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Orange-Volcanoes: A new open and collaborative platform to perform data-driven investigations and machine learning analyses in petrology and volcanology

Alessandro Musu [a,b], Valerio Parodi [c], Marko Toplak [d], Alessandro Carfì [c], Mónica Ágreda-López [b], Fulvio Mastrogiovanni [c], J. ZhangZhou [e], Diego Perugini [b], Donato Belmonte [f], Penny E. Wieser [g], Blaž Zupan [d], Maurizio Petrelli [b,*]

[a] Department of Lithospheric Research, University of Vienna, UZA2, Josef-Holaubek-Platz 2, 1090 Vienna, Austria
[b] Department of Physics and Geology, University of Perugia, Piazza dell'Università, 1, Perugia, 06123, Italy
[c] Department of Informatics, Bioengineering, Robotics and Systems Engineering, University of Genoa, Via Opera Pia 13, Genova, 16145, Italy
[d] Faculty of Computer and Information Science, University of Ljubljana, Večna pot 113, SI 1000, Ljubljana, Slovenia
[e] Research Center for Earth and Planetary Material Sciences, School of Earth Sciences, Zhejiang University, Hangzhou 310058, China
[f] Department of Earth, Environmental and Life Sciences (DISTAV), University of Genova, Corso Europa 26, Genova, 16132, Italy
[g] Department of Earth and Planetary Science, UC Berkeley, CA, 94720, United States of America

A R T I C L E I N F O

Dataset link: https://github.com/AIVolcanoLab/orange3-volcanoes

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A B S T R A C T

Orange-Volcanoes is an extension of the open-source Orange data mining platform specifically tailored for geochemical, petrological, and volcanological investigations. Orange-Volcanoes enhances the original platform by incorporating specialized tools to enable interactive data-driven investigations in geochemistry, such as performing Compositional Data Analysis (CoDA). Applying CoDA transformations enables the use of many standard and multivariate statistical methods like principal component analysis, discriminant analysis, and hierarchical clustering on compositional data. In this way, Orange-Volcanoes allows for the application of a wide range of data mining and statistical methods implemented in Orange using geochemical data. Moreover, Orange allows the use of advanced methods in the field of explainable artificial intelligence, such as feature importance and Shapley additive explanations. Also, within Orange-Volcanoes, we demonstrate the flexibility of the Orange platform by developing visual tools that allow for conducting mineral-liquid equilibrium tests and calculating thermo-barometric estimates. The Orange-Volcanoes supports collaborative efforts and reproducibility by offering a visual programming interface that requires no coding experience, making it accessible to a wide range of users, including scientists, educators, and students. We provide a series of case studies, including interactive petrological data exploration and clustering in tephra studies to highlight Orange-Volcanoes' potential and versatility in volcanological applications. Orange-Volcanoes can be downloaded using pip, and its documentation is available at https://orange3-volcanoes.readthedocs.io/en/latest/.

1. Introduction

New discoveries in science mainly consist of uncovering patterns and relations from the observation of still unexplained phenomena and, possibly, formalizing them in laws and equations (Montáns et al., 2019). Such laws and equations can sometimes be inductively derived from a few and highly-focused experiments designed to either demonstrate or refute a specific model (i.e., "model-driven" applications). This is a classical approach that has been widely used in Earth sciences, for example, in experimental petrology (Johannes and Holtz, 2012), or in classical volcanological studies (Sparks and Walker, 1977). Nowadays, new and complementary approaches based on the investigation of a large number of observations can support classical strategies in deriving new discoveries. For example, purely data-driven investigations consist of analyzing a possibly large number of raw, multi-dimensional, and sometimes heterogeneous observations to uncover hidden patterns, mostly without the presence of a specific theory to be demonstrated or refuted (Montáns et al., 2019). As reported by Montáns et al. (2019): "These procedures have the additional advantage of testing correlations between different variables and observations, learning unforeseen patterns in nature and allowing us to discover new scientific laws or

* Corresponding author.
E-mail address: maurizio.petrelli@unipg.it (M. Petrelli).

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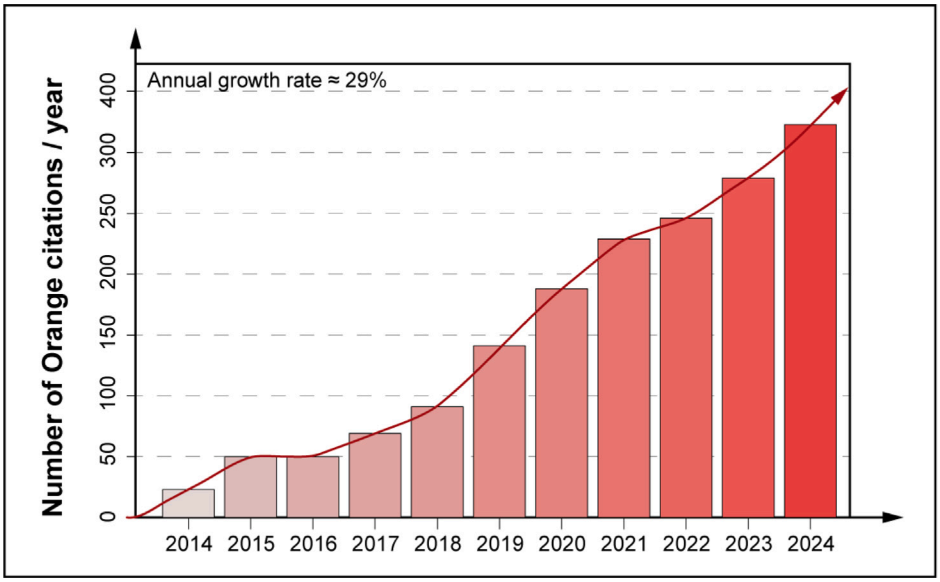

Fig. 1. Number of Orange citations per year, until December 2024. The annual growth rate was estimated by first fitting an exponential growth model (Price, 1963) and then following the procedure reported in Yáñez Dávila et al. (2023) yielding an estimated rate of approximately 29.

even more, performing predictions without the availability of such laws". The progressive and significant increase of the available computational power occurred over the past decades, and the continuous improvements of statistical tools like machine learning techniques fed the proliferation of studies relying on data-driven investigations, also involving petrology and volcanology (Boschetty et al., 2022; Caricchi et al., 2020; Petrelli and Perugini, 2016; Petrelli et al., 2017, 2020; Musu et al., 2023). The core process of data-driven investigation is data mining, which involves extracting relevant information not known *a priori* (and potentially useful) from a large data set (Witten et al., 2017; Montáns et al., 2019; Ishak et al., 2020; Ratra and Gulia, 2020; Thange et al., 2021). In detail, data mining consists of collecting and investigating large amounts of observations with a set of mathematical and statistical tools designed to: (i) filter out the complicated and redundant noise in the data; (ii) identify patterns and/or meaningful correlations, thereby excluding trivial or spurious correlations; and (iii) accelerate the route to data evaluation and decision-making (Witten et al., 2017; Thange et al., 2021).

However, data-driven investigations in petrology and volcanology are sometimes hindered by limiting factors (Petrelli, 2024) like: (i) interactive data mining platforms allowing for the joint application of both classical petrological approaches and new data-driven investigations are scarce; (ii) ready-to-use petrological and volcanological data sets are, sometimes, difficult to retrieve or of difficult access; (iii) machine learning methods are often perceived as mere "black-boxes" by Earth Scientists; (iv) results are not always easy to reproduce.

