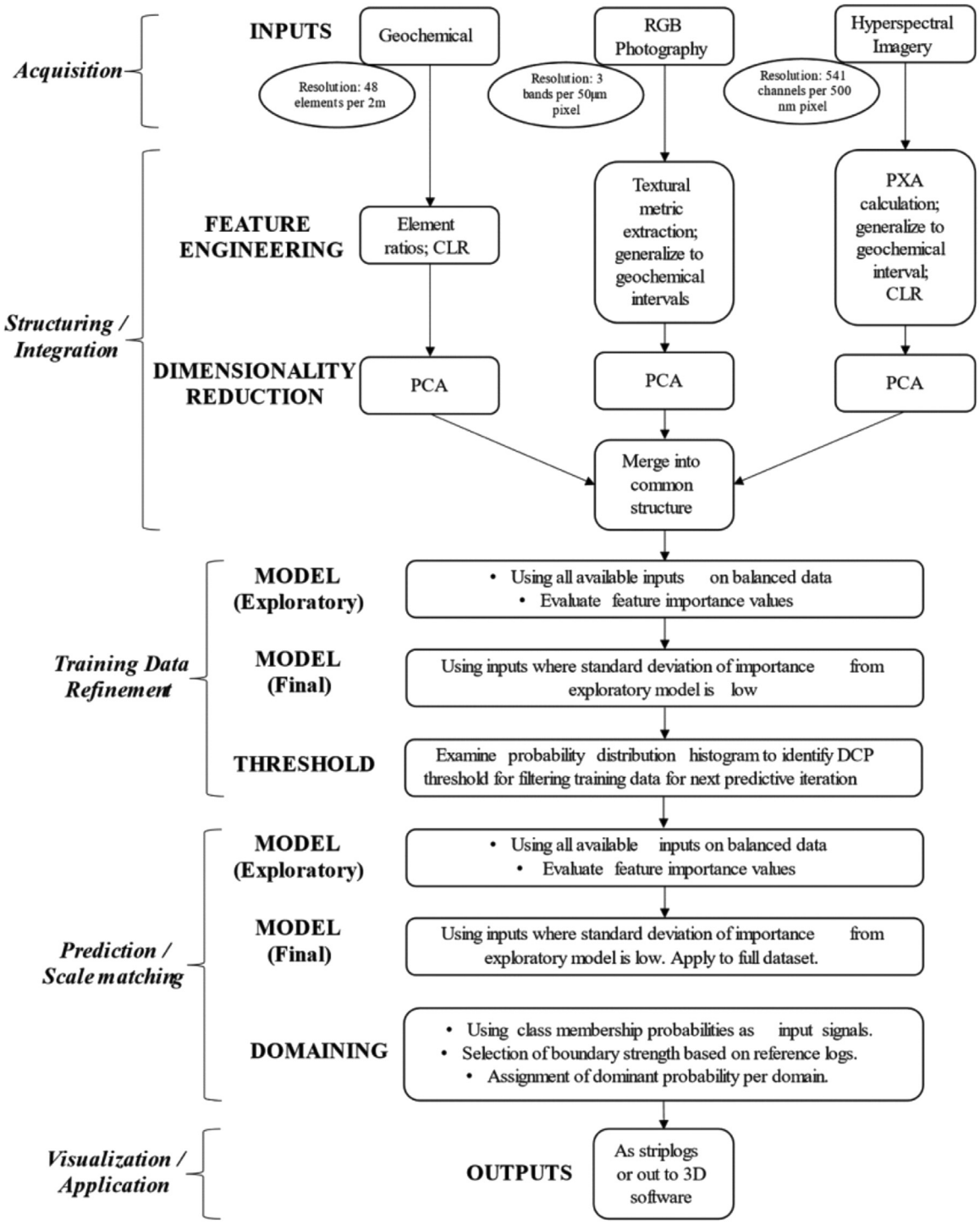

Fig. 3. Schematic visualisation of the workflow described in Trott et al. (2023). CLR, centred-log ratio; DCP, dominant class probability; PCA, principal component analysis; PXA, pixel abundance; RGB, red–green–blue.

of predictions that are not otherwise possible with categorical results (Fig. 4).

3.1.4. Multiscale multivariate continuous wavelet transform tessellation

Numeric data with a single spatial dimension (i.e., depth) can be denoised and domained using Multiscale multi-variate continuous wavelet transform tessellation (MMCWTT). This process, designed for boundary detection, consists of several chained techniques from the field of signal analysis (Hill et al., 2015; Hill and Uvarova, 2018; Trott et al., 2023). In soft terms, input signal(s), in this case Class Membership Probabilities (CMPs), are convolved with a gaussian kernel at a range of scales, to efficiently calculate zero crossings of the second derivative wavelet coefficients which highlight where these signals change in terms of depth and scale (boundary strength; Fig. 5a). A rectangular tessellation (Fig. 5b) is then generated using these depths and boundary strengths to facilitate identification of the depths where these changes occur at a given scale, or boundary strength (Hill et al., 2021). In the context of de-noising predictions for alteration types at the Josemaria por-

