

Machine Learning in Petrology: State-of-the-Art and Future Perspectives

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Abstract

The present manuscript reports on the state-of-the-art and future perspectives of Machine Learning (ML) in Petrology. To do that, it first introduces the basics of ML, including definitions, core concepts, and applications. Then, it starts reviewing the state-of-the-art of ML in petrology. Established applications mainly concern clustering, dimensionality reduction, classification, and regression. Among them, clustering and dimensionality reduction are particularly valuable for decoding the chemical record stored in igneous and metamorphic phases and to enhance data visualization, respectively. Classification and regression tasks find applications, for example, in petrotectonic discrimination and geothermobarometry, respectively. The main core of the manuscript consists of depicting the next future for ML in petrological applications. I propose a future scenario where ML methods will progressively integrate and support established petrological methods in boosting new findings, possibly providing a paradigm shift. In this framework, the use of multimodal data, data fusion, physics-informed neural networks, and ML-supported numerical simulations, will play a significant role. Also, the use of ML hypotheses formulation and symbolic regression could significantly boost new findings. In the proposed scenario, the main challenges are: a) progressively link machine learning algorithms with the physical and thermodynamic nature of the investigated petrologic processes, b) unblur deep learning algorithms that too often operate as black boxes, c) go ahead in exploring cutting edge tools that rise from researches in Artificial Intelligence, and overall, d) start a collaborative effort among researchers coming from different disciplines in research and teaching.

Keywords: machine learning, artificial intelligence, petrology, volcanology, geochemistry, deep learning, physics informed neural networks, generative ai, foundation models, symbolic regression.

1. INTRODUCTION

Machine Learning (ML) has become an increasingly popular and effective tool in Physical Sciences over the past 10 years (Wang *et al.*, 2023a). With its ability to analyze large data sets and identify patterns that may not be immediately apparent to the human eye, ML has the potential to affect drastically, and possibly revolutionize, many fields in Geosciences (e.g., Bergen *et al.*, 2019; Reichstein *et al.*, 2019; Dramsch, 2020; Bortnik and Camporeale, 2021; Fleming *et al.*, 2021; Arrowsmith *et al.*, 2022; Li *et al.*, 2023c), including petrology (e.g., Petrelli and Perugini, 2016). To start depicting the state of the art of ML in Petrology, Fig 1A shows the impact of manuscripts dealing with the application of ML to Earth and Planetary Sciences on the Scopus record by year, starting from 2000. Fig 1A highlights that a few publications have been published per year on ML until 2010. Then, the Scopus record experienced nearly exponential growth, highlighting the great interest of Earth Scientists in the field (e.g., Bergen *et al.*, 2019; Reichstein *et al.*, 2019; Dramsch, 2020; Bortnik and Camporeale, 2021). The observed trendline has been mainly driven by studies involving remote sensing and global Earth models (Reichstein *et al.*, 2019; Toms *et al.*, 2020; Bortnik and Camporeale, 2021; Fleming *et al.*, 2021; Geer, 2021; Li *et al.*, 2022a). Currently, the manuscripts record dealing with ML in Earth and Planetary Sciences is approaching the total number of manuscripts that have been published in Igneous and Metamorphic Petrology (Fig. 1A). In Petrology, we observe the same trend (Fig. 1B). However, ML petrological studies can be still considered niche, with the number of publications not exceeding 100/years yet. Observing Fig. 1B, it is not difficult to guess that ML will start playing a significant role in petrological studies soon in the future, as already occurred in many other scientific fields like large experimentations on particle physics (Karagiorgi *et al.*, 2022), biology (Webb, 2018), medicine (Deo, 2015; Rajkomar *et al.*, 2019), and engineering (Salehi and Burgueño, 2018; Montáns *et al.*, 2019). In particular, as reported by Wang *et al.* (2023a) ML methods are being

“increasingly integrated into scientific discovery to augment and accelerate research, helping scientists to generate hypotheses, design experiments, collect and interpret large datasets, and gain insights that might not have been possible using traditional scientific methods alone”.

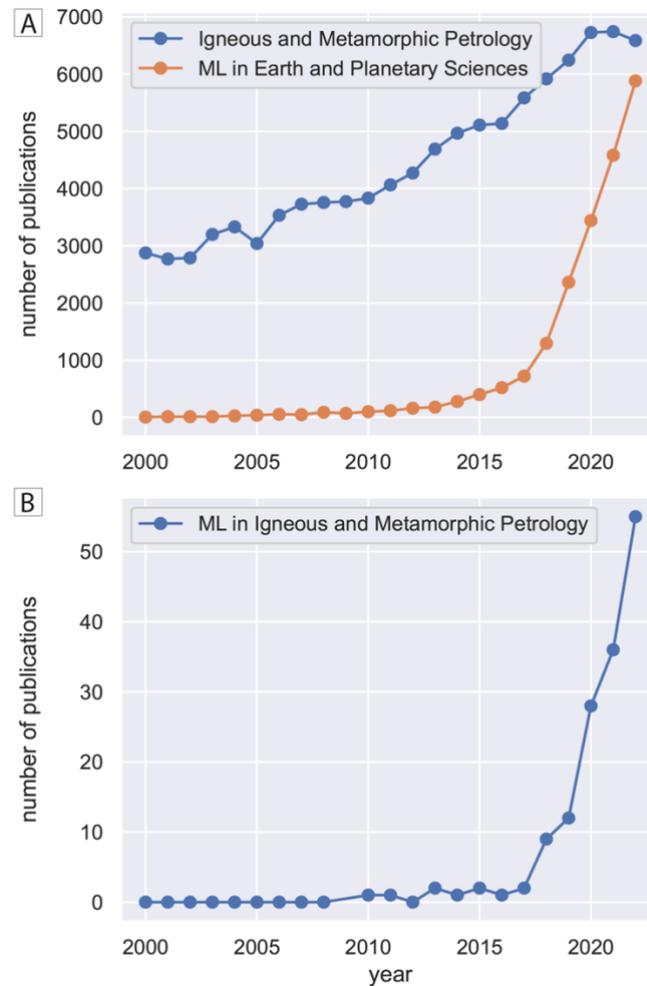


Figure 1: Scopus trends per year of the manuscripts published in: A) “Igneous and metamorphic petrology” and “Machine Learning in Earth and Planetary Sciences”; B) “Machine learning in igneous and metamorphic petrology”.

In principle, ML methods can support all the stages of petrological research, including, data acquisition, hypothesis formation, modeling, and uncertainty estimation (Wang *et al.*, 2023a). Nowadays, petrological applications of ML are mostly focused on data-driven pattern recognition (Fig. 2A), as depicted by Petrelli and Perugini (2016). In detail, Fig. 2A highlights a few interesting, but limited, applications of ML in petrology. These methods are currently well established and they include clustering, dimensionality reduction, classification, and

regression. Recent advances in the field, like the development of Deep Neural Networks (Aggarwal, 2018), including physics-informed algorithms (Karniadakis *et al.*, 2021), Generative AI (Ghosh and ATLAS collaboration, 2022), Transformer architectures (Vaswani *et al.*, 2017), and Foundation Models (Bommasani *et al.*, 2021), drastically pushed the potential of ML in petrology over the expectation reported by Petrelli and Perugini (2016).

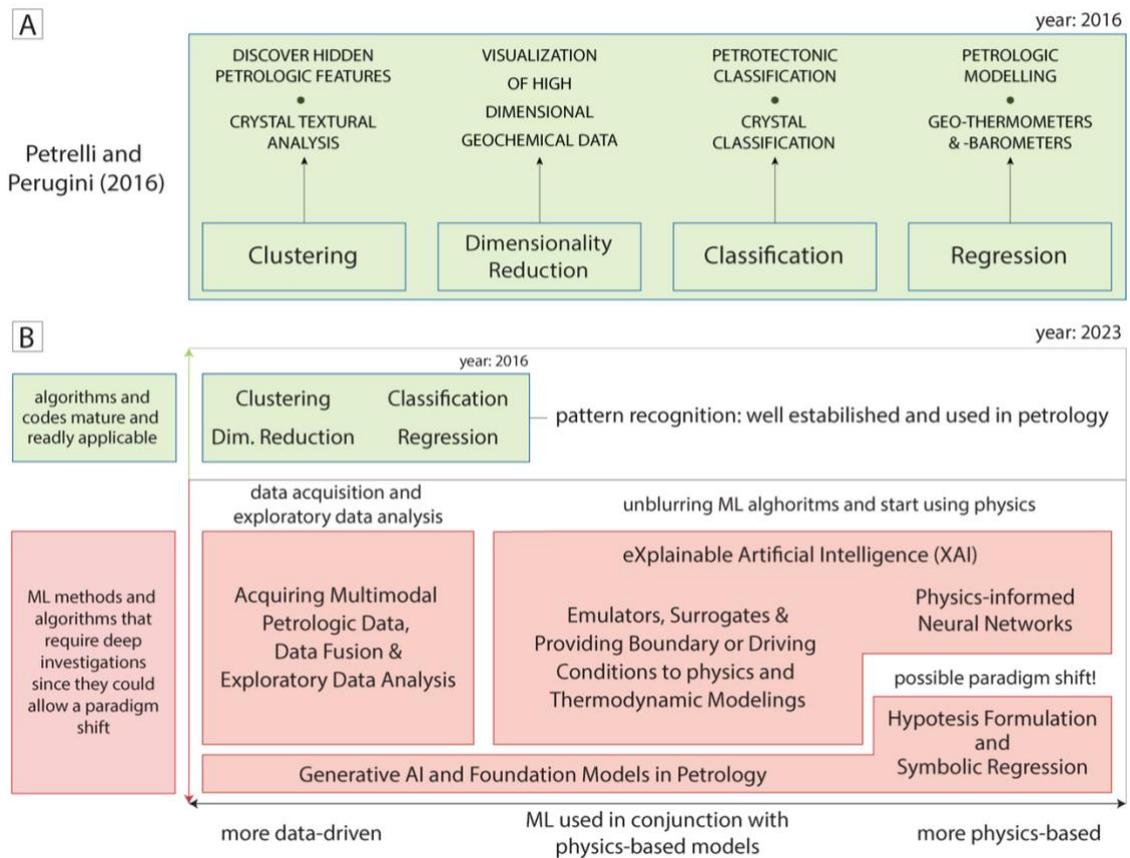


Figure 2: Two scenarios depicting the application of Machine Learning in petrology as A) reported by Petrelli and Perugini (2016) and B) proposed in the present manuscript (modified from Petrelli and Perugini, 2016 and Bortnik and Camporeale, 2019).