All these limitations could be potentially overcome using data mining platforms, for example, Orange (Demšar et al., 2013; Godec et al., 2019). Orange is a Python-based platform for interactive data visualization and modeling (Demšar et al., 2013; Godec et al., 2019). It enables high-quality qualitative and quantitative data-visualization and data-mining using a visual programming approach (Demšar et al., 2013; Godec et al., 2019). In detail, Orange enables interactive data mining, allowing the user to control, visualize, and interact directly with each stage of the workflow through a simple and intuitive interface (Demšar et al., 2013; Rojas-Galeano and Rodriguez, 2013; Godec et al., 2019; Mohi, 2020; Dobesova, 2024). By natively incorporating numerous advanced visualization tools, statistical methods, and machine learning algorithms, Orange potentially allows geochemists, petrologists, and volcanologists to focus their efforts on data-mining instead of coding (Demšar et al., 2013; Godec et al., 2019; Petrelli, 2024). Furthermore, it is based on a collaborative approach, allowing experienced Python programmers to contribute to Orange development and share new scientific tools (Demšar et al., 2013; Godec et al., 2019). For instance, it is possible to create new original packages of functions (add-ons) to solve specific problems, which users can add to their own collection of tools in Orange. In addition, the availability of many methods belonging to Explainable Artificial Intelligence in Orange (i.e., the ones contained in the Orange3 Explain add-on), like feature importance (Kaneko, 2022; Lundberg et al., 2019), Shapely additive Explanations (SHAP, Lundberg et al., 2019), and Individual Conditional Expectation (ICE, Goldstein et al., 2015), facilitates the transition from the so-called "black-box" modeling approach to transparent data modeling and interpretation (Gunning et al., 2019). Finally, its simple graphical form, combined with extensive documentation (comprising a variety of tutorials), speeds up the educational process, making it an excellent tool for teaching but also for facilitating communication and active cooperation between researchers and practitioners with different or no knowledge of programming languages (Demšar et al., 2013; Godec et al., 2019; Dobesova, 2024).

As a drawback, Orange still lacks tools that are of fundamental importance in petrology and volcanology. For example, Compositional Data Analysis (CoDA) has not been implemented yet. To note, CoDA allows the application of most of the advanced statistical methods implemented in Orange on geochemical data, otherwise not recommended due to their compositional nature (Aitchison, 1984). Access to petrological and volcanological data sets is not always straightforward, and a large library of different petrological and volcanological (experimental and natural) data sets has yet to be integrated into the Orange platform for easy accessibility. Furthermore, it misses fundamental petrological data cleaning options, such as quality filters commonly applied to mineral analyses (i.e., cation sum filter for clinopyroxene) and equilibrium tests (Putirka, 1999, 2008; Mollo et al., 2013; Neave et al., 2019).

To start filling this gap, we developed Orange-Volcanoes, an add-on that allows connecting Orange to the petrological and volcanological community. Orange-Volcanoes is minded on a collaborative basis, allowing all users to contribute or suggest improvements. For example, novices can support the Orange-Volcanoes development by suggesting improvements and experienced Python programmers can collaborate by adding new features and integrating existing tools within the Orange-Volcanoes GitHub repository: https://github.com/AIVolcanoLab/orange3-volcanoes.

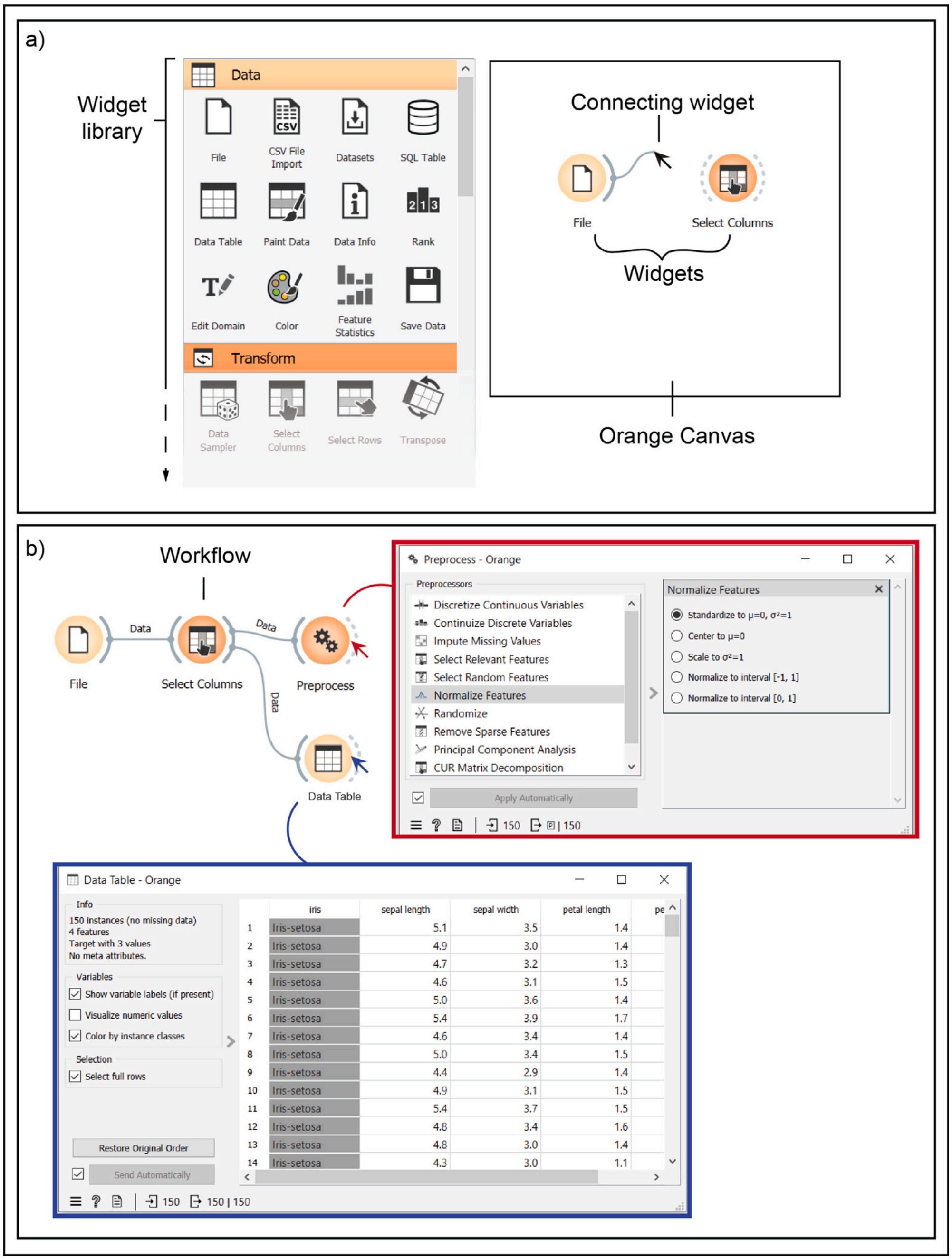

Fig. 2. Composing a workflow in Orange. (a) Screenshot of the widget library. The widgets can be dragged into the Orange Canvas and manually connected to form a workflow. (b) Simple workflow. It is possible to inspect each individual portion of the workflow. Clicking on individual widgets and using data tables allows users to visualize the data in the input and the output and change the function performed by each widget.