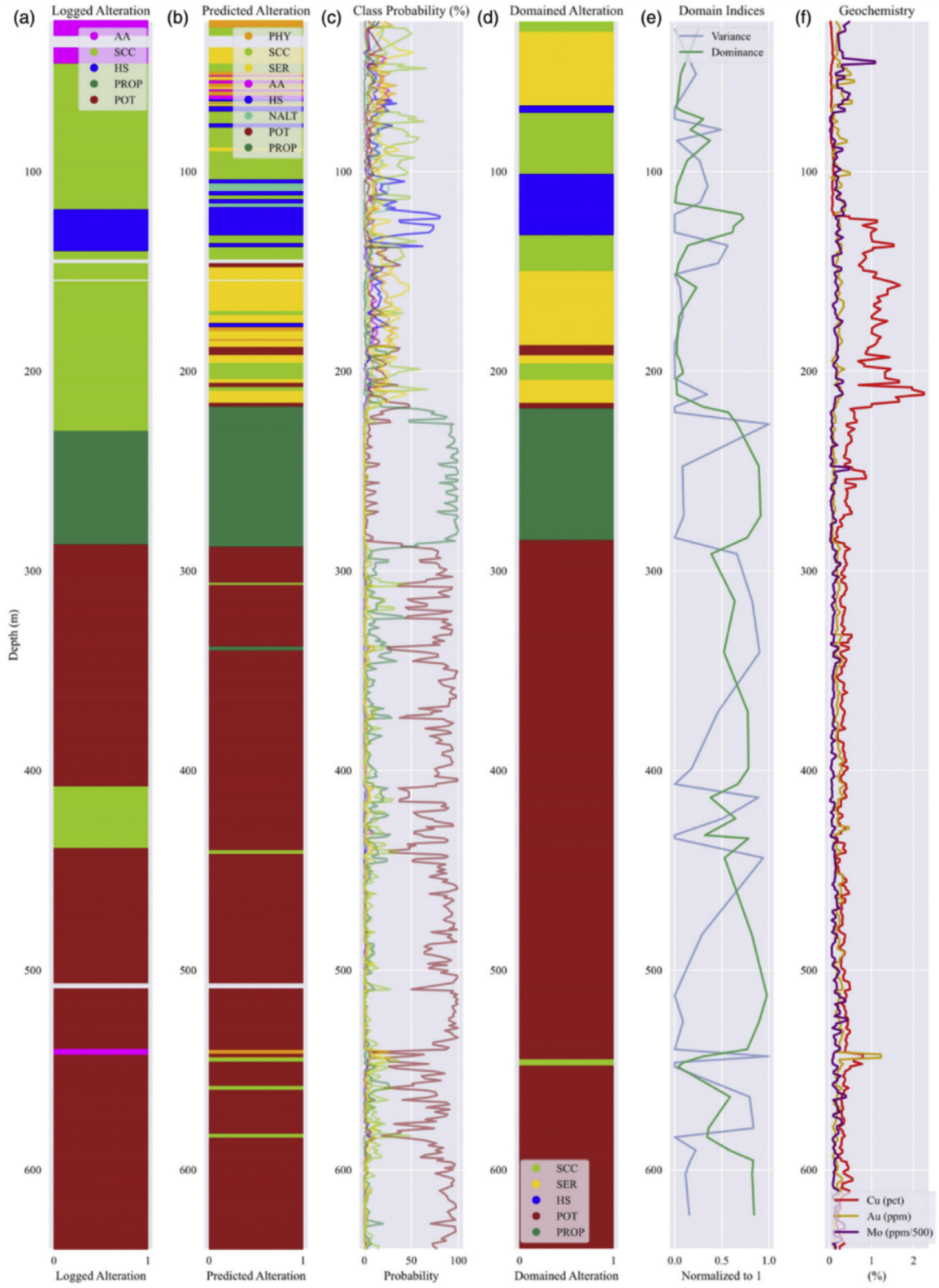

Fig. 4. Example from Trott et al. (2023) showing (a) logged alteration, (b) predicted alteration (noisy), (c) class probabilities for predicted alteration types, (d) denoised (domained) predicted alteration, (e) domain indices, and (f) geochemistry (mineralization elements for comparative purposes). AA, advanced argillic; HS, high sulfidation; NALT, sodic; PHY, phyllic; POT, potassic; PROP, propylitic; SCC, sericite-chlorite-clay; SER, sericitic.

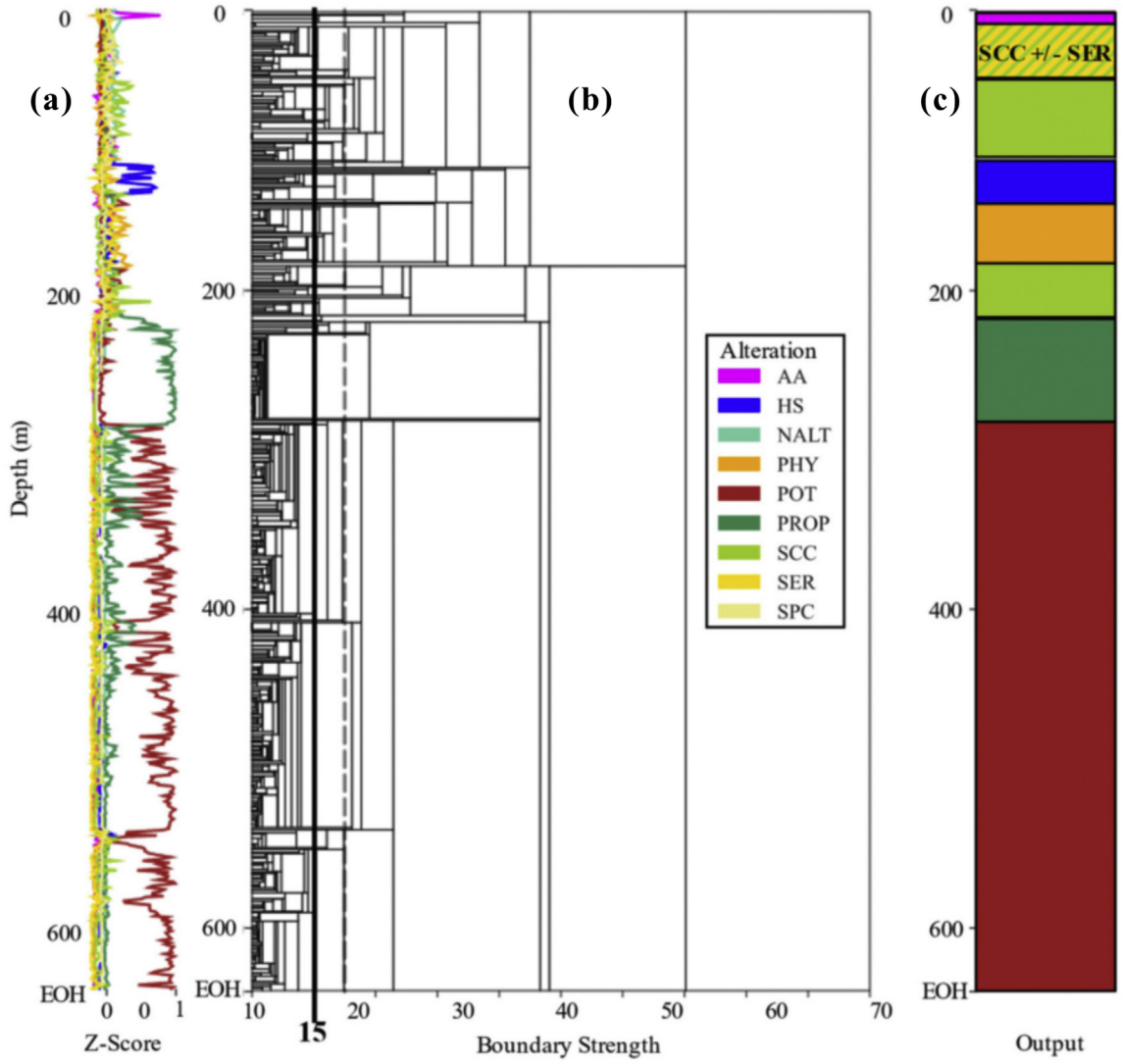

Fig. 5. (a) Class membership probability (CMP) traces (Trott et al., 2023). (b) The depths of tessellated boundaries (*y*-axis) with corresponding strengths (*x*-axis). (c) The denoised classification calculated at the selected boundary strength (15). SPC, sericite-pyrite-clay; please refer to Fig. 4 for explanations of other abbreviations.