Figure 2B reports the evolution of Fig. 2A and depicts, together with present uses, a future scenario for the application of ML in petrology, as currently proposed by the author of this manuscript. Fig. 2B is at the same time intriguing and challenging and it drastically expands the scenario reported in Fig. 2A. The main idea behind Fig. 2B is to push the current application of ML in petrology by progressively linking ML methods with the fundamental

laws of Physics and Thermodynamics, possibly producing a paradigm shift. Petrologists are currently deeply involved in the investigation, development, testing, and application of ML techniques making new models and solutions at a continuously increasing rate (Petrelli *et al.*, 2020; Zhang *et al.*, 2020; Le Losq *et al.*, 2021; Luo *et al.*, 2021a; Schönig *et al.*, 2021; Valetich *et al.*, 2021; Musu *et al.*, 2023; Wang *et al.*, 2023b; Zhong *et al.*, 2023a).

As a drawback, many of the applications reported in Fig. 2B are not fully mature yet and deserve further investigations and deeper understanding before being fully accepted by the petrological community. Also, many critical issues still persist. As an example, poor knowledge of the mathematics behind the investigated ML models and the management of the algorithms by non-experts could lead to biased models (Fleming *et al.*, 2021). Also, the quality of data is a fundamental prerequisite since it's almost impossible to have an effective ML model with bad data. In the following sections, I am going to review the state of the art for the application of ML in petrology and discuss its future potential. I start by providing an overview of ML techniques and their applications in petrology. Then, I discuss some of the challenges associated with using ML in petrology and highlight some recent advances that have been made in this area. Finally, I conclude by discussing some of the future directions that I believe ML research in petrology will take.

2. BASICS OF MACHINE LEARNING

This section provides basic definitions and concepts to allow all petrologists to start understanding ML algorithms and workflows.

2.1 Definitions

In one of the early attempts to define ML Samuel (1959) stated “a computer that can learn how to solve a specific task, without being explicitly programmed.” Later, Mitchell (1997) provided a more formal definition: “A computer program is said to learn from experience E with respect to some task T and some performance measure P if its performance on T , as measured by P , improves with experience E .” In other words, ML methods try to convert experiences to knowledge. Please note that, in physical sciences, the experience almost always coincides with data. Therefore, ML methods attempt to convert raw data into knowledge. In the so-called data-driven approach, ML algorithms attempt to solve problems relying on the provided data only (Shai and Shai, 2014). In other words, ML algorithms try to solve the problem even if the researcher cannot provide an explicit path to achieve the solution of additional physical constraints. For example, in regression tasks, ML algorithms can be trained to predict a dependent variable without knowing an equation to fit the experimental data set.

The main concept behind ML methods is the process of learning. During the learning process, ML algorithms attempt to transform experience (i.e., data) into “knowledge” (Shai and Shai, 2014). On the basis of the learning scenario, we can identify many different approaches. Examples are supervised, unsupervised, semi-supervised, self-supervised, reinforcement, and transfer learning (Shai and Shai, 2014; Bommasani *et al.*, 2021; Wang *et al.*, 2023a).

2.2 The Learning Process

2.2.1 Supervised learning

Supervised ML algorithms always use the desired solutions (i.e., the labels) to train the algorithm. Basic examples of supervised learning methods are regression and classification. In classification problems (Figs. 3A and 3B), ML algorithms assign new samples to a specific class (i.e., a set of observations characterized by the same label). In regression issues (Figs. 3C and 3D), the algorithms try to predict the value for one or more dependent variables in response to an observation.

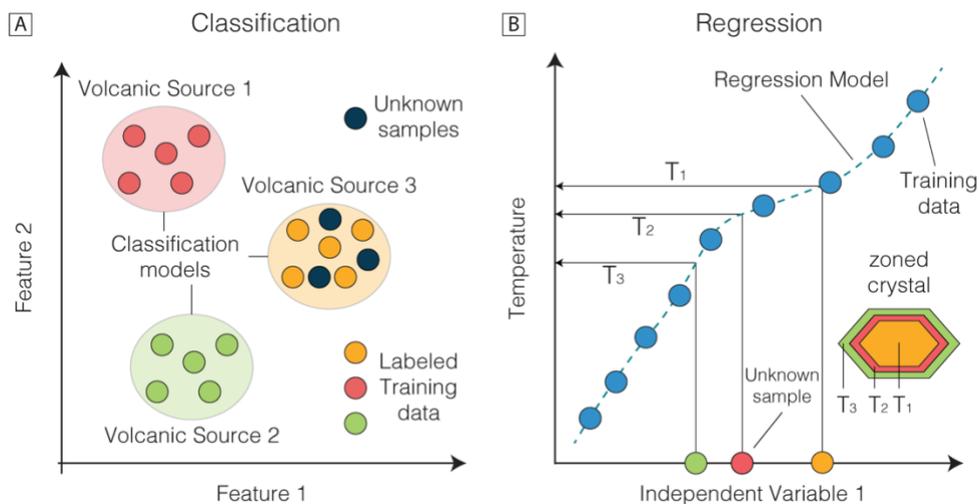


Figure 3: Machine Learning classification (A) and regression (B) in Petrology (modified from Petrelli, 2023).

2.2.2 Unsupervised Learning

Unsupervised learning works with unlabeled data and it attempts the identification of meaningful patterns in the analyzed data without the feeding of known solutions. The clustering, dimensionality reduction, the detection of outliers, and novelty observations are

examples of applications for unsupervised learning methods. In more detail, the clustering consists of collecting “similar” samples into “homogeneous” groups, i.e., clusters (Figs. 4A). The dimensionality reduction consists of reducing the number of variables (features in the ML jargon) to allow the visualization of high-dimensional data (e.g., Morrison et al., 2017) or to improve the efficiency of a ML workflow (Figs. 4B). The detection of outliers aims at determining whether a new observation belongs to a specific set (i.e., an inlier) or none (i.e., an outlier) by training the algorithm using both inliers and potential outliers. Novelty detection is similar to outlier detection, but it only uses inliers during the training. Therefore, an observation that is different from the training set is considered a novelty (e.g., Petrelli, 2023).

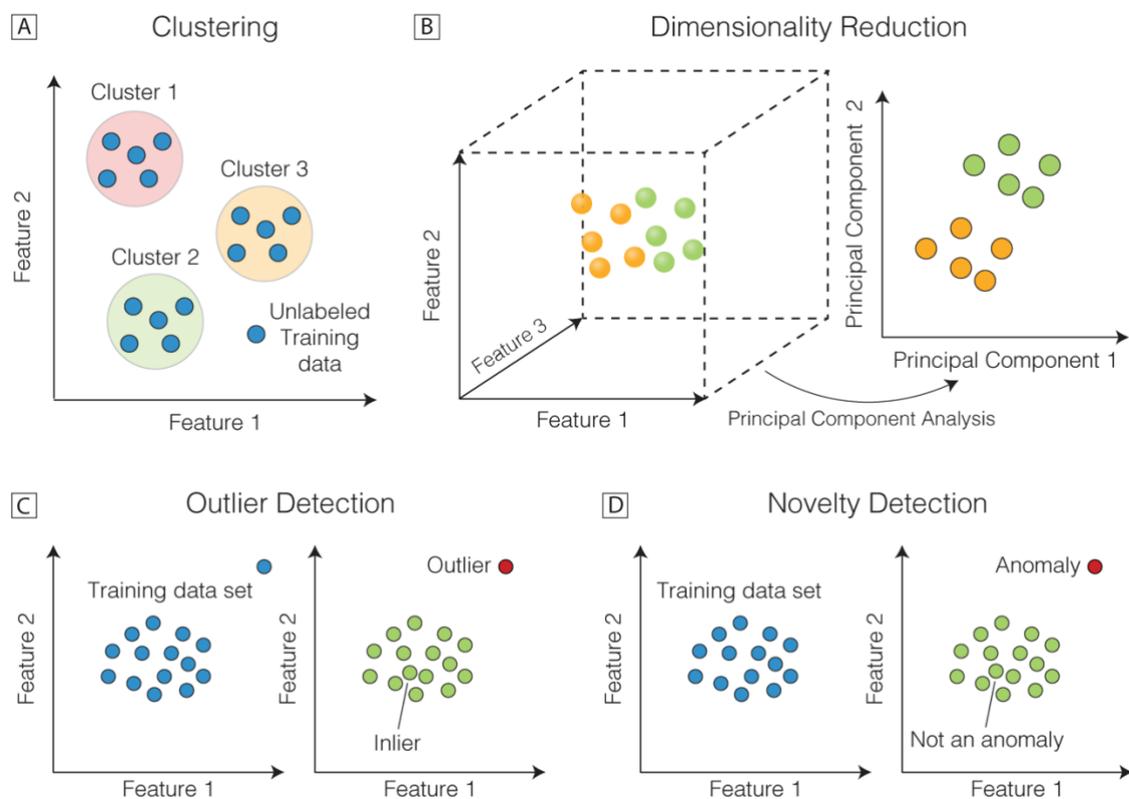


Figure 4: Examples of clustering (A), dimensionality reduction (B), outlier detection (C), and novelty detection (D) (modified from Petrelli, 2023).

2.2.3 Semi-Supervised Learning

Semi-supervised algorithms are in between supervised and unsupervised methods. Typically, semi-supervised methods use a small amount of labeled data for learning and they

support the training with a large number of unlabeled observations (Zhu & Goldberg, 2009).

Figures 5A and 5B highlight how semi-supervised algorithms work.

2.2.4 Self-supervised Learning

Self-supervised learning is a form of unsupervised learning where the algorithm generates its own labels from the data itself. It creates tasks that don't require human-labeled data and learns representations from these tasks (Wang *et al.*, 2023a).