The overall objective of Orange-Volcanoes is to provide a freely accessible and easy to use add-on within the Orange environment that is specifically intended to support the petro-volcanological community, regardless of the level of programming expertise of the user. In detail, Orange-Volcanoes currently implements fundamental data transformations in the framework of compositional data analysis (CoDA), like additive, centered, and isometric log-ratio transformations (Aitchison, 1986; Egozcue et al., 2003). Also, it provides direct access to selected petrological (e.g., Georoc, DIGIS Team 2024) and volcanological (e.g., Smith et al., 2011) data sets to reproduce the findings of the present work. Finally, it integrates data cleaning tools based on equilibrium between liquid-crystal pairs and geochemical data filtering. To demonstrate the potential of Orange-Volcanoes, we also developed a specialized widget to perform geo-thermometric and geo-barometeric estimates calling the Thermobar (Wieser et al., 2022) Python package. All Orange-Volcanoes tools are interactive, allowing for the development of exploratory data visualization and modeling. Within the manuscript, we demonstrate the potential of the proposed platform by applying Orange and Orange-Volcanoes to selected study cases in the framework of interactive petrological data exploration, clustering of geochemical data, and tephra studies.

2. Orange and Orange-Volcanoes

2.1. Orange

Orange (https://orangedatamining.com) is an open-source, Python-based, data mining platform that provides a simple and interactive

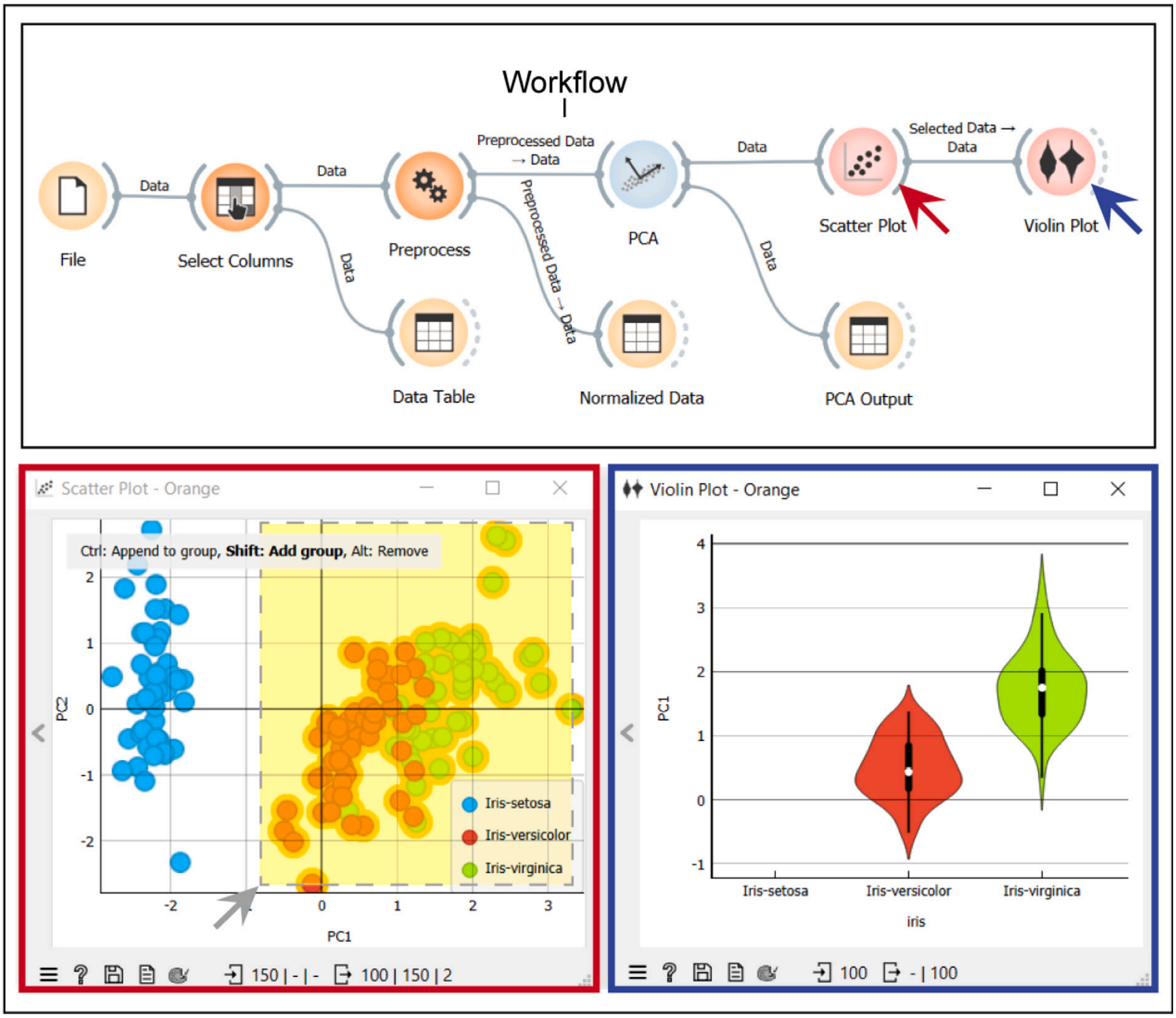

Fig. 3. Interactive workflows. Every change that is applied within a widget and every applied data selection (i.e., interactive selection of portions of data from a graph) is applied instantaneously to all following widgets, allowing immediate evaluation of the performed change or selection.

interface, allowing users to perform various tasks in data analysis and visual programming (Demšăr et al., 2013). In recent years, the interest and use of the Orange platform have been growing in several branches of scientific research (Fig. 1). The Orange library is structured hierarchically, comprising various components named "widgets". Each widget serves a specific function, such as data input, pre-processing, modeling, analysis, and visualization. Practically, widgets appear as visual elements that users can manually combine to construct a workflow (Fig. 2). In these terms, an Orange workflow consists of a network of interconnected widgets that can be easily assembled by manually dragging them onto a whiteboard interface (called Orange Canvas) and linking them together by drawing lines between them (Fig. 2a). This design enables users to interactively inspect each step of the workflow, including the input and output data for every widget. By clicking on a widget, an options menu appears, allowing users to select specific functions for that widget. For example, in the case of a normalization widget, users can choose the type of normalization to apply, such as standard scaling or [0,1] normalization (Fig. 2b). This step-by-step inspection gives users a better understanding and confidence in both the data set itself and the analytical methods employed.

Additionally, any modifications, such as choosing a specific data subset or adjusting parameters within a widget, are instantly applied throughout the entire workflow, leading to an immediate update in the final data display (Fig. 3). For instance, if we select a group of observations in a figure or a data table, all the following widgets will automatically adjust, reapplying the analysis to the selected sub-data set and updating all the results in real-time (Fig. 3). This extreme interactivity allows users to dynamically explore their data and methodologies, facilitating the extraction of insights and enabling easy comparison of different approaches in a visual and efficient manner. Ultimately, Orange's structure supports the creation of reproducible and comparable workflows, promoting a transparent and reproducible scientific approach.

Orange can be managed at three different levels: (i) as an end user, requiring no knowledge of the Python programming language and enabling the direct application of Orange widgets to the investigated data set; (ii) as an expert user, with the ability to incorporate Python scripts as widgets within the workflow, thereby enabling the addition of customized functions or formulas not available in Orange (Fig. 4); and (iii) as a developer, with the capability to expand or create custom add-ons that can then be shared and freely used by all within the Orange platform (e.g., Orange-Volcanoes).