phyry copper-gold deposit, this method was used to identify the appropriate scale and consistently simplify predictions into the domains defined at that scale by taking the class with the highest average CMP for any given interval, as shown in Fig. 5d.

This allows the granularity of the initial predictions (Fig. 5b) to be removed consistently across a very large dataset, and result in predicted alteration intervals predicted in an internally consistent fashion. The model accuracy, if recalculated using the domained output for test holes, rather than initial predictions, would be a more valid measure of the real-world applicability of the workflow.

3.2. Lithological mapping

Lithological mapping of an area is a fundamental starting point of any exploration venture aiming towards a mineral deposit discovery. Typically, these lithological maps are produced by interpreting and combining multiple different overlaying datasets, including different types of field observations and geophysical dataset collected in ground, airborne or satellite surveys (El-Omairi and El Garouani, 2023). Geophysical datasets have been found to be increasingly important during this initial stage of exploration work, with mineral exploration being conducted in remote areas and in locations with limited outcrop. Producing lithological maps has typically relied on geoscientists manually interpreting these datasets, and while expert geoscientists are able to combine and overlay multiple datasets and make meaningful and insightful interpretations, the process is time-consuming and is often a subjective interpretation by one geoscientist which can lead to significant discrepancies (Davies et al., 2020a). ML models have proven to be useful in supporting geoscientists in finding subtle patterns across different, seemingly non-associated features in overlaying datasets (Singh et al., 2024).

When a ML model is trained on appropriately distributed and scaled training data, it can be applied to, for example: (1) validating and querying pre-existing interpreted lithological maps and (2) assisting geoscientists in testing their lithological interpretations. Samples in training datasets such as field observations are usually clustered and not appropriately distributed, due to limiting factors in obtaining the samples such as outcrop exposure and time constraints. Therefore, field observations have an inherent spatial bias, and ML algorithms will erroneously model the closer samples to be more related than samples that are farther apart. To counter this issue, it is possible to use some form of neighbourhood model during the pre-processing stage of setting up a supervised ML classification scheme (Gahegan, 2000).

Lithological maps are often based on sparse field observations, combined with geophysical datasets. ML models provide a robust tool to test pre-existing maps, which are often misleadingly taken

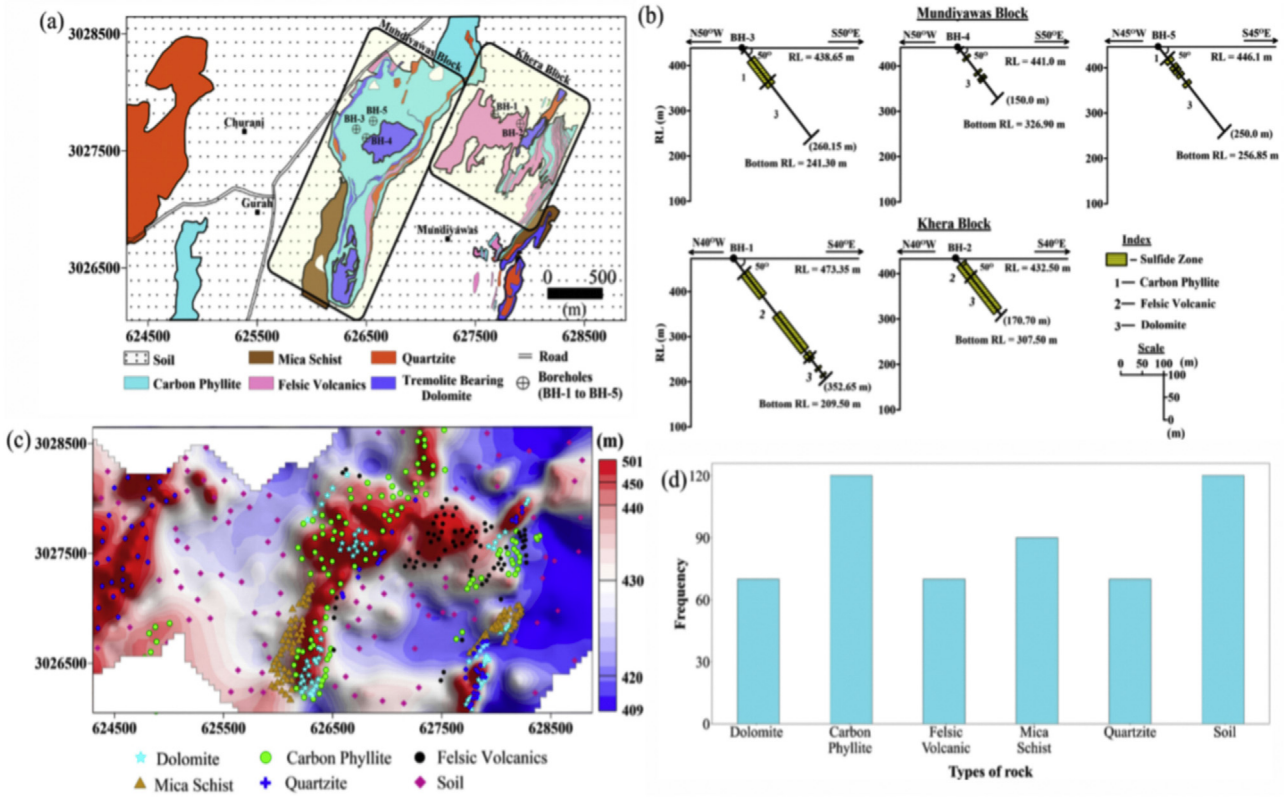

Fig. 6. (a) Geology map, (b) drillhole information, (c) topography map of Mundiyawas-Khera Cu deposit, Alwar basin (taken from Rao et al. 2019), (d) count plot of each lithology. The location of samples considered for the study is shown in (c) (from Singh et al., 2024).

as truth and not an interpretation. By running different iterations, a geoscientist can figure out how the original authors came to their conclusions, find weak spots in the interpretation, and come up with new interpretations in a rapid and cost-effective manner. Such desktop studies can lead the geoscientist to ask the right questions and, for example, pull out relevant drill core to query and develop the existing exploration model. By querying pre-existing lithological maps an ML model can highlight unrecognised locations for potential mineralisation and downgrade others that had been considered prospective. This can significantly advance geological understanding, point an exploration team in the right direction, and save critical exploration dollars.