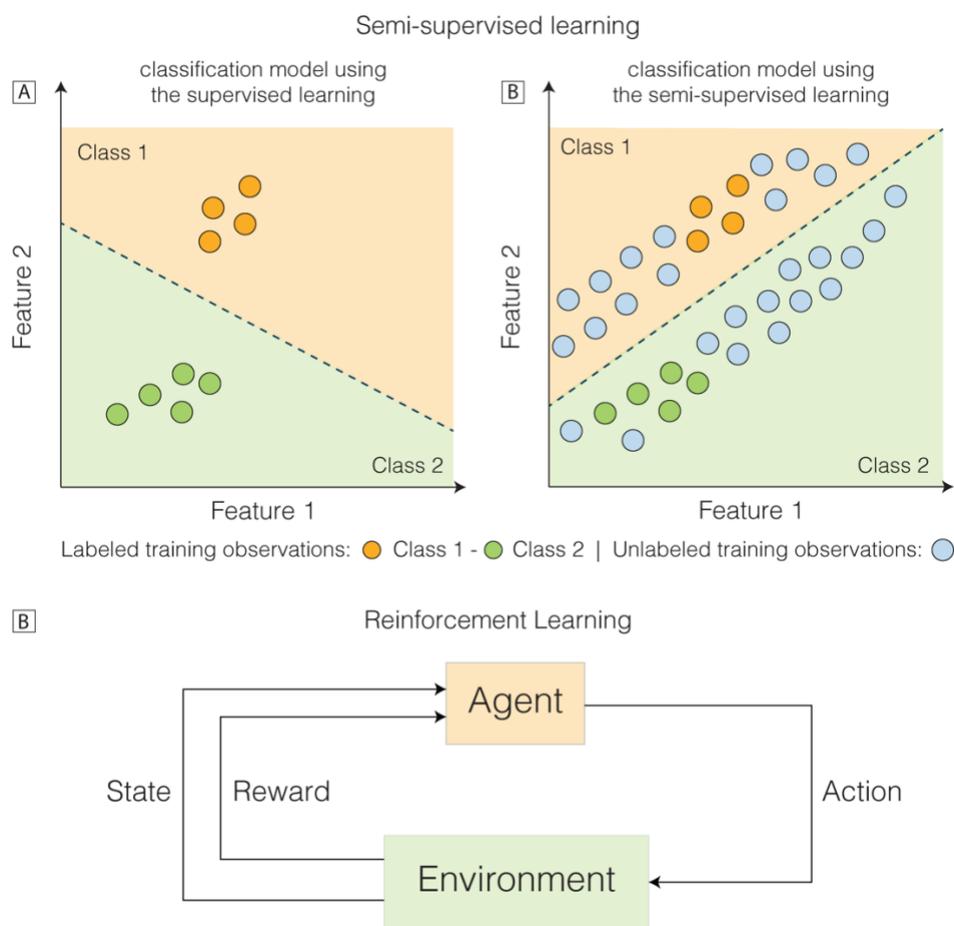


Figure 5: Examples of (A-B) semi-supervised and (C) reinforcement learning (modified from Petrelli, 2023 and Sutton and Barto, 2018).

2.2.5 Reinforcement Learning

Reinforcement learning (RL; Figure 5C) aims at enhancing the learning process by interacting with the state of the environment (Sutton and Barto, 2018; Matsuo *et al.*, 2022). To

achieve this goal, an agent observes the environment's state and takes actions to improve future predictions (Figure 5C) (Sutton and Barto, 2018; Matsuo *et al.*, 2022).

2.2.6 Transfer Learning

Transfer learning involves training a model on one task and then fine-tuning it on another related task. This leverages knowledge gained from one domain to improve performance in another (Bommasani *et al.*, 2021).

2.3 Machine Learning Architectures

2.3.1 Shallow Learning Algorithms

The terms shallow and deep learning refer to the architecture of a ML algorithm. Shallow learning typically consists of an input layer, a single processing step, and an output. Examples of supervised ML algorithms are: Logistic Regression, Least Absolute Shrinkage and Selection Operators (LASSO), Support Vector Machines (SVM), Discriminant Analysis, k-nearest neighbors, Naïve Bayes, and tree-based methods like Decision Trees, Random Forests, or Extremely Randomized Trees (Tab. 1 and references therein). For unsupervised learning, examples are: Principal Component Analysis (PCA), Manifold Learning, Hierarchical cluster analysis, Density-Based Spatial Clustering of Applications with Noise (DBSCAN), K-Means, and Gaussian Mixture Models (Table 1 and references therein).

Algorithm	Type of Learning	Method Reference	Example Applications Using Petrologic Data
Logistic Regression	Supervised	Wright (1995)	Hardman et al. (2018); Ueki et al. (2018); Ren et al. (2019); Fontaine et al. (2023)
LASSO	Supervised	Tibshirani (1996)	Dyar et al. (2016); Breitenfeld et al. (2018); Sutton et al. (2020)
Kernel ridge regression	Supervised	Saunders et al. (1998)	Le Losq et al. (2019)
Discriminant Analysis	Supervised	Klecka (1980)	Pearce (1976); Le Maitre (1982); Agrawal et al. (20204); Vermeesch (2006a); Agrawal et al. (2008); Agrawal et al. (2010); Kalkreuth et al. (2010); Verma (2013); Brandmeier and Wörner (2016); Hardman et al. (2018); Tolosana-Delgado et al. (2018); Han et al. (2019); Lukács et al. (2021); Uslular et al. (2022)
Support Vector Machines	Supervised	Cortes and Vapnik (1995)	Savu-Krohn et al. (2011); Abedi et al. (2012); Kuwatani et al. (2014); Petrelli and Perugini (2016); Petrelli et al. (2017); Ueki et al. (2018); Han et al. (2019); Le Losq et al. (2019); Wang et al. (2020); Ferreira da Silva et al. (2021); Chen et al. (2021); Guo et al. (2021); Uslular et al. (2022); Valetich et al. (2021); Wang et al. (2021); Lei et al. (2022); Li and Zhan (2022); Nakamura (2023); Zhong et al. (2023)
Decision Tree	Supervised	Breiman et al. (1984)	Griffin et al. (2002); Vermeesch (2006b); Wang and Pedrycz (2015); Akkaş et al. (2015); Han et al. (2019); Petrelli et al. (2020); Lei et al. (2022)
Gradient Boosted Decision Trees	Supervised	Friedman (2001)	Petrelli et al. (2020); Saha et al. (2021); Zou et al. (2021); Uslular et al. (2022); Lei et al. (2022); Qin et al. (2022); Fontaine et al. (2023); Nakamura (2023); Yu et al. (2023)
Random forests	Supervised	Breiman (2001)	Ueki et al. (2018); Gregory et al. (2019); Ren et al. (2019); Petrelli et al. (2020); Hong et al. (2021); Schöning et al. (2021); Thomson et al. (2021); Wang et al. (2021); Gion et al. (2022); Higgins et al. (2021); Huang et al. (2022); Lei et al. (2022); Zou et al. (2022); Fontaine et al. (2023); Nakamura (2023); Zhong et al. (2023); Lang et al. (2023); Li et al. (2023a); Zhou et al. (2023)
Extremely randomized trees	Supervised	Geurts et al. (2006)	Petrelli et al. (2020); Schöning et al. (2021); Jorgenson et al. (2022); Lei et al. (2022); Li and Zhang (2022)
k-nearest neighbors	Supervised	Bentley (1975)	Petrelli et al. (2020); Li and Zhang (2022); Lei et al. (2022); Uslular et al. (2022); Fontaine et al. (2023); Nakamura (2023)
Naïve Bayes	Supervised	Rish (2001)	Han et al. (2019); Ren et al. (2019); Uslular et al. (2022)
Hierarchical cluster analysis	Unsupervised	Ward (1963)	Dawson and Stephens (1975); Le Maitre (1982); Templ et al. (2008); Kalkreuth et al. (2010); Caricchi et al. (2020); Gleeson et al. (2021); Boschetty et al. (2022); Musu et al. (2023)
Principal Component Analysis	Unsupervised	Jolliffe and Cadima (2016)	Le Maitre (1982); Hart et al. (1992); Stracke (2012); Krippner et al. (2014); Brandmeier and Wörner (2016); Yoshida et al. (2018); Ueki and Iwamori (2017); Iwamori et al. (2017); Hamada et al. (2020); Rummel et al. (2020); Cone et al. (2020); Sutton et al. (2020); Li et al. (2020a); Li et al. (2020b); Lin et al. (2022); Musu et al. (2023)
Indipendent Component Analysis	Unsupervised	Hyvärinen and Oja (2000)	Iwamori and Albarède (2008); Iwamori and Nakamura (2012); Iwamori and Nakamura (2015); Yasukawa et al. (2016)
Manifold Learning	Unsupervised	Cayton (2005)	Rummel et al. (2020); Wang et al. (2022); Stracke et al. (2022); Li et al. (2023)
DBSCAN	Unsupervised	Ester et al. (1996)	Rummel et al. (2020); Ferreira da Silva et al. (2021)
Gaussian Mixture Models	Unsupervised	McLachlan and Peel (2000)	Lucero-Álvarez et al. (2021); Sheldrake and Higgins (2021)
K-means	Unsupervised	MacQueen (1967)	Templ et al. (2008); Brandmeier and Wörner (2016); Yoshida et al. (2018); Iwamori et al. (2017); Cone et al. (2020); Hamada et al. (2020); Müller et al. (2021); Sheldrake and Higgins (2021); Valetich et al. (2021)
Factor Analysis	Unsupervised		Yoshida et al. (2018)

Table 1: Application of shallow machine learning methods using petrologic data. For each algorithm, a reference manuscript is also reported.

Shallow ML algorithms are nowadays widely explored in petrology. As an example, Table 1 reports some representative shallow ML algorithms with example applications to petrological data. As reported by Xu *et al.* (2021) the application of shallow ML methods comes with many advantages.

For example, there are a plethora of ready-to-use tools, allowing their easy application (e.g., Petrelli, 2023). In addition, they are typically highly interpretable, also, they can work successfully using little data (Xu *et al.*, 2021). As a drawback, they also have some shortcomings. For example, linear models can easily underfit the data, i.e., the hypotheses are too simplistic, resulting in poor accuracy. On the contrary, other models (e.g., decision trees) are prone to overfitting, i.e., the trained models work exceptionally well in fitting the training set, but their performances with real data are scarce (Shai and Shai, 2014). Finally, the tuning of model hyperparameters is often a difficult task (Xu *et al.*, 2021).

2.3.2 Deep Learning Algorithms

Deep learning algorithms allow the development of complex computational models, able to extract meaningful data representations with different levels of abstraction (Lecun *et al.*, 2015). The ability to capture the essential features of input data and generate a representation of the investigated data sets names “deep representation learning” (Wang *et al.*, 2023a). These representations typically consist of dense and compact vectors, named embeddings or latent vectors, aimed at capturing the essential structures and patterns of input data (Wang *et al.*, 2023a).

Deep learning algorithms typically consist of an input layer, more than one hidden processing layer, and an output. To keep some basic concepts, Figures 6 and 7 report seven deep learning architectures, nowadays widely utilized in Scientific applications (Lecun *et al.*, 2015; Raissi *et al.*, 2019; Abdar *et al.*, 2021; Matsuo *et al.*, 2022), as well as by the industry in

solving many everyday challenging applications like, web searches, shopping chart recommendations, user support in consumer products such as smartphones (Lecun *et al.*, 2015), and AI chatbots, e.g., ChatGPT, Bard, and CoPilot (Ebert and Louridas, 2023).