2.2. Orange-Volcanoes

Orange-Volcanoes (https://git.new/orange-volcanoes) consists of a set of widgets in Orange allowing the user to perform several fundamental tasks in geochemistry, petrology, and volcanology (Fig. 5). In detail, Orange-Volcanoes includes dedicated widgets for:

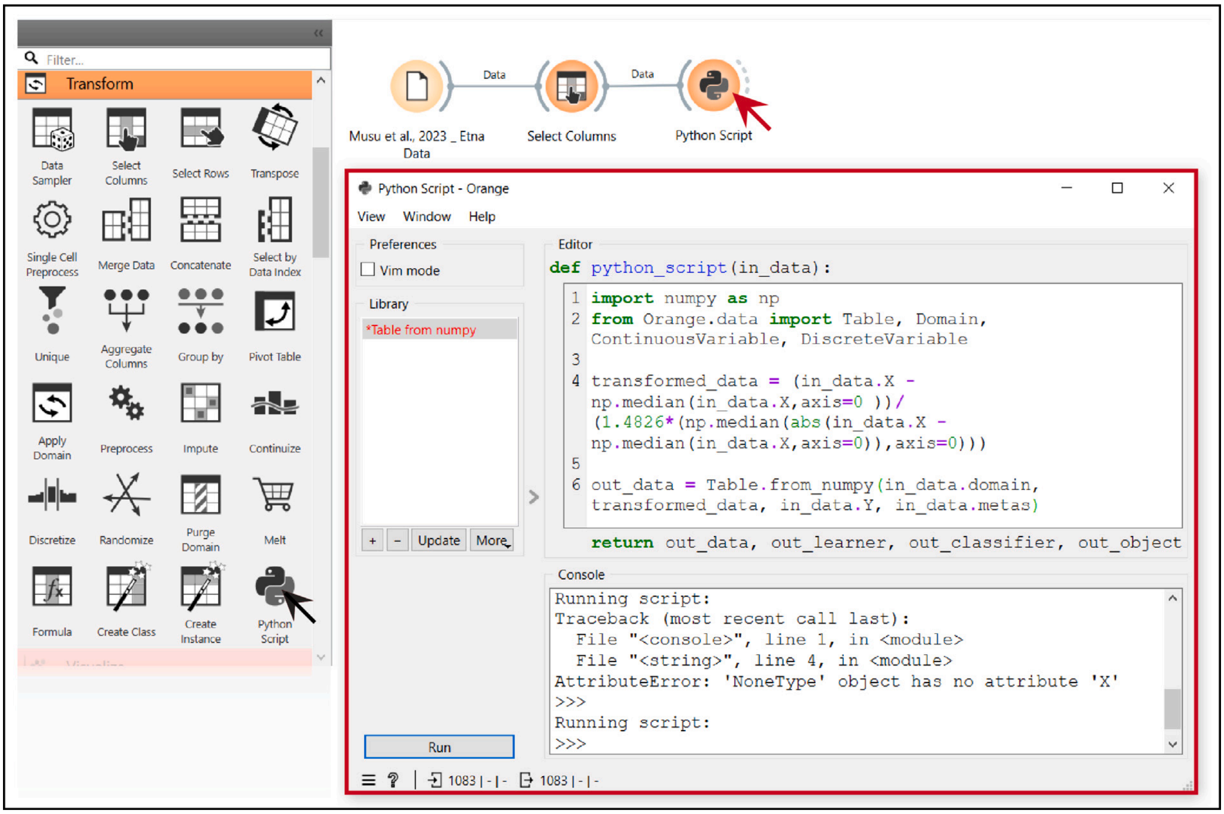

Fig. 4. Python script. Orange includes a widget that allows users to insert a custom Python function or script. In the example, we apply a robust normalization function (Media-MAD Normalization; Templ et al. 2008, Rousseeuw and Hubert 2011, Eesa and Arabo 2017) to a selected data set (Musu et al., 2023).

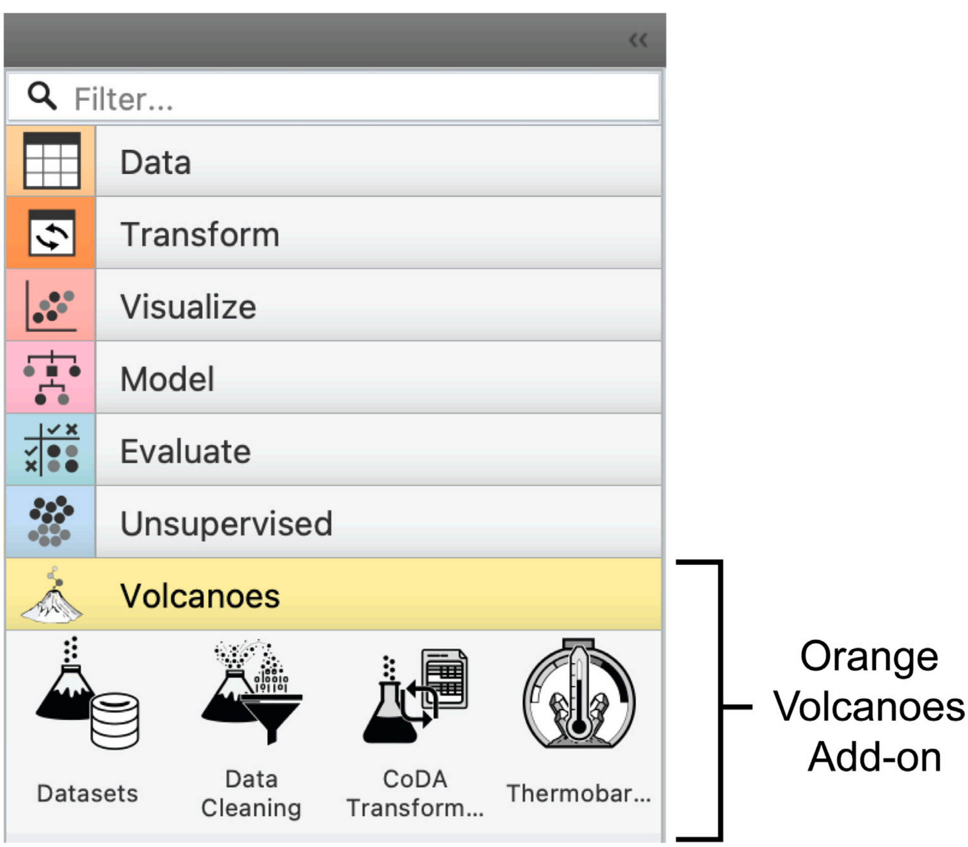

Fig. 5. Orange-Volcanoes. Orange-Volcanoes is an “add-on”, a package containing a set of widgets allowing users to pre-process, filter and analyze geochemical, petrological and volcanological data.