It is essential for the geoscientist working with the ML model to understand the benefits and limitations of different datasets. For example, analytical signal and derivates of geophysical datasets such Bouger gravity and magnetic data are sensitive to the edges of lithological units (Dentith and Mudge, 2014). Singh et al. (2024) and Cracknell and Reading (2014) conducted lithological mapping studies to compare the performance of multiple ML algorithms. These studies involved the supervised classification of lithology, using potential field geophysical datasets. The study areas comprised Mundiyawas-Khera area of the Alwar basin in Rajasthan, India (Fig. 6) and an approximately 160 km^2 region located near Broken Hill, far western New South Wales, Australia. Both studies found that, in this context, the random forest (RF) algorithm either matched or outperformed Naive-Bayes (NB), k-nearest neighbors (kNN), support vector machines (SVM), multi-layer perceptron (MLP), gradient boosting (GB), and artificial neural networks (ANN) algorithms. Random forest was considered straightforward to train, computationally efficient, highly stable with respect to variations in classification model parameter values, and as accurate as, or substantially more accurate than the other ML algorithms trialled.

Many lithologies can be distinguished by their relatively high or low response in geophysical surveys. However, expert geoscientists can make more accurate predictions by studying an image of a geophysical survey, taking specific interest in the texture of geological units as they are represented in the survey. A potential future research direction for ML applied to lithological mapping would be to incorporate textural information alongside absolute values from potential field geophysical surveys, such that this existing technique is better integrated with machine vision methods.

3.3. Mineral analyses for metallogenic fertility

Igneous rock suites associated with porphyry copper (Cu) deposits typically exhibit a distinctive whole-rock geochemical signature, which has been recognized as an indicator of metallogenic 'fertility.' This term refers to the predisposition of magmas with such signatures to form porphyry Cu mineralization. Several geochemical characteristics have been identified as markers of magma fertility, including high Sr/Y, high La/Yb, high Eu/Eu*, high Sr/MnO, and high Al_2O_3/TiO_2 (Baldwin and Pearce, 1982; Richards, 2011; Wilkinson, 2013; Loucks, 2014; Ahmed et al., 2020; Mafra et al., 2024). These features are increasingly being utilized in porphyry Cu exploration (Cooke et al., 2020).

The distinctive geochemical composition is thought to arise from processes that are significant in the generation of magmas responsible for porphyry Cu deposits. These processes are typically associated with strongly compressional tectonic regimes that promote crustal thickening and prolonged magma storage at deep crustal levels (Sillitoe, 2010; Richards, 2011; Chiaradia and Caricchi, 2017; Wu et al., 2024). Such conditions lead to the differentiation of magmas at high pressure and elevated melt H_2O contents, thereby stabilizing amphibole and, to a lesser extent, garnet, which

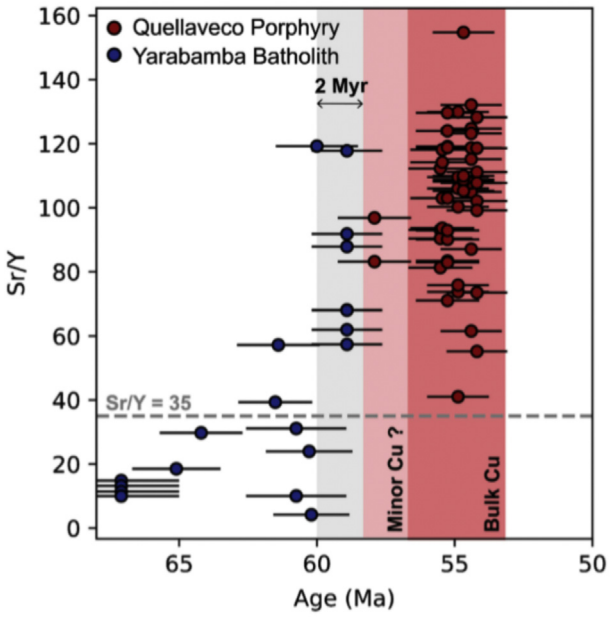

Fig. 7. Scatterplot showing whole-rock Sr/Y in the Quellaveco district, Southern Peru (data from Nathwani et al., 2021) as a function of emplacement age determined by zircon U–Pb LA ICP-MS data. Error bars are 2σ errors on the weighted mean with a propagated 2 % systematic uncertainty. Dashed line indicated the 'fertile' threshold for Sr/Y proposed by Loucks (2014). Shaded regions indicated the time periods of bulk Cu minerasation (darker red) at Quellaveco (Simmons, 2013; Nathwani et al., 2021). Plot indicated that high Sr/Y ('fertile') compositions were present in the ~2 Myr period to the onset of Cu mineralisation (grey shaded region) and peaked during bulk Cu mineralisation (from Nethwani et al., 2022).