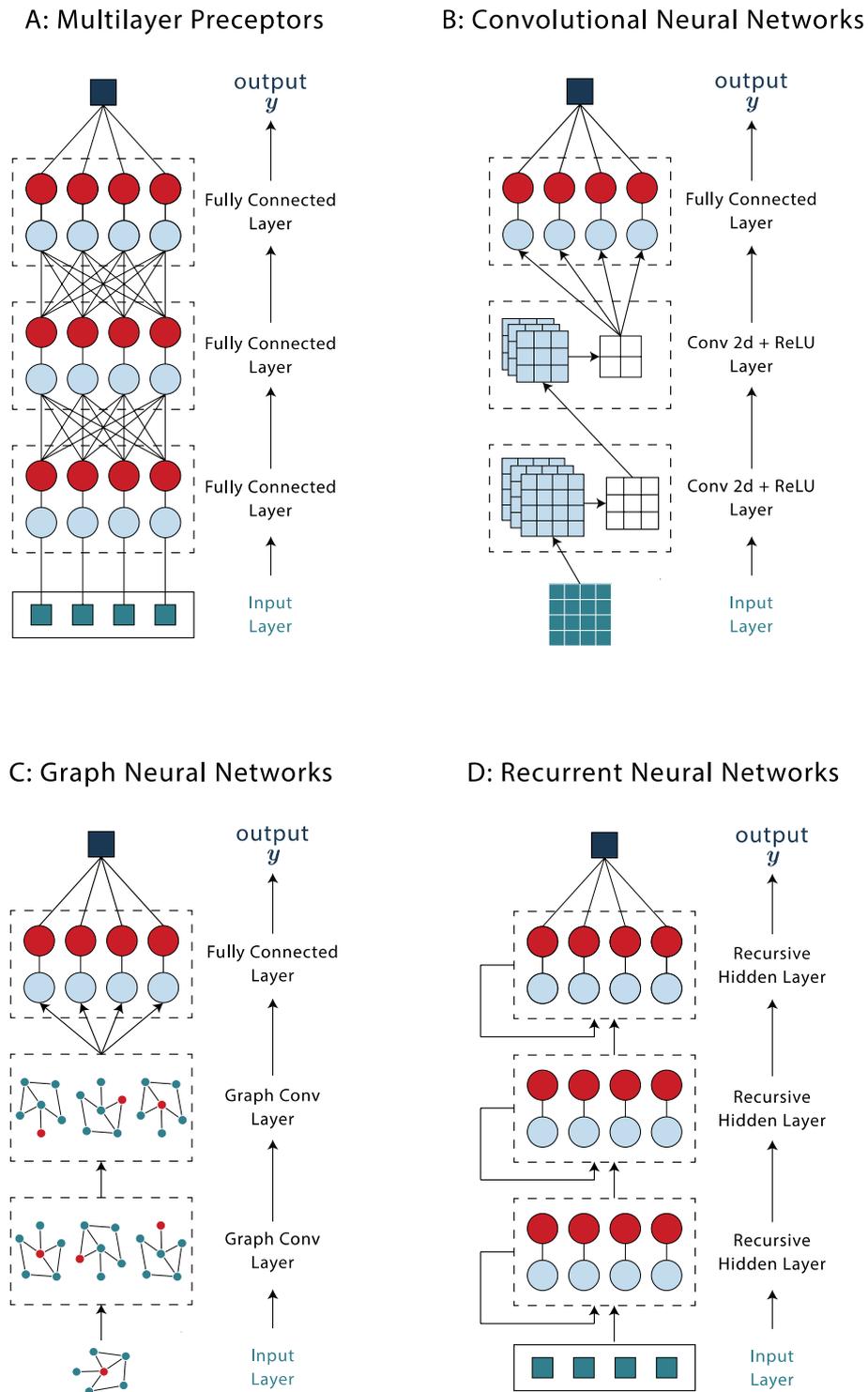


Figure 6: Showcase of deep learning architectures: A) Multilayer Perceptrons, B) Convolutional Neural Networks; C) Graph Neural Networks; D) Recurrent Neural Networks.

Multilayer Perceptron: A multilayer perceptron (Fig 6A) is typically composed of an input, one or more hidden layers, and an output. In the simplest cases, the input consists of vectors (e.g., geochemical analyses) or 2D matrices (e.g., elemental maps). Hidden layers are composed of a combination of very simple functions (e.g., sigmoids, steps, or ReLUs) modulated by weights (i.e., the parameters that vary during the learning process). The final layer is the output, which reports the results of the elaboration (Goodfellow et al., 2016).

One of the key concepts behind multilayer perceptrons relies on the “universal approximation theorem” (Hornik et al., 1989; Cybenko, 1989). It states that “feedforward networks with a linear output layer and at least one hidden layer can approximate any continuous function on a closed and bounded subset of \mathbb{R}^n ” (Goodfellow et al., 2016). However, please note that there is no assurance that the model, during the training process, will learn the target function properly (Goodfellow et al., 2016). Mathematically, a multilayer perceptron is a function $f(x; \theta)$ that aims at approximating some unknown function f^* (Goodfellow et al., 2016). During the training, the multilayer perceptron learns the values of θ that result in the most accurate approximation of f^* (Goodfellow et al., 2016).

Convolutional Neural Networks (CNNs): CNNs (Fig 6B) are deep learning architectures developed to manage data in the form of multiple arrays, like images, signals, and videos (Lecun *et al.*, 2015). CNNs utilize specific vectorial operations in convolutional and pooling layers to capture spatial hierarchies and reduce the complexity of the data (Lecun *et al.*, 2015). CNNs have been applied successfully in several scientific fields including time-series prediction, signal identification, image classification, object detection, image segmentation, and face or object Recognition (Li et al., 2022b and references therein).

Graph Neural Networks (GNNs): GNNs (Fig 6C) are deep learning architectures designed to work with graph-structured data (Scarselli *et al.*, 2009). Graphs are mathematical

structures composed of nodes (vertices) and edges (connections between nodes), and they are used to represent relationships and connections in various domains, such as social networks, recommendation systems, biology, and more (Wu *et al.*, 2021).

Recurrent Neural Networks (RNNs): RNNs (Fig 6D) are deep learning algorithms designed to process sequential data, such as time series, natural language, and speech (Lecun *et al.*, 2015). They are characterized by connections that loop back on themselves, allowing them to maintain a hidden state that captures information from previous steps in the sequence. In other words, RNNs can maintain, in their hidden units, information about the history of past components of a sequence (Lecun *et al.*, 2015). RNNs find strong applications in time series investigations, speech recognition, acoustic modeling, trajectory prediction, sentence embedding, and correlation analysis (Yu *et al.*, 2019 and references therein).

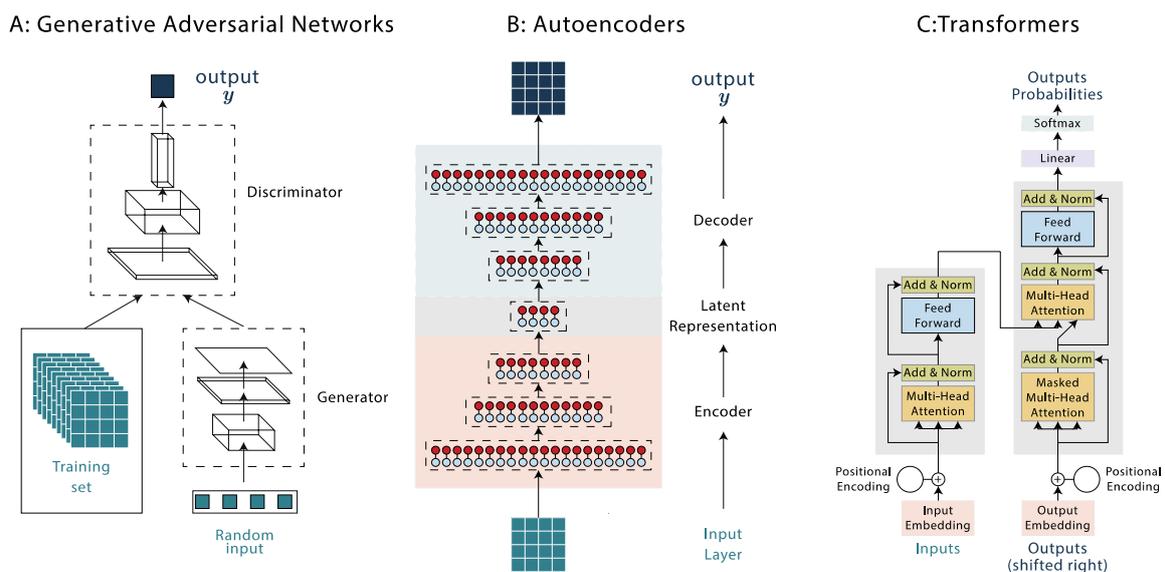


Figure 7: More Deep learning architectures: A) Generative Adversarial Networks, B) Autoencoders, C) Transformers.

Generative Adversarial Networks (GANs): GANs (Fig 7A) consist of two neural networks (i.e., a generator, and a discriminator) that are trained competitively. GANs can manage large data sets of vectors, matrices, or sequences, and find applications in medicine

(Lee et al., 2020), biology (Wan and Jones, 2020), data augmentation (Sandfort *et al.*, 2019), and more (Gui *et al.*, 2023).

Autoencoders: Autoencoders (Fig 7B) consist of an encoder and a decoder that learns how to represent data in a lower dimensional space and reconstructs the learned representation of the inputs, respectively (Lopez Pinaya *et al.*, 2020). The main goal of autoencoders is to get a compressed and meaningful representation of the investigated data set (Lopez Pinaya *et al.*, 2020). Denoising, Contractive, and Variational Autoencoders are popular variants (Lopez Pinaya *et al.*, 2020). Autoencoders find applications in classification, clustering, anomaly detection, recommendation systems, and non-linear dimensionality reduction (Lopez Pinaya *et al.*, 2020 and references therein).

Transformers: Transformers (Fig 7C) are a relatively recent deep learning architecture that has revolutionized natural language processing tasks (Vaswani *et al.*, 2017). They use a self-attention mechanism to process input data in parallel and have achieved state-of-the-art results in tasks like computer vision, text generation, image processing, and time-series analysis (Vaswani *et al.*, 2017; Ahmed *et al.*, 2023; Li *et al.*, 2023a).

3. APPLICATIONS OF MACHINE LEARNING IN PETROLOGY

Observing Figure 2B and Table 1, it emerges that some ML applications in petrology are well established and used (highlighted in green): they are clustering, dimensionality reduction, classification, and regression (Petrelli and Perugini, 2016). The application of these methods in petrology is currently straightforward since algorithms and codes are mature and robust libraries are available in most programming languages (e.g., R, Python, and Matlab). Together with established methods, Figure 2B reports some challenging applications of ML in petrology (highlighted in red). They are the use of multimodal petrologic data, fusion techniques, and exploratory data analysis. Also, the application of methods and techniques like

model interpretability for black-box algorithms (i.e., eXplanaible AI, XAI), surrogates, emulators, and physics-informed neural networks could significantly boost petrological research. In addition, the application of ML hypothesis Formulation methods and ML symbolic regression techniques to provide hypothesis candidates and symbolic regression could provide significant support in petrologic investigations. Finally, the investigation of generative AI and foundation models surely deserves attention. In the following sections, I will start reviving established ML methods in Petrology. Then, I will introduce and discuss current challenges and future perspectives for the application of ML in Petrology.