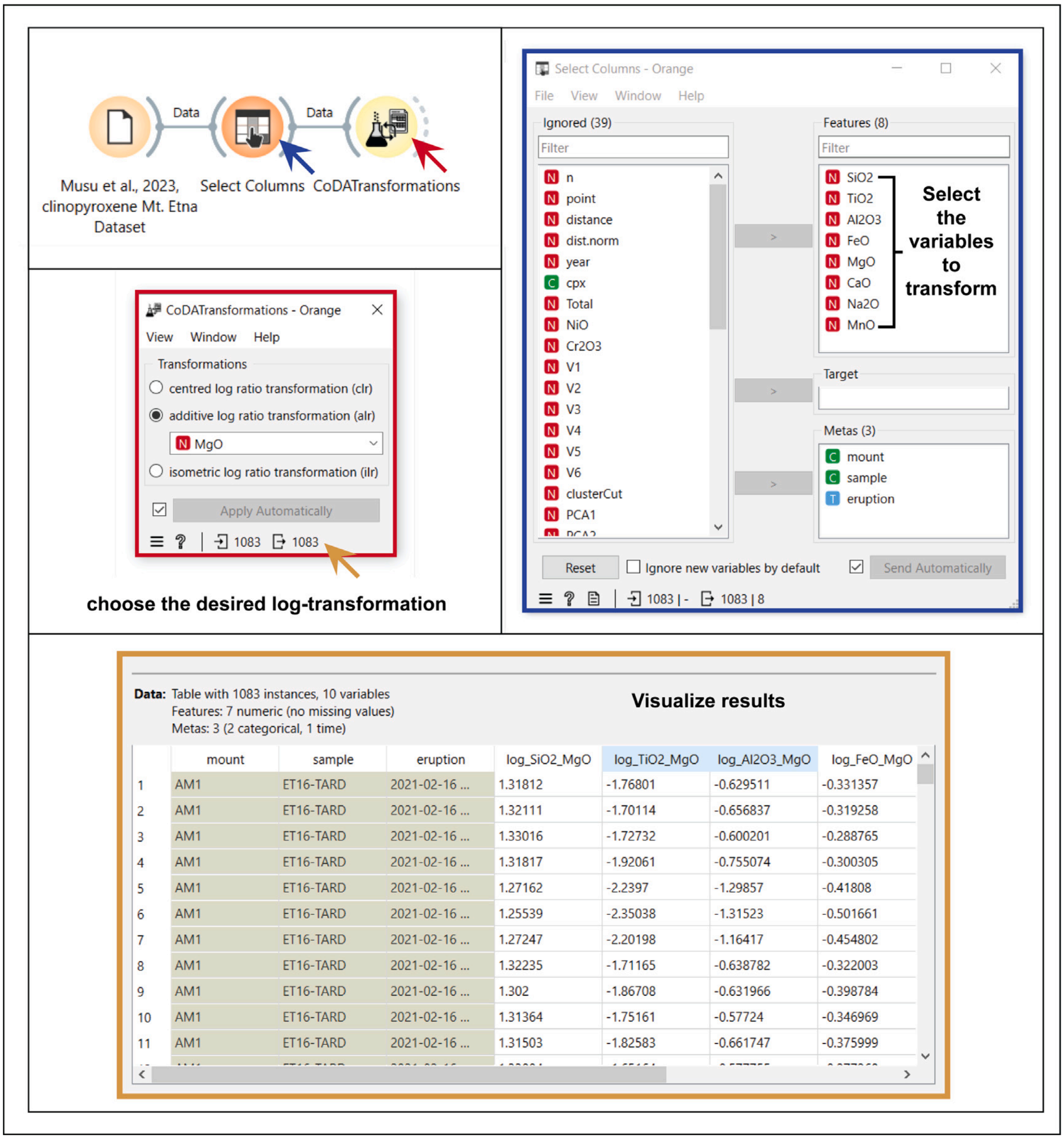

Fig. 6. CoDA transformation. The “CoDATransformations” widget allows the user to transform the starting data set with three different log-ratio transformations: (i) centered log-ratio (clr); (ii) additive log-ratio (alr); and (iii) isometric log-ratio (ilr) transformations. Users can upload an already pre-prepared data set on the Orange canvas with the widget “File” or upload the raw data set (with the widget “File”) and then select the desired column to transform using the widget “Select Columns”.

- Data import of geochemical, petrological, and volcanological data sets;
- CoDA pre-processing (i.e., centered, additive and isometric log-ratio transformations);
- Data cleaning of geochemical analyses performed on volcanic glasses and minerals (e.g., filter for total oxides and filter for sum of cations);
- Data cleaning based on mineral-liquid equilibrium tests;
- Classic and machine-learning-based thermobarometry estimates based on mineral only, mineral-liquid pairs, and liquid-only.

2.2.1. Data import

To import a personal data set into the Orange environment and process it through the dedicated Orange Volcanoes widgets, the user can simply employ the “File” widget within Orange (which allows the user to insert a custom .txt, .csv or . xlsx file). Alternatively, Orange-Volcanoes provides access to a list of open-source volcanological and petrological data sets, which the user can open through the “data sets” widget and immediately consult and analyze. In detail, the first release of Orange Volcanoes contains: (i) The experimental data set used to train machine-learning-based themobarometry (i.e., Petrelli et al., 2020); (ii) The glass major element analysis from the Campanian Volcanic Province product published by Smith et al. (2011); (iii) Selected clinopyroxene major element composition of Colli Albani Volcano and from the Campanian Volcanic Province (collected from Georoc; DIGIS Team, 2024); (iv) a single point geochemical analyisis example used by Pawlowsky-Glahn and Egozcue (2006) to explain and test different log-ratio transformations; (v) example dataset for Cpx-Liq, Opx-Liq and Opx-Cpx thermobarometry.

2.2.2. Compositional Data Analysis (CoDA)

The study of compositional data, such as the major element chemical compositions of volcanic glass and minerals, belongs to the field of Compositional Data Analysis (CoDA; Greenacre, 2021; Ágreda-López et al., 2024; Petrelli, 2023, 2024). Compositional data present two specific characteristics: (i) they consist of strictly positive values, and (ii) their components are interdependent, summing to a fixed total (e.g., 1 or 100), a concept referred to as the “closure” problem (Aitchison,

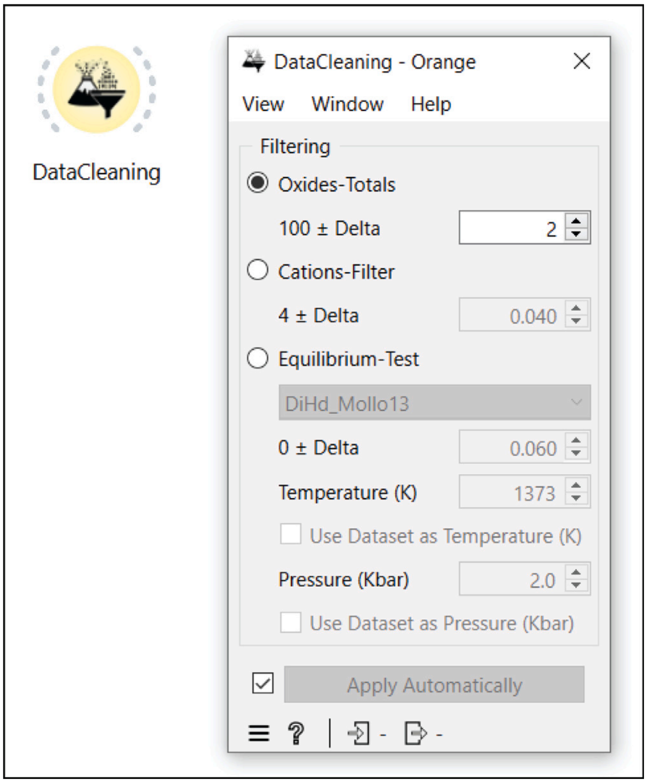

Fig. 7. Geochemical data cleaning. The "DataCleaning" widget allows the user to filter the starting data set for (i) oxide - totals, (ii) cation per formula unit sum, and (iii) crystal-melt pair disequilibrium.

1984, 1986). Many statistical multivariate methods, such as Hierarchical Clustering analysis, require data sets with independent variables that can range from $-\infty$ to $+\infty$, a requirement not met by compositional data (Greenacre, 2021; Ágreda-López et al., 2024). Therefore, to analyze glass and mineral chemistry using these statistical methods, including machine learning tools, data must be transformed ("opened") to satisfy the assumptions of these analytical techniques. Several transformations have been proposed to address the closure issue in geochemical data sets, including the additive log-ratio (alr), centered log-ratio (clr), and isometric log-ratio (ilr) transformations (Aitchison, 1986; Egozcue et al., 2003). These log-ratio transformations also have the added benefit of reducing skewness in data distributions, which enables the transformed data to leverage the advantages of Gaussian distributions (Zheng et al., 2021; Zhao et al., 2022). In Orange-Volcanoes, we implemented the alr, clr, and ilr transformations in a widget named "CoDATransformation", which allows users to easily apply these transformations to their selected data sets (Fig. 6). The use of the "CoDATransformation" widget enables users to conduct several multivariate analyses (e.g., hierarchical clustering, k-means, PCA, etc.) on geochemical, petrological, and volcanological data sets.