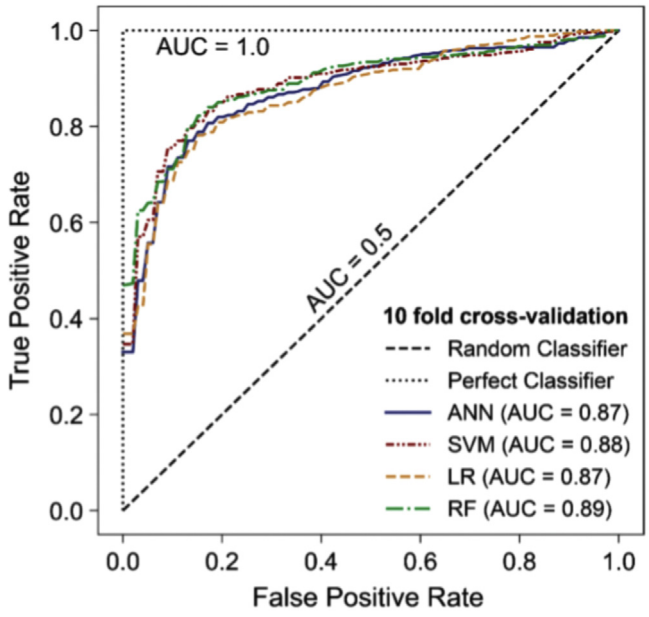

Fig. 8. Receiver operating characteristics (ROC) curves for each machine learning technique, showing the true positive rate versus false positive rate as the classification threshold is varied between 0 and 1. The ROC curve for each model is an average of 10 curves from the tenfold cross-validation, determined by the trapezoid rule. This gives an Area Under Curve (AUC) value between 0.0 and 1.0. For reference, a random (AUC = 0.5) and perfect classifier (AUC = 1.0) are shown (from Nethwani et al., 2022). ANN, artificial neural networks; SVM, support vector machine; LR, linear regression; RF, random forest.

are compatible with Y, middle rare earth elements (MREEs), and heavy rare earth elements (HREEs). In contrast, plagioclase, which is compatible with Sr and Eu, is suppressed. These conditions give rise to the geochemical characteristics described above, which can be discriminated from typical arc rocks using bivariate thresholds (e.g., Loucks, 2014; Ahmed et al., 2020; Wells et al., 2021).

Although such classification methods are useful, they have limitations. Specifically, they overlook additional variables that could potentially provide fertility signals and may result in false positives, as other processes can generate similar geochemical signatures. Furthermore, some parameters may be subject to alteration due to hydrothermal processes. False negatives also remain common in porphyry-related rocks, particularly those with less evolved compositions (e.g., SiO_2 < 65 wt%; Loucks, 2014) or in more variable tectonic settings associated with alkaline magmas and gold-rich porphyry deposits (Chiaradia, 2020).

In a study conducted by Nethwani et al. (2022), four ML algorithms—random forest (RF), logistic regression, artificial neural networks (ANN), and support vector machine (SVM)—were tested to classify the metallogenic fertility of rocks using a global whole-rock geochemical dataset (Fig. 7). The objective was to differentiate samples associated with porphyry Cu deposits from those not linked to known mineralization. The study's findings indicated that all algorithms, except for SVM, achieved similar high accuracy scores (81–83 %), surpassing the performance of traditional bivariate classification methods, which yielded accuracy scores between 65 % and 69 % (Fig. 8). Among the tested algorithms, random forest was preferred due to its ability to easily evaluate feature importance and visualize results.

3.4. Mineral prospectivity mapping

Mineral prospectivity analyses have emerged as powerful tools for spatially mapping the potential distribution of minerals across regional to camp scales (McCuaig et al., 2010; Yousefi and Nykänen, 2017; Cheng et al., 2024). Traditionally, these analyses were qualitative, relying on expert judgment to combine geological, geochemical, and geophysical datasets with deposit models to define prospective targets. However, advancements in statistical modelling and GIS software have revolutionized the field, enabling more robust and quantitative approaches (Fig. 9).

Modern prospectivity analyses leverage both data- and knowledge-driven methods to identify and evaluate key mineral system processes and their influence on mineral distribution. Data-driven techniques are based on empirical associations between known deposits and underlying mineralizing processes (e.g., Singer, 1975; Porwal et al., 2003; Joly et al., 2012). In contrast, knowledge-driven approaches rely on conceptual models and expert input to define key processes and assign relative importance to them (e.g., Joly et al., 2012; Chudasama et al., 2016; Levaniemi et al., 2017). Recent advancements have integrated these approaches, combining data-driven insights with knowledge-driven frameworks to enhance analytical accuracy and incorporate uncertainty measures (e.g., Porwal et al., 2006; Lisitsin et al., 2014; Hronsky and Kreuzer, 2019).

A notable evolution in assessment models is the shift from deposit-based to process-based approaches, where the focus is on understanding mineralizing systems and mapping their constituent processes (e.g., Porwal and Kreuzer, 2010; Yousefi et al., 2019; Groves et al., 2022). While various datasets are utilized to represent these processes, many analyses prioritize structural architecture and data closely related to mineralization, such as geochemical pathfinder elements, rather than explicitly mapping broader system processes.

Mineral prospectivity mapping is essential for delineating and ranking areas favourable for mineral deposit exploration (Bonham-Carter, 1994; Carranza, 2009, 2011). Machine learning (ML) extends GIS-based mapping by training models with known deposit locations to identify geoscientific features indicative of mineraliz-