3.2 Established ML Applications in Petrology

Established ML techniques in petrology mainly consist of shallow ML methods (Table 1; Fig. 2) in the fields of clustering, dimensionality reduction, classification, and regression. They almost exclusively rely on a purely data-driven approach. In other words, they do not use any prior knowledge about the physical rules that govern the investigated process.

3.2.1 Clustering and Dimensionality Reduction

As previously reported, clustering methods and dimensionality reduction techniques allow the grouping of “similar” observations and reduce the number of features (variables) with minimal loss of information, respectively. They are all unsupervised methods; therefore, they work on unlabeled data.

In petrology, unsupervised machine learning methods can support us in unraveling the chemical record stored metamorphic phases (e.g., Yoshida et al., 2018; metamorphic petrology) and in the crystal cargo of a single eruption or multiple volcanic events (e.g., Caricchi et al., 2020; Costa et al., 2023; Musu et al., 2023; igneous petrology). This record often includes the chemistry of different minerals such as olivine, ortopyroxene, clinopyroxene,

plagioclase, amphibole, quartz, and garnet (Boschetti *et al.*, 2022). Each of these phases provides clues to decode the dynamics and the evolution of volcanic plumbing systems (Costa *et al.*, 2020; Petrelli and Zellmer, 2020; Ubide *et al.*, 2021). For example, Boschetti *et al.* (2022) report a nice example of the application of unsupervised ML methods in igneous petrology. In detail, Boschetti *et al.* (2022) investigated magma dynamics through chemical analyses of the crystal cargo carried by erupted magmas during the Villarrica's recent activity (14 ka-present). The main goal was to understand why, in the last 14ka, the Villarrica volcano displayed near-constant basalt to basaltic andesite bulk-rock composition, but large variations in eruptive styles. By the application of hierarchical clustering on chemical analyses of olivines, plagioclases, and clinopyroxenes, Boschetti *et al.* (2022) detected previously unseen zonation patterns, highlighting the occurrence of compositionally distinct clusters within each crystal phase. Then, they successfully incorporated thermodynamic modeling in the study to relate the outcome of clustering analyses to intensive magmatic variables like temperature, pressure, water content, and oxygen fugacity. Finally, by combining the outcomes of unsupervised ML methods with the thermodynamic modeling, Boschetti *et al.* (2022) highlighted the existence of multiple discrete magma reservoirs in the volcanic plumbing system of Villarrica volcano that were separated in space and time. Within these reservoirs, melts differentiate and sometimes mix, when the refilling of the system by more primitive magma occurs. Finally, they hypothesized that the process of mixing between less evolved and differentiated magma drove the explosive activity at Villarrica volcano. Similar investigations have been performed by Costa *et al.* (2023) and Musu *et al.* (2023).

In the field of metamorphic petrology, Yoshida *et al.* (2018) reported the investigation of metamorphic rocks' evolutive paths during subduction-related metamorphism using Principal Component Analysis, Factor Analysis, and *k*-means clustering. The investigated rocks belonged to the Sanbagawa metamorphic belt in central Shikoku (Japan) and were

characterized by metamorphic conditions ranging from the pumpellyite-actinolite to epidote-amphibolite facies. Cluster analyses on geochemical data revealed the occurrence of five clusters and four end-members, respectively (Yoshida *et al.*, 2018). Cluster analyses were then successfully integrated with thermodynamic modeling that allowed the definition of a link between the chemical evolution of the rocks and the metamorphic grade with the compositional variations within the data set, as defined by cluster analyses (Yoshida *et al.*, 2018).

Table 1 reports many additional examples of Clustering and Dimensionality Reduction in petrology.

3.2.2 Classification

Classification tasks find many applications with petrological data sets. Examples are the petrotectonic classification (e.g., Petrelli and Perugini, 2016), tephra correlation (e.g., Petrelli *et al.*, 2017; Bolton *et al.*, 2020; Lukács *et al.*, 2021), the characterization of porphyry Cu deposits (e.g., Zou *et al.*, 2022), volcanic rock classification (e.g., Lang *et al.*, 2023), and the investigation of mantle metasomatism worldwide (e.g., Qin *et al.*, 2022).

For example, Petrelli and Perugini (2016) developed a classification method based on Support Vector Machines to study the intriguing and debated subject of discrimination among different tectonic environments using petrologic data. The application of the Support Vector Machines resulted in high accuracy (93%, on average), highlighting the power of the proposed method.

Tephra correlation is another field where ML classification methods found large applications (e.g., Petrelli *et al.*, 2017; Bolton *et al.*, 2020; Uslular *et al.*, 2022). For example, Bolton *et al.* (2020), suggested the use of machine learning classifiers on tephra correlation. In detail, Bolton *et al.* (2020) trained 11 supervised classification algorithms on about 2000 major element determinations of glass shards, representing 10 volcanic sources. Then, they developed

an ensemble classifier, i.e., a model deriving from the combination of all the investigated ML algorithms to successfully correlate tephra from Eklutna Lake (south-central Alaska). To note Bolton et al. (2020) pointed out that ML classifiers are robust and effective tools. However, “they should aid expert analysis, not replace it” (Bolton *et al.*, 2020).

Zou et al. (2022) explored the use of Random Forest and Feed Forward Neural Network algorithms to characterize magma fertility for porphyry Cu deposits. Their research focused on a trace-elements data set of magmatic zircons. Feature importance analysis highlighted that Eu/Eu^* , $\text{Eu}/\text{Eu}^*/\text{Y}$, Ce/Nd , Ce/Ce^* , Dy, Hf, and Ti hold significant relevance in distinguishing between zircons that are “fertile” and those that are “barren”. Finally, Zou et al. (2022) highlighted that ML models can successfully discriminate zircons from igneous rocks associated with porphyry Cu deposits from those in non-mineralized systems with high accuracy and irrespective of geological context.

Qin et al., (2022) applied machine learning methods to classify the chemical compositions of clinopyroxenes from mantle xenoliths and explore their connection with mantle metasomatism. In detail, Qin et al. (2022) compiled a training dataset of 21,605 and 2,967 analyses of clinopyroxenes for major and trace elements, respectively. Samples were labeled as “positive” if affected by metasomatism based on petrographic evidence, and “negative” if unaffected by metasomatism. Then, they trained several ML algorithms, including Random Forest, Support Vector Machines, and Gradient Boosted Decision Trees. Results highlighted several locations characterized by high mean probabilities of mantle metasomatism and large variabilities in the probability distributions observed across different areas worldwide. Finally, Qin et al. (2022) suggested that metasomatism events are globally widespread, but they do not find evidence of correlation with geophysical parameters such as crustal thickness, lithospheric thickness, or mantle *S*-wave velocity.

3.2.3 Regression

ML Regression in petrology found example applications in thermo-barometric investigations (e.g., Petrelli et al., 2020; Higgins et al., 2021; Thomson et al., 2021; Jorgenson et al., 2022; Li and Zhang, 2022). In the first attempt, Petrelli et al. (2020) investigated several shallow ML models to unravel pre-eruptive temperatures and storage depths using clinopyroxene-only and clinopyroxene-melt pairs chemical compositions. Petrelli et al. (2020) demonstrated that ML models can outperform classical methods, based on simplified thermodynamic rules (Putirka, 2008). They finally utilized the proposed approach to Icelandic Volcanoes, providing further constraints on the architecture of volcanic plumbing systems in Iceland. Several applications followed (Higgins *et al.*, 2021; Thomson *et al.*, 2021; Jorgenson *et al.*, 2022; Li and Zhang, 2022). Using a deep learning approach, Chicchi et al. (2023) also provided an additional clinopyroxene P-T regressive model.

ML shallow regression models have been also applied to estimate ferric iron content in clinopyroxenes (Huang *et al.*, 2022), to predict (Breitenfeld *et al.*, 2018) olivine composition using Raman spectroscopy, and to investigate iron redox state using X-ray absorption spectroscopy (Dyar *et al.*, 2016).

Lei et al., (2022) trained selected shallow machine learning models (e.g., extremely randomized trees, Random Forest, XGBoost, Support Vector Machines, Decision Trees, AdaBoost, K-Nearest Neighbors, Polynomial, Linear, Bayesian Ridge, and Partial Least Squares) and a deep learning algorithm (i.e., a feedforward neural network) to predict carbon solubility in Fe-Ni-S-C melts. The results reported by Lei et al., (2022) highlighted a significant improvement in the accuracy of carbon solubility predictions than classical regression models. Finally, Lei et al. (2022) suggested that diamond and Fe-Ni-S-C melts could be the primary hosts of carbon in the convecting deep upper mantle and throughout most of the mantle

transition zone. However, Lei et al., (2022) also suggested carbide is likely to precipitate at adiabatic temperatures in the deepest parts of the transition zone of C-rich mantle sources.

Using a Deep Learning algorithm (i.e., a feedforward Neural Network), Lin et al., (2022) provided a regression model to predict $\epsilon_{\text{Hf}}(t)$ values. In detail, the input data were 35 chemical elements in igneous rocks and the target output was the corresponding mean zircon $\epsilon_{\text{Hf}}(t)$ value of each sample. The results reported by Lin et al. (2022) support the evidence of a significant contribution of syn-collisional felsic magmatism to net continental crust growth.

Graph Neural Networks also found applications in regression tasks of potential petrologic interest. For example, Hong et al., (2022) developed a GNN model to predict the melting temperature at atmospheric pressure of natural minerals and synthetic materials.

To note, purely ML data-driven modelings do not help in understanding the physics behind the problem. However, such models can still support classical physics or thermodynamic predictors by providing independent constraints, sparking a constructive debate, and suggesting new directions. This is the case of the study proposed by Petrelli et al. (2020) that trained a statistical model based on ML to estimate magma storage pressures and temperatures and sparked a complete revision of the errors associated with thermo-barometric investigations (Wieser *et al.*, 2022b, 2022c, 2023a, 2023b).

3.3 Challenging Machine Learning Applications in Petrology

The lower portion of Fig. 2B highlights promising but challenging ML applications in petrological studies. They mostly involve, but not exclusively, deep learning algorithms.