2.2.3. *Data the cleaning widget*

Raw geochemical data typically sum to a nominal value (e.g., 100%). Any significant deviation from this sum may indicate that one or more elements have not been included within the analytical protocol, poor data quality, or both. To ensure accuracy, a filter is often applied to the totals of selected mineral phases. For example, in the case of anhydrous minerals (such as clinopyroxenes), an acceptable range for the sum of the analyzed oxides is usually between 98 wt% and 102 wt%. Another commonly used filter is the cation sum filter. Using clinopyroxene as an example, its mineralogical formula consists of 4 cations and 6 oxygens. It is considered good practice to recalculate the composition of pyroxenes in terms of cations based on 6 oxygens. After this recalculation, the cation sum should be approximately 4. A significant deviation from this value could suggest that the mineral analyzed is not the target mineral or that the analysis point is located in a mixing zone between the mineral of interest and surrounding phases (e.g., clinopyroxene-plagioclase or clinopyroxene-glass interfaces). In Orange-Volcanoes, we have implemented both types of filters, providing an interactive tool that recalculates oxide totals and the cation content on a stoichiometric basis, by calling stoichiometric functions from Thermobar. This allows the user to choose how narrowly or widely to set the filter around the desired sum (Fig. 7).

In Orange-Volcanoes, data cleaning can be also performed using disequilibrium filters for mineral-liquid pairs. The chemical composition of mineralogical phases is frequently employed to reconstruct the conditions of deep crystallization, including pressure (P), temperature (T), and initial magma composition (X). To obtain accurate estimates of deep-forming conditions, it is essential to determine whether the analyzed crystal has reached equilibrium with the surrounding melt. Several equilibrium tests have been developed in recent years (Putirka, 2008; Mollo et al., 2013; Neave et al., 2019). We have implemented a specialized tool, utilizing equilibration functions from Thermobar (Wieser et al., 2022), that enables users to select the appropriate equilibrium test and specify the threshold for filtering their geochemical data (Fig. 7).

2.2.4. *Mineral and liquid thermobarometry*

Assessing the pressures (P) and temperatures (T) at which magmas are stored in volcanic systems is fundamental for understanding eruptive dynamics and the overall behavior of magmatic systems across different tectonic settings (Petrelli et al., 2020; Neave and Putirka, 2017; Higgins et al., 2022; Jorgenson et al., 2022; Wieser et al., 2022; Ágreda-López et al., 2024). Investigating the chemical composition of magmatic crystals and residual glass through thermobarometry provides insights into the dynamics of deep magma reservoirs, the origins of magmatic crystals, and the timescales of magmatic processes. This knowledge is crucial not only for anticipating volcanic activity but also for identifying the conditions under which critical elements such as Li, Cu, Mo, and rare earth elements (REEs) are concentrated (Wieser et al., 2022; Ágreda-López et al., 2024). Additionally, understanding magma storage depths provides essential information on the evolution and structure of the Earth's crust (Wieser et al., 2022). A comprehensive collection of all available thermobarometers is already implemented in Python within the Thermobar package (Wieser et al., 2022). To demonstrate the potential of Orange-Volcanoes in democratizing petrologic tools for non-experts in coding, we integrated the Thermobar library (Wieser et al., 2022) into Orange-Volcanoes through a dedicated widget. This widget allows users to estimate crystallization P and T from chemical analyses of mineral–liquid pairs, liquid-only, and mineral-only data (Fig. 8).

We tested the performance of Orange-Volcanoes thermobarometry widgets for each implemented model against Thermobar estimates (performed with the Jupyter Notebook web-based platform; Figure S1). The results of the comparison confirm that the algorithms implemented in Orange-Volcanoes correctly estimate the pressure (P) and temperature (T), producing as output the exact same values as when using Thermobar directly in Python.

2.2.5. *Usage and limits*

A detailed tutorial for the installation of Orange and Orange-Volcanoes, as well as for the use of each new widget, is available in the Orange-Volcanoes documentation (https://orange3-volcanoes.readthedocs.io). The documentation also provides downloadable Orange project files containing the original workflows used in this manuscript.

This release still presents some limitations. The CoDA transformation is already available for any type of geochemical dataset, enabling users to explore the full potential of Orange across a wide variety of

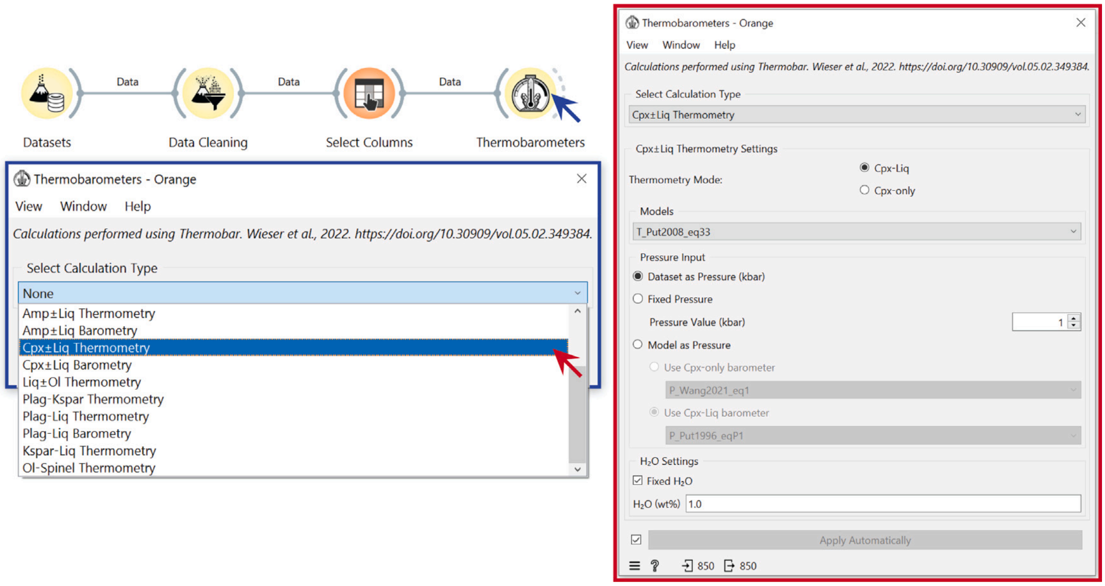

Fig. 8. Thermobarometry with Orange-Volcanoes Orange-Volcanoes enables thermobarometric calculations on mineral-only, mineral–liquid, and liquid-only analyses through a dedicated widget, "Thermobarometers". This widget directly calls the full Thermobar library (Wieser et al., 2022), allowing users to select the appropriate mineral or mineral–liquid pair, choose specific equations, and define input parameters such as pressure, temperature, and H_2O content when required.

data. The thermobarometry widget supports a broad range of mineral phases and thermobarometric models, allowing users to access the complete Thermobar library within the Orange framework. However, the DataCleaning widget is currently implemented only for clinopyroxene and liquid compositions and cannot yet be applied to other mineral phases. The Dataset widget is also being expanded, and additional datasets still need to be included (such as multi-mineral and glass compositions from GEOROC and novel experimental data). Despite these initial limitations, this release establishes a solid foundation for data-driven analysis of geochemical, volcanological, and petrological data within an open-source framework. Orange-Volcanoes is under active development. We are currently working to expand its capabilities to additional mineral phases. Importantly, this first release is intended as a starting point for collaborative development. We welcome contributions from other research groups and encourage collaboration aimed at broadening the application of Orange-Volcanoes to address a wider range of petrological and volcanological challenges. In this regard, researchers interested in contributing to the further development of Orange-Volcanoes are invited to contact us by email or by submitting a request through our GitHub page (https://git.new/orange-volcanoes).