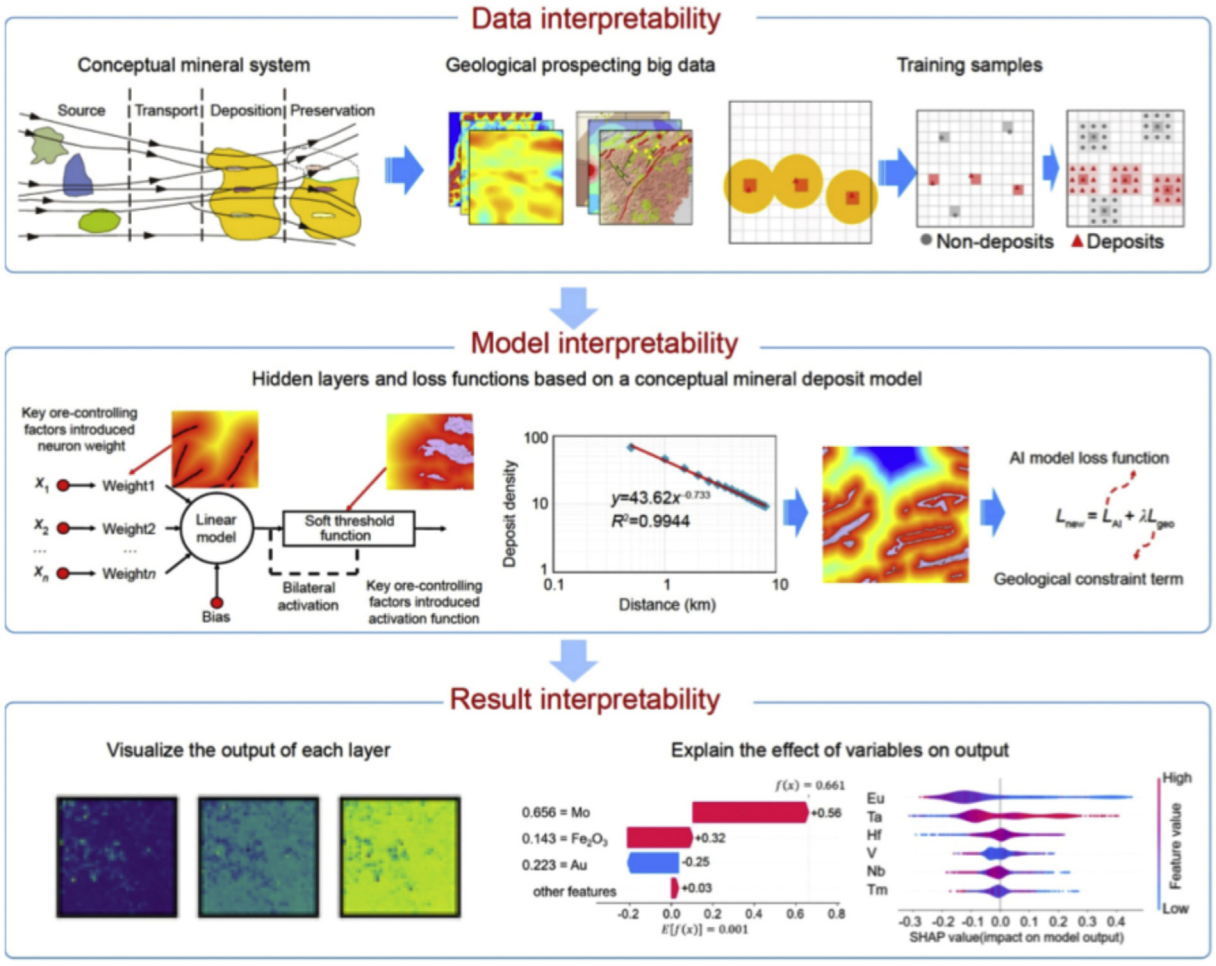

Fig. 9. Schematic representation of interpretability in the context of ML models used for mineral prospectivity mapping (Zuo et al., 2024).

ing processes or ore body footprints. This data-driven predictive modelling is particularly effective in moderately to well-explored (brownfield) regions.

Common multivariate techniques for data-driven mapping include logistic regression (e.g., Chung, 1983; Carranza and Hale, 2001), random forest regression (Carranza and Laborte, 2016; Costa et al., 2019), and artificial neural networks (e.g., Singer and Kouda, 1996, 1999; Harris et al., 2003). These methods analyse spatial associations between training locations and evidential datasets to predict prospective areas. For example, the random forest regression algorithm uses training data consisting of 1s (deposit locations) and 0s (non-deposit locations) to construct multiple regression trees. This generates predictions as likelihood values (0–1) for deposit occurrence, which can be classified using threshold values to distinguish prospective from non-prospective areas (Rodriguez-Galiano et al., 2014).

Emerging methods, such as time-series modelling, are gaining attention in geosciences. Farrar et al. (2023), for instance, combined ML with time-series modelling of plate reconstruction models to predict both spatial and temporal aspects of porphyry copper mineralization associated with plate tectonics in the central Andes, offering new dimensions to mineral prospectivity research.

4. Application of machine learning to critical mineral exploration: future direction and recommendations

Following the AI boom of the late 2010's, significant funding has been invested into developing ML models within the minerals industry. However, this is yet to translate into significant exploration success, as greenfield discovery rates remain much the same or even in decline over the last 20 years (Schodde, 2023). Despite the technological advances and increased exploration spending this century, the root cause of declining discovery rates is primarily the decreasing number of orebodies that remain outcropping and undiscovered on the surface (McCuaig and Hronsky, 2014; Farrar et al., 2023). Most future discoveries of critical mineral deposits will therefore be either wholly or partially obscured at surface by post-mineralisation cover. As yet, the exploration industry has not demonstrated the tools or knowledge to systematically make repeatable and predictive discoveries of ore deposits through post-mineralisation cover. The transition from making predictions in a geologically data rich, outcropping environment, to a 'blind' covered environment, presents a significant challenge to the exploration industry. ML techniques are expected to play an increasingly greater role in leveraging all available data to assist predictive exploration (Kwan et al., 2025).

Several factors may help to explain the underperformance or lag of ML applications contributing to exploration success, these include: high-complexity/dimensionality of geoscience problems combined with datasets of inconsistent quality and coverage; paucity of positive training data due inherent scarcity of economic ore deposits; reduced access to data science practitioners due to competition for talent with other industries such as technology; limited cross-disciplinary collaboration within the geosciences, leading to poor performance of generalised models; remote location of worksites making access to high-speed internet and computation difficult; and inherent scepticism within the extractive mining industry, where ML is can be traditionally viewed

as irrelevant, too high-risk and/or too uncertain. Additionally, much of the application of ML within the exploration industry has been focussed on improving orebody knowledge, or drilling and mining efficiencies (see Sections 3 and 4), rather than explicit prediction of undiscovered orebody location via prospectivity mapping.

There are a number of review papers on ML applied to the minerals industry (e.g. Jung and Choi, 2021; Jooshaki et al., 2021; Woodhead and Landry, 2021). These provide a comprehensive overview of existing literature and research efforts, but contain only limited comments on how we might better apply this technology going forwards, particularly with regards to overcoming specific challenges that the industry faces. The discussion below attempts to make progress on this front.

4.1. Limitations of machine learning

Creative thinking is fundamental to devising innovative solutions to complex, high-dimensional challenges. In mineral exploration, past explorers focused on testing specific hypotheses. Since mining involves sampling without replacement, the economic discoveries made by previous explorers are no longer available within the search space (Davies et al., 2020b). As a result, it is essential for future exploration to examine new hypotheses that address different search areas or concepts involving slightly modified deposit types. Additionally, exploring under-developed search spaces requires navigating data-poor environments (Davies et al., 2020c), where explorers must bridge significant gaps in existing geoscientific datasets to predict outcomes and integrate with ongoing exploration efforts (Aitken et al., 2018).