3.3.1 Multimodal Data Mining and Data Fusion in Petrology

Petrologic data include many categories. They could be textual (e.g., textural description), tabular (e.g., single spot EPMA or LA-ICP-MS analyses), imagery (e.g., crystal

mappings), and volumetric (e.g., 3D phase modeling) to cite a few. Each category of data is a modality (Ramachandram and Taylor, 2017; Stahlschmidt *et al.*, 2022). In petrology, we usually provide investigation and modeling for every single modality (e.g., a textural description first, then major elements, trace elements, and isotope modeling). Then, we compare and evaluate the results deriving from different modalities separately, at the discussion level within manuscripts. This strategy takes the name of unimodal approach (Ramachandram and Taylor, 2017; Stahlschmidt *et al.*, 2022). Data fusion (Figure 8) deals with the combination and modeling of data from different modalities (Ramachandram and Taylor, 2017; Stahlschmidt *et al.*, 2022).

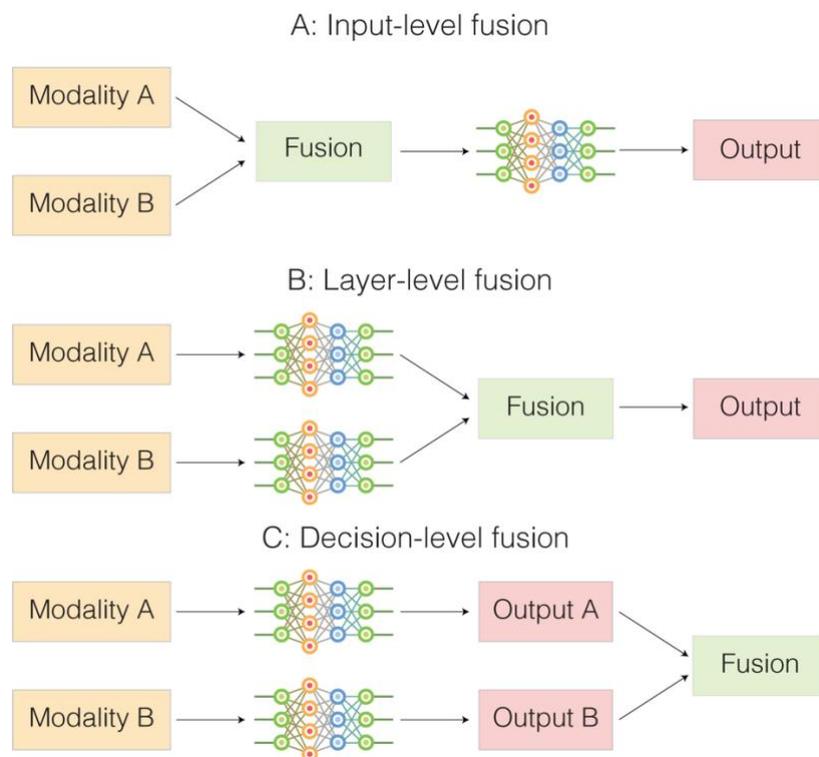


Figure 8: Working principles of Data Fusion: A) input-level fusion, B) layer-level fusion, C) decision-level fusion (modified from Behrad and Saniee Abadeh, 2022).

The main idea behind data fusion is to solve a specific problem with fewer errors than unimodal approaches would (Ramachandram and Taylor, 2017; Stahlschmidt *et al.*, 2022). In the literature, the authors categorize the advantages of data fusion as complementary,

redundant, and cooperative features (Ramachandram and Taylor, 2017; Stahlschmidt *et al.*, 2022). The advantages of multimodal data mining and data fusion have been widely demonstrated in many fields including medicine (Behrad and Saniee Abadeh, 2022), biology (Stahlschmidt *et al.*, 2022), remote sensing (Li *et al.*, 2022a), geological mapping (Lindsay *et al.*, 2014), and disaster response (Algiriyage *et al.*, 2021). When working with multimodal data, the process of data fusion could occur at three different levels (Figure 8; Behrad and Saniee Abadeh, 2022): input-level fusion, layer-level fusion, and decision-level fusion. At Input-level fusion (Figure 8A), different modalities are combined at the raw level, before the modelling (Behrad and Saniee Abadeh, 2022). For the layer-level fusion (Figure 8B), the different modalities feed the model independently (Behrad and Saniee Abadeh, 2022). Then the fusion occurs at the modeling level. Finally, decision-level fusion (Figure 8C) consists of training different models for each single modality. Then, the outcomes of different models are fused to make the final decision (Behrad and Saniee Abadeh, 2022). Each fusion strategy comes with benefits and drawbacks. For example, one advantage of input-level fusion is that it intimately combines different modalities in a single data set. As a drawback, all modalities must be known for each sample in the training set, a condition that is not easy to achieve in practice (Behrad and Saniee Abadeh, 2022).

Combining and modeling tabular (e.g., single spot analyses) or mapping data from different modalities (e.g., EPMA, LA-ICP-MS, SIMS, or LIBS) is a potential direct application of data fusion in petrologic studies. However, more sophisticated approaches involving different modalities like the outcome of numerical simulations, and analytical data on natural and experimental samples could possibly arise.

3.3.2 Exploratory Data Analysis and Uncertainty Quantification

Exploratory Data Analysis (EDA) is a process that helps identify hidden patterns in data and provides meaningful information to make critical decisions (Hodeghatta and Nayak, 2023). It is a way to summarize and visualize a data set to better understand its characteristics. EDA can help in identifying trends, relationships, and anomalies in a data set that may not be promptly apparent. EDA is not new (Tukey, 1977), and it is strictly related to the established techniques reported in section 3.2 (i.e., clustering, dimensionality reduction, classification, and regression). However, the possible use of new data-driven techniques (Godec *et al.*, 2019) and the recent growth of user-friendly tools for exploratory data analysis (Demšar *et al.*, 2013) make the development of effective EDA tools in petrology a promising perspective.

For example, visual programming toolboxes, like Orange (Demšar *et al.*, 2013), allow the democratization of data visualization, image analysis, and the application of machine learning methods (Godec *et al.*, 2019). They simplify the construction of machine learning workflows by visually assembling elements for data preprocessing, visualization, and modeling (Godec *et al.*, 2019). They typically deal with shallow ML algorithms. However, they allow widget development to expand their applications to deep learning models (Godec *et al.*, 2019). Also, specific widgets can be derived to allow petrologic investigations. For example, it is possible to equip them with existing petrological models, like thermobarometers (Wieser *et al.*, 2022c), phase saturation (Wieser and Gleeson, 2023), and solubility models (Iacovino *et al.*, 2021; Wieser *et al.*, 2022a), allowing their combined use and integration with ML methods.

Also, ML algorithms can be trained to explicitly predict the confidence interval, or inherent uncertainty (Abdar *et al.*, 2021; Hüllermeier and Waegeman, 2021). Uncertainty quantification methods should be associated with any classification and regression task, improving current ML petrologic models. Once developed, uncertainty quantification models can be easily added, as components, to visual programming EDA toolboxes.

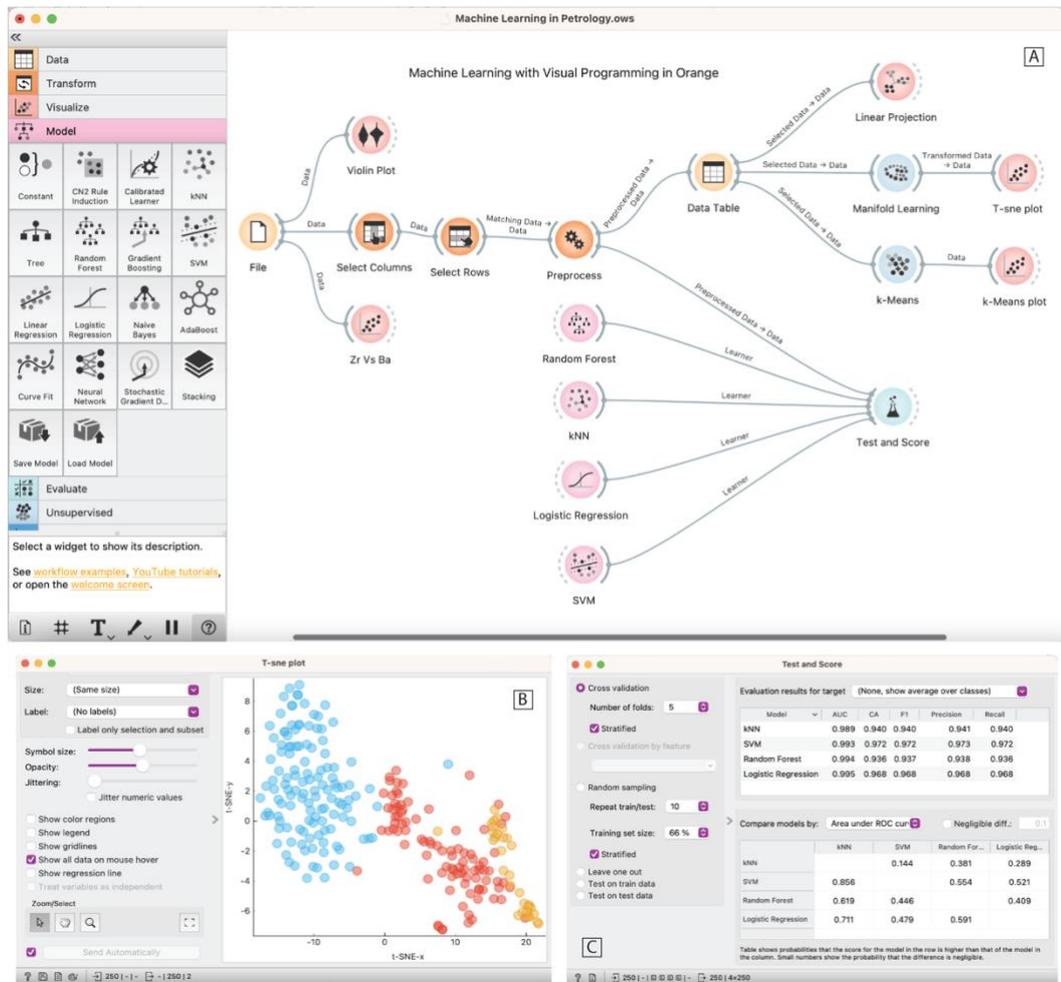


Figure 9: Exploratory Data Analysis (EDA) with Orange (Demšar et al., 2013). A) Visual coding workflow depicting an example application of simple plotting (i.e., violin and binary plots), clustering (i.e., t-sne and k-means), and classification (random forest, kNN, logistic regression, and support vector machines) on petro-volcanological data. B) detail showing the application of t-sne clustering. C) Scores of the classification algorithms.

Figure 9 reports an example application of a ML workflow to petrologic data. In detail, Figure 9 highlights how to apply data visualization by clustering analysis and data classification by different supervised methods on the major element analyses by EPMA of glass samples belonging to the recent activity of the Campi Flegrei Caldera (Smith et al., 2011).