3. Defining reproducible machine learning workflows on volcanic data

3.1. Clustering analysis on tephra glasses

In order to illustrate a practical application of Orange-Volcanoes on natural volcanic data, we developed a machine learning workflow to import, pre-process, and model by clustering analysis a data set consisting of glass chemical analyses from the recent activity of the Campi Flegrei caldera reported by Smith et al. 2011.

Fig. 9 reports the Orange workflow divided into four different steps:

1. Uploading and selecting data. The data set is first loaded, and only the columns necessary for clustering analysis (e.g., major element compositions) are selected using the "Select Column" widget. Rows containing zeros or not-a-number values – unsuitable for logarithmic transformations or clustering – are excluded using the "Select Row" widget.
2. Data Pre-processing. The major element compositions are transformed through an isometric log-ratio (ilr) transformation using the "CoDATransformations" widget (implemented within Orange-Volcanoes). The transformed data set is then normalized using the "Preprocess" widget with a standard scaler. Notably, the ilr transformation enables the application of clustering algorithms to geochemical data sets within the Orange environment.
3. Clustering Analysis. Once the data are loaded, filtered, transformed, and normalized, the clustering analysis is performed. First, Euclidean distances (the distance between two points in space, computed as the square root of the sum of squared coordinate differences; Dokmanic et al. 2015) are calculated using the "Distances" widget. Subsequently, hierarchical clustering is carried out using the "Hierarchical Clustering" widget. It is worth noting that other clustering algorithms (e.g., k-means and Louvain Clustering) are also available within the base Orange widget collection.
4. Data merging, visualization and export. In this step, the original, untransformed major element composition is merged with the transformed data set and clustering results into a single data set. The clustering outcomes are then visualized using simple binary chemical scatterplots (Fig. 9b). Additional plots are generated to explore the cluster chemical compositions (Fig. 9c) and to identify which eruptive products correspond to specific clusters (Fig. S2). In this final step, it is possible to export the merged clustered data set using the widget "Save Data".

As shown in Fig. 9, we identified four distinct clusters based on Euclidean distances. Most volcanic products from the first eruptive epoch of Campi Flegrei belong to Clusters 1 and 2. Cluster 3 compositions dominate the second eruptive epoch and the later eruptive period (Epoch 3b and the Monte Nuovo eruption, Fig. S2). Finally, Cluster 4 primarily corresponds to products from the third epoch, with some product from the first epoch.

The application of this workflow to the data of Smith et al. (2011) is purely illustrative, serving to demonstrate one of the many analytical applications that can be performed with Orange-Volcanoes on

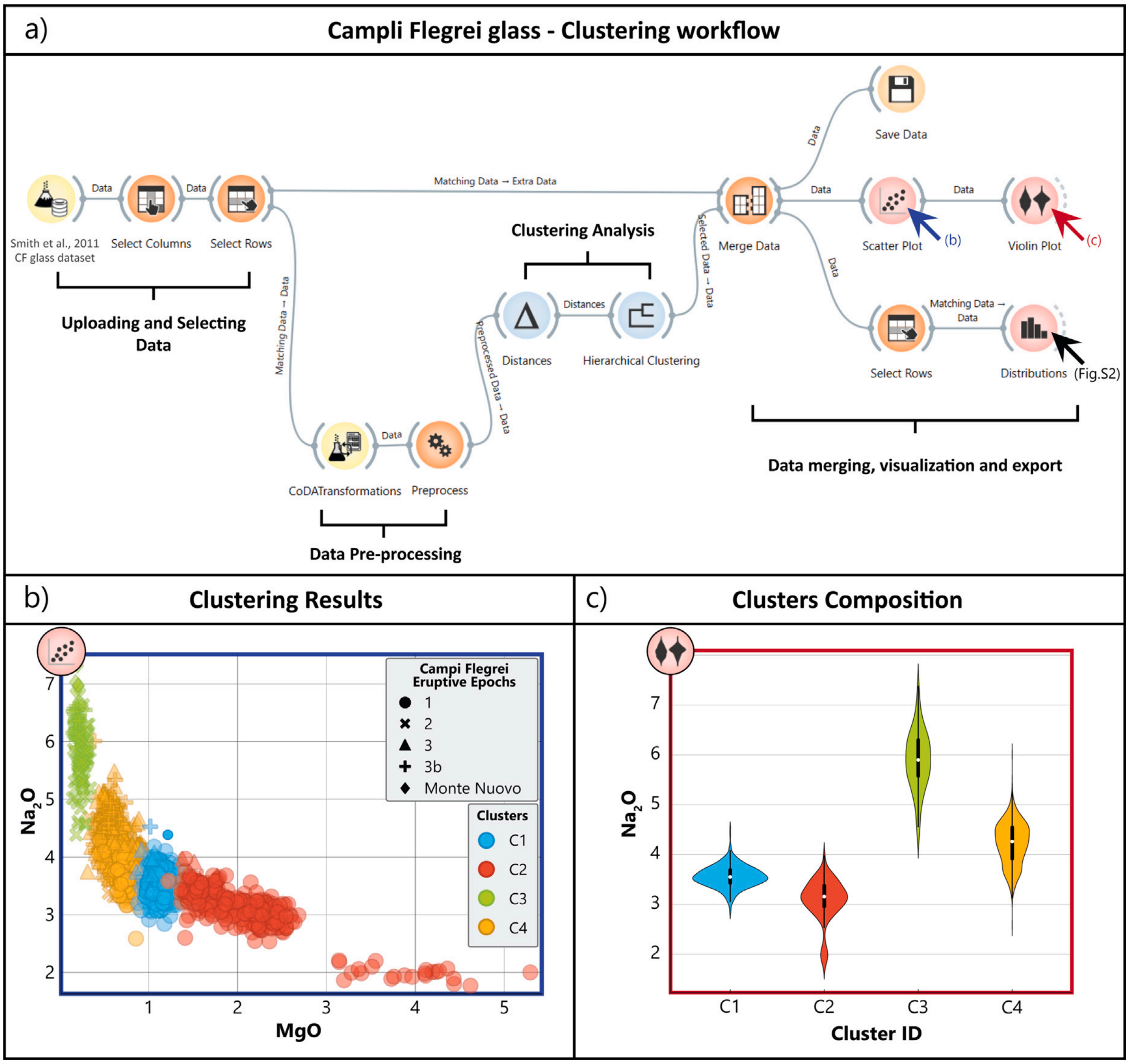

Fig. 9. Hierarchical Clustering algorithm applied to the glass chemical composition of Campi Flegrei samples (Smith et al., 2011). (a) Clustering workflow divided into the main sessions: (i) uploading and selecting data; (ii) data pre-processing (including the CoDA transformation implemented in Orange-Volcanoes, which allows for the very first time to apply clustering algorithms on geochemical data within the Orange Environment); (iii) clustering analysis; and (iv) data merging, visualization and export. In (b) we can observe the clustered observations plotted in the MgO vs Na_2O compositional space, while in (c) we display the Na_2O composition of the different clusters. The distribution histogram is displayed in Fig. S2.

geochemical datasets. As noted by Smith et al. (2011), glass chemistry alone is not sufficient to robustly correlate most tephra deposits (specifically in the case of Campi Flegrei). It is therefore essential to complement chemical data with stratigraphic, chronological, and volcanological information. In this context, we consider that the use of robust static tools available in Orange can enable not only objective, reproducible, and rigorous classification of chemical data, but also the integration of large multivariate datasets, where geochemical data can be jointly analyzed with stratigraphic, chronological, and volcanological parameters, thereby supporting more robust classification and interpretation based on multidisciplinary observations.