Focusing solely on technological advancements overlooks the critical role of human innovation in generating and evaluating multiple predictions based on diverse datasets (Davies et al., 2020d). Techniques like 'deep learning' have significantly advanced AI's ability to explore creative domains (Schmidhuber, 2015). However, this creativity has been criticized for merely replicating existing patterns rather than producing truly novel outcomes (Davis and Marcus, 2015; Marcus, 2018). In terms of evaluating predicted hypotheses, current AI systems face limitations in understanding correlations and avoiding biases, as their deep learning methods are often poorly aligned with prior knowledge (Fjelland, 2020).

With the right training data, AI and machine learning can effectively predict the locations of well-known deposits in data-rich environments. However, AI is still far from capable of identifying new deposit types or search areas based on a holistic understanding of Earth sciences. In conclusion, mineral exploration is recognized as a complex, non-linear process. While AI and technological advancements offer promising opportunities to improve exploration targeting, a combination of technology and human creativity is vital for achieving sustainable, long-term success (Davies et al., 2021).

4.2. Issues related to team structure

As for major advances in geochemistry and geophysics, there is an expectation that the application of ML in mineral exploration should result in a significant discovery. The lack of any notable ML-led discoveries is sometimes used as an argument against further uptake of this technology by industry. This, however, misses a fundamental characteristic of ML. It represents a mathematical technique, not a new geoscientific dataset within which geoscientists might realise the location of an undiscovered orebody. Discoveries are the result of collecting new data or re-analysing existing data in a new or novel manner, but the underlying dataset remains geoscientific in nature. Within mineral exploration, ML is best employed in a supporting role to help geoscientists better understand conventional geoscientific datasets.

Applying ML to existing geoscientific datasets requires effective collaboration between data scientists and experts in each sub-discipline of geoscience. Data scientists versed in the application of ML are required to work closely and consistently with a diverse team of geoscientists, made up of individuals specialising in geochemistry, geophysics, structural geology, economic geology, resource geology, mineralogy, etc. The augmentation of machine computing power and human expertise has only more recently become a focus of AI researchers (e.g., Marcus, 2020). There are a number of actions that we as an industry can do to maximise the effectiveness of such a combination.

According to Page (2008), the Diversity Prediction Theorem states that 'when the diversity in a group is large, the error of the crowd is reduced.' In practice, this suggests that exploration teams perform better when they have greater diversity in skills and background experience. Additionally, Woodall (1994) presented the argument that empirical and conceptual strategies should be balanced within exploration teams, and Nemeth and Wachtler (1983) called for industry to promote open discussion and dissent in order to avoid closed-mindedness and 'groupthink' leading to defective decision-making (Janis, 1972).

Explorers require a degree of autonomy and a safety-net in order to be confident enough to take risks and test novel search ideas (Davies et al., 2020d). Clear goal-oriented strategies provide a focus of attention to relevant information, and management can provide a framework to mitigate and challenge excessive risk-taking and minimise consequences of inevitable failures. Bond et al. (2012) found that having a MSc or PhD qualification significantly improved expert performance in interpreting a geoscientific dataset. The development of practical scenario-based training courses is identified as a significant opportunity to improve the effectiveness of exploration teams (Davies et al., 2020d), and integration of ML tools into such courses would improve their understanding, uptake, and implementation, thus benefitting exploration outcomes.

Adoption of these concepts by industry is required to current working environments that allow for effective application and integration of ML tools into existing exploration teams and their targeting practices.

4.3. Data challenges

Despite the lack of 'big data' being used within geoscience research, it would be remiss to assume mineral exploration comprises simple datasets. Data employed within exploration is both highly complex and, from a statistical perspective, poorly and inconsistently sampled.

For larger study areas, budget limitations typically require the collation of historical open-source datasets. Typically, each of these datasets differs enough to make direct comparison challenging. For example, geochemical surveys (e.g. soil sampling) may use different analytical methods to determine elemental concentrations for the same elements, or samples can be extracted from a subtly different medium or depth. These subtle differences make direct comparison of elemental concentration values between datasets unreliable. Geophysical datasets (e.g. airborne magnetic surveys) collected adjacent to each other are often stitched together to be used as a combined dataset. However, there are almost always differences in their collection parameters, for example, flight height and speed, line orientation and spacing, atmospheric conditions, sensor model and settings, etc. An expert geoscientist may be able to accommodate for these differences when visually analysing data. However, unless carefully handled and mitigated during the data preparation stage, such variability can lead ML models astray.

In addition to technical survey differences, sampling bias is often introduced during the design and planning of each survey. Due

to limited budgets, explorers select specific areas of interest for conducting surveys or may conduct a higher resolution survey in a spatially constrained location, with a preconceived expectation of what the results will present. These decisions can lead to discrepancies in data density, spatial distribution, and quality. There are often biases towards locations considered more prospective by previous explorers, and particularly areas containing known orebodies (Hronsky and Groves, 2008). When conducting exploration in less mature regions, areas with post-mineral cover, or with a new targeting concept in mind, it can be counter-productive to use detailed datasets from well-endowed regions as analogies. The same detailed datasets have typically not yet been collected and so do not exist outside of the well-explored domains. An ideal survey from a statistical perspective would involve randomly sampling both training and study areas and applying consistent methods of analysis. For commercial reasons, however, this approach is rarely taken in mineral exploration.

Significant mineral discoveries are a rare event in exploration, representing a significant deviation from the norm. Statistics, in general, is notoriously poor at handling outliers, and has proven even less effective at predicting them (e.g., economic forecasting unable to predict stock market crashes; Martin, 2009). The number of known orebodies available as a training set is extremely limited, and data collected on these orebodies is often unsuitable for direct comparison with less well-explored regions. Despite the opportunity afforded to develop greater contextual understanding at the more regional scale, deposit-scale datasets are rarely collected beyond the footprint of an orebody. Due to a combination of poor sampling with a lack of 'big data,' in terms of data quantity, the minerals industry faces a very difficult challenge to implement ML within exploration programs.

4.4. Philosophical differences in exploration

Mineral exploration poses unique challenges for the application of machine learning (ML), differing fundamentally from its use in more conventional contexts. Unlike traditional applications, where ML models aim to identify patterns with high accuracy, mineral exploration requires searching a finite space for subtle variations that may signal undiscovered ore deposits. This process involves training models to recognise patterns derived from known orebodies, to predict the locations of undiscovered orebodies. However, contrary to conventional applications of ML, an emphasis on achieving high accuracy may paradoxically hinder success.