3.3.2 Explainable Artificial Intelligence

Most of the established shallow learning methods in petrology are almost transparent and easily interpretable. As an example, three-based methods allow the identification of feature importance by: a) Gini Importance, Permutation Based Variable Importance, and depth

importance (Qi, 2012). However, the rise of deep learning methods, together with exciting opportunities, comes with new challenges. These methods are mostly opaque and they easily achieve the status of a black box as the complexity of the deep learning architecture increases. However, in scientific applications, the ability to explain the rationale behind the output of a model is crucial.

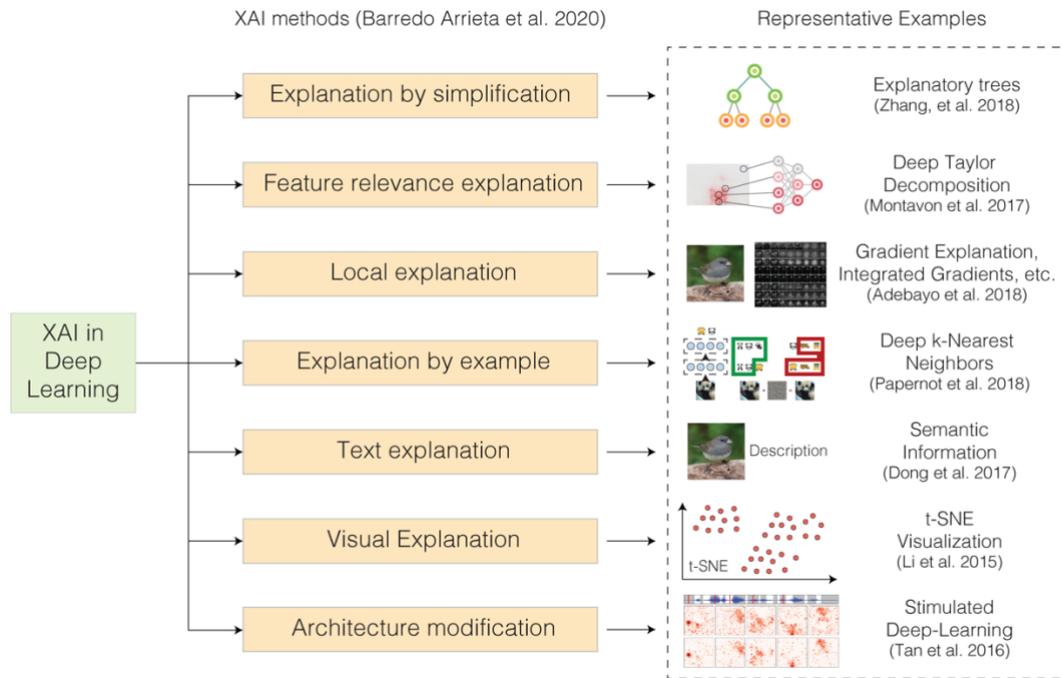


Figure 10: eXplainable AI (XAI) methods of possible interest in petrology.

EXplainable AI (XAI) incorporates a suite of ML techniques that a) produce more explainable models while maintaining a high level of learning performance, and 2) enable humans to understand complex deep learning models (Gunning *et al.*, 2019; Barredo Arrieta *et al.*, 2020). In petrology, the development of XAI tools should come together with the development of any new applications of deep learning methods. To note, Barredo Arrieta *et al.* (2020) efficiently clarify the terminology behind XAI, which I think could be of interest to the petrology community. For example, the term *understandability* measures the ability of humans to understand a model, *comprehensibility* refers to the ability of humans to understand the learned knowledge of a deep learning model, and *interpretability* is the ability

to explain or provide meaning in understandable terms to a human. Regarding the term *explainability*, Barredo Arrieta *et al.* stated “An explainable Artificial Intelligence is one that produces explanations about its functioning.” Finally, a model is considered to be *transparent* if by itself it is understandable (Barredo Arrieta *et al.*, 2020). Figure 10 reports some XAI tools that should be adopted during the development of deep learning models in petrology.

3.3.3 Physics-informed Neural Networks

An effective approach to boost scientific applications is to enhance ML algorithms by incorporating physical equations or constraints in the modeling (Wang *et al.*, 2023a). These equations could be fundamental laws of physics, thermodynamic constraints, or principles of molecular structures (Wang *et al.*, 2023a). One of the deriving deep learning algorithms takes the name of physics-informed Neural Networks. The main aim of physics-informed Neural Networks is to account for the physics of the problem, rather than attempting to deduce the solution based exclusively on data as in the case of purely data-driven approaches (Cuomo *et al.*, 2022). Also, incorporating physical constraints in ML modeling allows for reducing the number of training examples needed to achieve a satisfactory level of accuracy, and performing scale analyses to large hypotheses spaces (Wang *et al.*, 2023a).

As an example of petrologic interest, Chen *et al.* (2021) utilized physic-informed Neural Networks to investigate X-ray diffraction analyses and unravel the Bi-Cu-V oxide phase diagram. In detail, Chen *et al.* (2021) formulate Bi-Cu-V phase mapping as an unsupervised pattern demixing problem to be solved by training a specific deep-learning algorithm named Deep Reasoning Networks. To constrain the model, Chen *et al.* (2021) applied two types of prior knowledge: prototypes of the X-ray diffraction component signals and rules that govern their mixtures.

Also, Le Losq et al. (2021) and Le Losq and Baldoni (2023) trained a physics-informed neural network that incorporated thermodynamic equations to predict several latent and observed properties of melts and glasses. In detail, the deep learning model trained by Le Losq et al. (2021) can predict: a) viscosity values in the 10^0 - 10^{15} \log_{10} Pa·s range with a precision equal to, or better than, $0.4 \log_{10}$ Pa·s; b) density and optical refractive indexes with errors equal or lower than 0.02 and 0.006, respectively; c) Raman spectra for the investigated system with a mean error of $\sim 25\%$; d) the glass transition temperature with an error of 19 K; e) the melt configurational entropy at the glass transition within $0.8 \text{ J mol}^{-1}\text{K}^{-1}$.

3.3.3 Emulators, Surrogates & Providing Boundary or Driving Conditions

Emulators and surrogate modeling can be used as an alternative to computationally costly methods to reduce computational loads (Angione *et al.*, 2022). In the literature, the terms ‘surrogate model’ and ‘emulator’ are sometimes used interchangeably. However, as reported by Angione et al. (2022) term ‘emulator’ should be specifically used for methods that provide full probabilistic predictions of simulation behavior, not only approximate results. Natural use of emulators and surrogate is in computational flow dynamic simulations, a scientific tool that found large applications in petrology (Katz, 2008; Gutiérrez and Parada, 2010; Petrelli *et al.*, 2011, 2016; Parmigiani *et al.*, 2014, 2016, 2017; Robertson *et al.*, 2015; Keller and Katz, 2016; Brogi *et al.*, 2022; Longo *et al.*, 2023). As an example, using the output of costly computational flow dynamic simulations, we can train deep ML surrogates or emulators that can predict the outcomes of the modeling. Also, we can replace computationally heavy building blocks in the simulation with lighter ML models to speed up the computation (Bortnik and Camporeale, 2021).

As an example of petrologic interest, Prasianakis et al. (2020) reported the development of a surrogate model to speed up the modeling of geochemically reactive transport (GRT). GTR

simulations combine, at each time step, the computation of the advective-diffusive flow field, chemical reactions, and resulting chemical speciation at each point in the spatial grid. In these simulations, the computation of chemical reactions and speciation usually acts as a bottleneck, significantly increasing computational costs. Prasianakis et al. (2020) reported the use of a deep learning surrogate for accelerating geochemical calculations in a cross-scale reactive transport model. The results reported by Prasianakis et al. (2020) highlighted the ability of the deep learning surrogate to significantly reduce the computational cost (~4 orders of magnitude) with practically no loss in accuracy. As a result, chemical computations were no longer the bottleneck of the simulations opening new perspectives in GTR simulations (Prasianakis *et al.*, 2020).

Also, ML models have been successfully trained to constrain, improve, and speed up molecular dynamics modeling and *ab initio* computations (Botu and Ramprasad, 2015; Noé *et al.*, 2020; Zhang *et al.*, 2020, 2021; Li and Voth, 2022; Gao *et al.*, 2023). To note, many researchers have been involved in the last years in integrating atomic simulations with ML to perform petrologically relevant investigations like, for example, the mechanisms governing noble gas solubility, element partitioning, and isotopic fractionation in silicate melts (e.g., Zhang et al., 2020, 2022; Deng and Stixrude, 2021; Luo et al., 2021a, 2021b; Wang et al., 2023b). In atomic simulations, accurate force field estimations are mandatory to accurately simulate melt structures and their interactions with noble gases. As reported by Wang et al. (2023b), in state-of-the-art Molecular Dynamics simulations, the force fields were either derived by experimental data at low pressures or estimated on limited density functional theory modeling. However, these methods may introduce inaccuracies under high pressure (Wang *et al.*, 2023b). In theory, performing full-density functional theory calculations would provide more accurate results. As a drawback, the resulting computational cost will be prohibitively expensive. To overcome this limitation, many authors reported the use of ML-based force field

estimations to accurately model atomic interactions with the same level of accuracy of full density functional theory calculations but significantly lowering the computational cost (e.g., Wang et al., 2023b and references therein). In detail, Wang et al., (2023b) reported the use of a machine learning-based force field estimator named Deep Potential to investigate the effect of pressure and temperature on the solubility of noble gases (He, Ne, and Ar) in silicate melts (up to ~30 GPa and 2500 K) for the melt of molten basalt, olivine, and enstatite. The results reported by Wang et al. (2023b) highlighted that: a) the solubility of all noble gases (He, Ne, and Ar) increases with temperature; b) the solubility of noble gases increases with pressure until a maximum solubility threshold located at 5 GPa. Beyond 5 GPa, the solubility progressively decreases as pressure continued to increase; c) the modeling showed a significant increase in the self-diffusivity of oxygen atoms in silicate melts from atmospheric pressure to ~5-8 GPa, which can be attributed to the formation of Si/Al-O5-6 in the melts upon compression.

To note, ML-boosted MD simulations are not limited to solubility problems, and they are nowadays a fundamental tool for the investigation of the petrologic properties of the Earth's and other planets' interiors, from magma oceans to cores (Zhang *et al.*, 2020, 2022; Deng and Stixrude, 2021; Luo *et al.*, 2021b, 2021a; Deng *et al.*, 2023; Wang *et al.*, 2023b).

4. PERSPECTIVES FOR A PARADIGM SHIFT

As reported by Wang et al. (2023a), Machine learning is progressively becoming more intertwined with the process of scientific exploration, enhancing and expediting research. This integration aids scientists in formulating hypotheses, devising experimental plans, amassing and analyzing extensive datasets, and unearthing insights that might have remained elusive through conventional scientific approaches alone (Wang *et al.*, 2023a).

4.1 Generative AI and Foundation Models

Generative AI is a broader field that encompasses a wide range of AI techniques and models designed to generate new content. This content can be in various forms, such as text, images, audio, and videos. Also, Generative AI involves creating models that can produce data that is similar to what they were trained on. For example, generative AI has proved its utility in “data generation” and “data refinement” (Wang *et al.*, 2023a). In “data generation”, generative adversarial networks have proven to effectively support many scientific domains like particle collision events (Ghosh and ATLAS collaboration, 2022), pathology slides (Mahmood *et al.*, 2020), chest X-rays (Teixeira *et al.*, 2018), magnetic resonance contrasts (Lee *et al.*, 2020), and three-dimensional (3D) material microstructure (Kench and Cooper, 2021). In petrology, “data generation” could support the augmentation of existing petrological datasets and support the development of more reliable ML models. Also, they could boost the investigation of structural and topological features at small length scales (i.e., the microstructure). Finally, they could effectively support cutting-edge 4D petrological studies, as already occurred in medical sciences (e.g., Moghari *et al.*, 2019; Chang *et al.*, 2021). For example, Ferreira *et al.* (2022) trained a generative adversarial network (GAN) model, named PetroGAN, to create synthetic petrographic datasets across different rock types, highlighting the potential of Generative AI in supporting geoscientific ML applications, particularly in the presence of limited datasets. In “data refinement”, ML algorithms can enhance spatiotemporally resolved measurements by reducing noise and improving resolution (Wang *et al.*, 2023a). In microscopy, deep learning algorithms are an effective tool already (e.g., Hoffman *et al.*, 2021; Qiao *et al.*, 2021; Yang *et al.*, 2022), ready to be used in petrological applications.

Foundation models are a subset of Generative AI algorithms, mainly based on the transformer architecture, that have been “trained on broad data at scale and are adaptable to a

wide range of downstream tasks (Bommasani *et al.*, 2021)". On top of a foundation model, it is possible to develop more specialized and focused models, tailored to specific applications or domains. Transfer learning (Thrun and Mitchell, 1995) is one of the main concepts at the base of foundation models (Bommasani *et al.*, 2021). As reported in section 2.2.6, the idea behind transfer learning is to use the "knowledge" that is learned from one task and apply it to solve a different problem. In deep learning, transfer learning is often achieved by the so-called "pretraining" (Bommasani *et al.*, 2021) on large data sets. More specifically, a deep learning model is typically trained to solve a non-specific task and then adapted to the problem of interest through fine-tuning, drawn by a specific and more focused data set (Bommasani *et al.*, 2021). Foundation models are driving the current revolution in AI applications. Examples are BERT (Devlin *et al.*, 2018), DALL-E (Ramesh *et al.*, 2022), and GPT-4 (OpenAI, 2023).

To my knowledge, foundation models have not been directly applied to petrology yet. However, their application to petrologic applications could support, for example, the development of reliable labeled data sets for the training. Also, they could support us in demanding tasks like, e.g., 2D, 3D, and 4D phase segmentation in natural and experimental samples. As an example, the Segment Anything Model (Kirillov *et al.*, 2023) could be effectively used in petrologic applications like the segmentation of experimental samples and the investigation of the crystal cargo belonging to volcanic eruptions. Also, the application of foundation models could push "Multimodal Data Mining and Data Fusion in Petrology" (cf. sec 3.3.1) to a superior level. Indeed, a big challenge could be the reliable combination of textural descriptions, petrographic imaging, chemical analyses, and numerical data to provide hybrid models by data fusion.

4.2 Hypothesis Formulation and Symbolic Regression

The generation of testable hypotheses and the identification of physical governing laws are central points in scientific research where ML methods have demonstrated the ability to play a significant role (Wang *et al.*, 2023a). For example, ML algorithms can identify promising hypotheses within a large pool of candidates (i.e., hypothesis formulation) or find candidate symbolic expressions (i.e., symbolic regression).

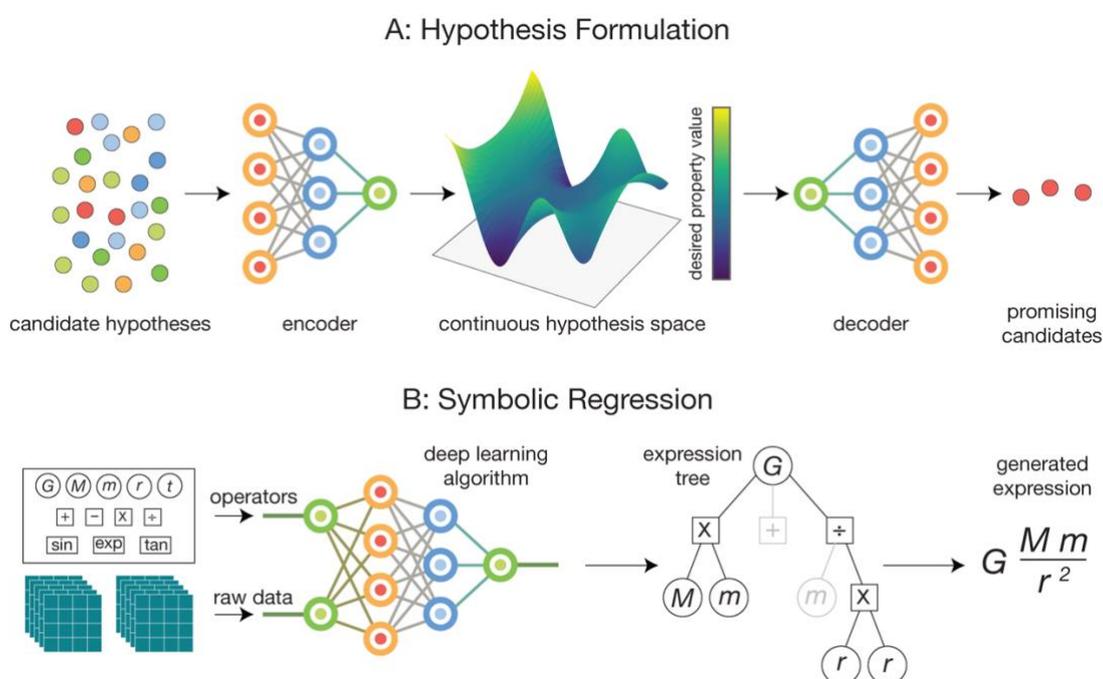


Figure 11: (A) Generation of testable hypothesis using autoencoders and (B) the identification of physical governing laws by symbolic regression (modified from Wang *et al.*, 2023a).

4.2.1 Hypothesis Formulation

As reported by Wang *et al.* (2023a), deep learning methods for hypothesis formulation have been effectively applied in many scientific fields like chemistry (Gómez-Bombarelli *et al.*, 2016), genomics (Avsec *et al.*, 2021), and particle physics (Ball *et al.*, 2022) to cite a few. For example, autoencoder models (Fig. 11A) can map discrete objects, such as chemical mixtures, to coordinates in a continuous and differentiable space describing a desired property

(Wang *et al.*, 2023a). Optimization algorithms are then able to find maxima or minima of the mapped space to effectively solve the problem in such differentiable space (Shen *et al.*, 2023). A petrological application for ML hypothesis formulation could be the investigation of thermodynamic and structural properties of magmas.

4.2.2 Symbolic Regression

Symbolic regression (Fig. 11B) consists of predicting the mathematical expression of a function from the observation of its values (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). Symbolic regression usually starts by predicting a “skeleton” (i.e., a parametric function) using a pre-defined list of operators, like basic operations (+, ×, ÷) and functions (log, sqrt, exp, sin, etc...) (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). Then, the constants in the *skeleton*(a, b) are estimated using optimization techniques (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). In classic symbolic regression, the leading algorithms rely on genetic programming (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). Genetic programming evolves by generations. At each generation, the algorithm predicts a population of candidates (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). Among them, the most promising candidates are selected and mutated to build the next generation (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). The iteration proceeds until achieving the desired accuracy level (Schmidt and Lipson, 2009; Angelis *et al.*, 2023). Deep learning algorithms, like recurrent neural networks and transformer architectures, have been also successfully applied to symbolic regression (Petersen *et al.*, 2021; Kamienny *et al.*, 2022; Angelis *et al.*, 2023). Intriguing applications in petrology rise on unraveling hidden thermodynamic rules of magmas as the chemical partitioning of elements among different phases, laws governing phase saturation, and governing equations for volatile elements’ solubility.

CONCLUSIONS

Machine learning algorithms are currently widely applied in petrology, mainly relying on shallow architectures. This approach comes with advantages and limitations. The main advantages include the possibility to work with little data and get results that are easy to explain. As a drawback, these models are often prone to over- and under-fitting issues. Most importantly, they mainly operate on a purely data-driven approach. Therefore, they are almost always unlinked to the physical rules governing the investigated petrological system. As a consequence, they do not support us in understanding or depicting the physics that govern the investigated petrologic problems.

Deep learning algorithms have demonstrated their ability to boost new scientific discoveries. However, deep learning algorithms often operate as black boxes, meaning that scientists are not able to explain the mechanisms leading to a specific output. In most scientific applications, including petrology, the understanding of how the modeling works is mandatory. As a consequence, each petrological study involving the application of deep learning algorithms should also involve the potentials of EXplainable AI (i.e., XAI), to ensure model interpretability.

Most importantly, to achieve challenging results and provide a paradigm shift, we should start linking machine learning algorithms with the physical nature of the investigated petrologic process (e.g., physic-informed neural networks, hypothesis formulation, and symbolic regression). In that direction, promising applications have already been developed to unravel, for example, the structure and properties of silicate melts (Le Losq et al., 2021). Moreover, one of the most promising petrological applications that links ML with the physical and thermodynamic nature of the system is ML-boosted Molecular Dynamics (Zhang et al., 2020, 2022; Luo et al., 2021a, 2021b). The exploration of foundation models and symbolic regression surely deserves attention, since they could support the achieving of thrilling results.

As a final remark, in agreement with Fleming et al. (2021), I would like to point out the need to enhance education and research efforts to train the next generation of geoscientists in understanding and proficiently using ML in Earth Science, including petrology. Currently, the learning experience in ML for geoscience students almost exclusively relies on self-teaching, short courses, or picking a thesis supervisor with knowledge of ML (Fleming et al., 2021). However, most of the students in geoscience receive no training in ML. Therefore, a strong collaborative effort, also involving expert data scientists, is needed to effectively train the new generation of petrologists, achieve new discoveries, and possibly achieve a paradigm shift.

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