A significant limitation arises from the scarcity of training data, since only a small number of known ore deposits are available, and these deposits are unlikely to perfectly resemble those yet to be discovered. Since mining involves sampling without replacement, undiscovered deposits will likely exhibit variations that diverge from the training dataset. Consequently, a different philosophical approach is necessary. Instead of prioritising model accuracy, practitioners are encouraged to adopt an exploratory mindset when applying ML in mineral exploration.

Studies by Jung and Choi (2021) and Jooshaki et al. (2021) devote substantial attention to comparing model types, output accuracies, and evaluation metrics. However, an excessive focus on these metrics risks diverting efforts from the development of practical and effective ML models for exploration purposes. Instead, interdisciplinary collaboration between data scientists and geoscientists is recommended to test hypotheses and tailor models to address specific geological questions or theories. This approach involves running multiple models with varying parameters and training datasets, allowing for subjective comparisons of their outputs. While this strategy may not yield a single high-accuracy model, it fosters collaboration and the creation of a diverse ensemble of imperfect models, each offering unique insights into the problem at hand.

Furthermore, data scientists are urged to prioritise innovative methods for presenting and communicating results to experts in other disciplines. This effort should be reciprocated by geoscientists, who can work to simplify complex geological terminology. ML algorithms that offer straightforward interrogation (e.g., random forest; Cracknell and Reading, 2014; Singh et al., 2024) and tools such as exploratory data analysis (EDA), data wrangling, missing data enrichment, and dimensionality reduction can be particularly valuable in this context. These techniques enable the manipulation and exploration of datasets, facilitating the generation and communication of deeper insights essential to advancing mineral exploration.

4.5. Conventional statistics

In general, geoscientists lack comprehensive training in statistics. Options for overcoming this limitation include the formation of multidisciplinary teams containing data science experts, and wider availability of additional statistics and ML modules as part of university geoscience courses. It is also suggested that a specific focus on AI and ML is limiting, and a broader approach would be beneficial. Although currently out-of-favour with many practitioners and the media, it is advised that analytical techniques are incorporated from across data science and traditional statistics.

Several authors (e.g., Hronsky and Groves, 2008; McCuaig and Hronsky, 2014; Lisitsin, 2015; Hagemann et al., 2016; Wyman et al., 2016; Davies et al., 2020a) have emphasized the importance of developing integrated spatial mineral system models. Porwal and Kreuzer (2010) highlighted that exploration models consist of two critical components: (1) the probability that a specific location hosts mineralisation, which depends on factors such as fertility, geodynamics, and first-order architectural features; and (2) the estimated quantity of mineralisation at a location for each probability level, influenced by second- and third-order architecture and preservation processes.

An integrated spatial model aims to support exploration decision-making by generating resource potential maps (Davies et al., 2020b). These maps enable practitioners to estimate the approximate cost-benefit, expressed as the risk-adjusted dollar value, associated with exploring a particular location (Porwal and Kreuzer, 2010). Complex systems modelling (e.g., weather, climate, groundwater, tidal) often incorporates computational, probabilistic and time-series modelling methods. These can be used to integrate multiple system components, each requiring individual sub-models (e.g., probabilistic time-series modelling of rainfall, as an input to a wider groundwater model). Focusing on a single area of data analytics, such as ML, reduces our options to effectively model, understand, and predict the behaviours of complex systems.

For challenges that cannot currently be fully modelled through analytical methods, the introduction of subjective Delphi or Judgemental modelling approaches would likely provide improved predictive outcomes (Kahneman and Klein, 2009). These involve collecting the opinions of experts in a structured manner. The results from ML models can be presented to a group of experts, who then make subjective assessments, where their opinions are polled and combined. Examples of these methods applied in geoscience include Polson and Curtis (2010) and Bond et al. (2012), with Singer and Menzie (2010) and Davies et al. (2020d) applying them to mineral exploration specifically.

5. Conclusions

The application of ML in the mineral exploration industry has primarily focussed on improving orebody knowledge, and drilling

and mining efficiencies, within data-rich environments. To date, ML is yet to demonstrate material impact in reversing declining discovery rates of critical minerals deposits, at a time when an increase in discoveries is required to provide the raw materials to sustain a global energy transition. This ongoing inability to leverage ML to drive discovery of new critical minerals deposits can be attributed to the following: an unrealised necessity to explore in areas of post-mineralisation cover; low training data quality and abundance, limited access to data science practitioners; insufficient interdisciplinary collaboration; high complexity of geoscientific problems; and the extractive nature of the mining industry, that can lead to scepticism regarding technological uptake. While existing review papers provide valuable overviews of ML applications, they often lack actionable recommendations to address industry-specific challenges.

Mineral exploration differs fundamentally from traditional ML applications, as it focuses on subtle variations in finite search spaces rather than high-accuracy pattern recognition. Exploration datasets are highly complex and inconsistently sampled. Budget constraints often lead to the use of historical datasets with variability in sampling methods, analysis, and collection parameters. Moreover, sampling biases, particularly in well-explored regions, limit the applicability of detailed datasets to less mature areas. Scarcity of training data, and the potentially unique deposit-scale characteristics of undiscovered deposits, necessitate an exploratory rather than accuracy-driven approach. While ML tools like deep learning are powerful, they often replicate existing patterns rather than generating novel solutions. Furthermore, current models struggle with understanding complex correlations and avoiding biases. Collaboration between data scientists and geoscientists, with expertise in sub-disciplines like geochemistry and structural geology, is essential to test hypotheses and create diverse ensembles of models.

The integration of ML into mineral exploration requires a paradigm shift toward multidisciplinary collaboration, innovative data handling, integration with conventional statistical techniques, and philosophical alignment with the field's unique challenges. A combination of advanced technology, human creativity, and robust statistical methods is crucial for improving discovery rates and achieving sustainable exploration success. As discussed by several papers in this Special Issue, most critical metal supply comes from finite resources in existing mines and adjacent brownfield exploration (e.g., Guj and Schodde, 2025) and there is limited critical metal recycling (Schodde and Guj, 2025). In the short-term, greenfield exploration must play an important role and limitations with the application of AI and ML need to be resolved to aid discovery. Human creativity remains essential to achieving these aims, with ML acting as a supportive tool rather than a standalone solution.

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.

CRediT authorship contribution statement

Rhys S. Davies: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **McLean Trott:** Writing – review & editing, Writing – original draft, Methodology, Conceptualization. **Jaakko Georgi:** Writing – original draft, Conceptualization. **Alexander Farrar:** Writing – review & editing, Conceptualization.

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