Fig. 9c shows how Orange can display the chemical composition of each cluster. As an example, we plot only the Na_2O contents of four clusters. This exercise demonstrates how Orange and Orange-Volcanoes can be used to investigate a geochemical data set. The workflow is intuitive and user-friendly, giving researchers complete control over the chemical meaning of identified clusters or groups. It also enables quick tests of different transformations, normalizations, and clustering methods in an interactive manner.

3.2. Testing different machine learning classification models in tephra investigations

Combining Orange and Orange-Volcanoes allows users to test and compare the performance of different machine learning classification models, for example in tephra studies. It can cross-validate multiple models at the same time and evaluate their scores. The built-in “Test & Score” widget enables the computation of various accuracy and precision metrics for the applied models, facilitating direct comparison of their results. Fig. 10 shows a practical example of how to test different classification methods on geochemial observations belonging to the recent activity of the Campi Flegrei Caldera (Smith et al., 2011). Based on chemical composition, we classified which eruptive epoch the

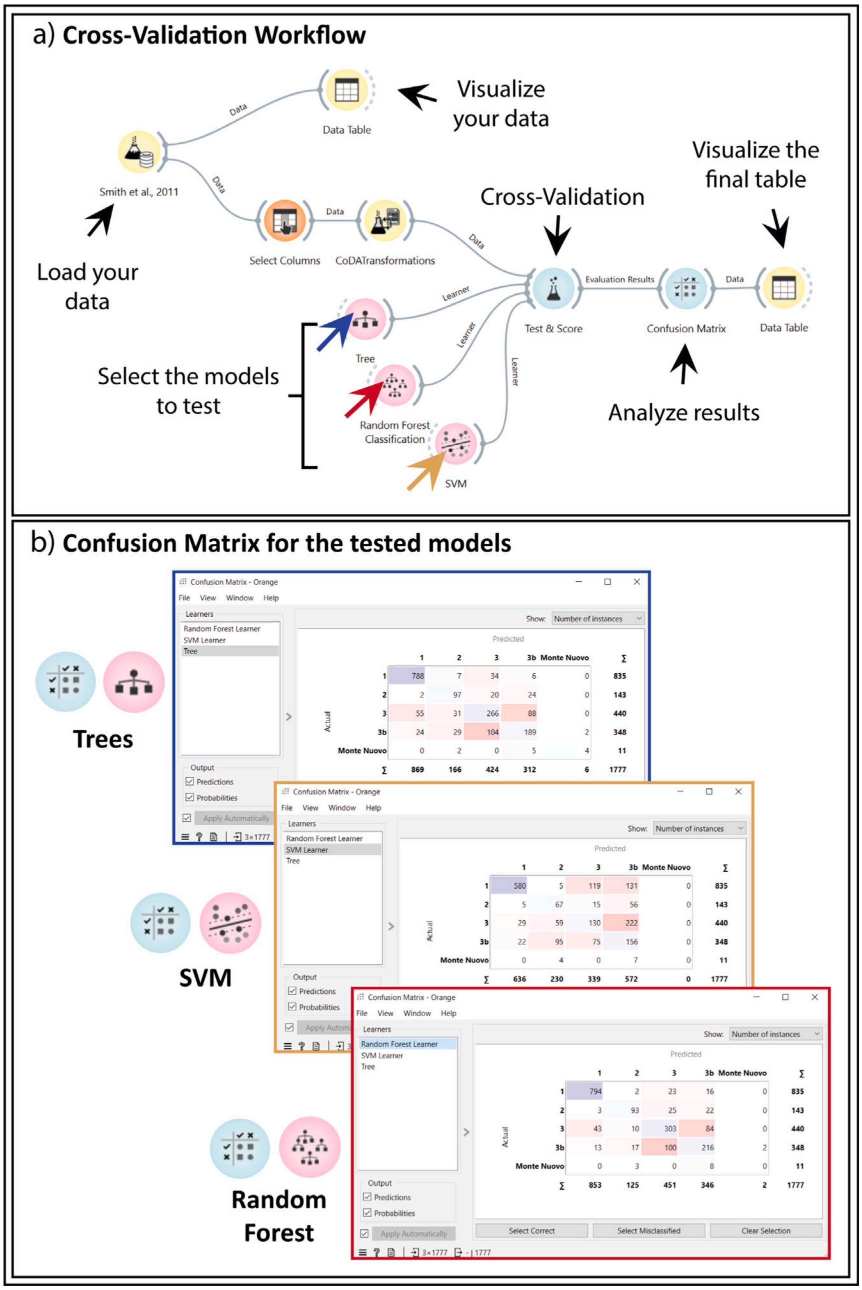

Fig. 10. Cross validation of multiple classification models (Tree, Support Vector Machine [SVG] and Random Forest) applied on the same Campi Flegrei glass chemical data set from Smith et al. (2011). (a) Cross validation workflow; (b) Confusion Matrix visualization for the three applied methods.

glasses belonged to. We applied three methods: Decision Trees, Random Forest, and Support Vector Machine.

As shown in Fig. 10, Orange can test all three methods simultaneously. It also displays the results in a confusion matrix (a table that summarizes the performance of a classification model by comparing predicted and true class labels; Powers 2020), so it is possible to quickly analyze how well each model performs. This feature lets user decide which algorithm works best for the studied data set. Cross-validating multiple models at once gives users the control over model performance. It also makes it easy to review the scores and build a robust analysis workflow for any given data set. The procedure is simple and intuitive, as outlined in Fig. 10. The complete workflow example is provided in the “Tephra Classification” section of the documentation (https://orange3-volcanoes.readthedocs.io/). Additionally, Orange provides various evaluation widgets, such as the Confusion Matrix and Performance Curve. These can be linked to the score results and visualization widgets like the scatterplot. In this case study, we observed that among the three tested models, the Random Forest classifier achieved the best performance, with accuracy and precision metrics of approximately 80% for this specific case and starting dataset.

4. Conclusions

The development of Orange-Volcanoes represents a significant contribution to the application of data-driven discovery in geochemistry, petrology, and volcanology. It extends the functionality of the Orange platform by providing customized tools (i.e., widgets) to address key challenges in geochemical data analysis, including compositional data analysis (CoDA), mineral data filtering, mineral-liquid equilibrium testing, and thermobarometric calculations. As a key feature, Orange-Volcanoes enables integration between machine learning techniques and classical petrological methods, promoting a deeper understanding of magmatic systems through accessible, interactive, and reproducible workflows. Moreover, the user-friendly design of the platform removes barriers for researchers with limited or no programming knowledge while maintaining the flexibility for advanced users to customize and expand its functionality. These characteristics also make Orange and Orange-Volcanoes well suited for education, allowing students to engage with geological data through structured, visual workflows. This approach helps learners interact with each analytical step, focus on data interpretation, and develop a clearer understanding of data structure and method selection, all without requiring any coding experience.

While several robust platforms exist for data mining and machine learning in geochemical, petrological, and volcanological research (e.g., Geochemistry π and XMapTools; Lanari et al. 2014, Li et al. 2020, Li and Costa 2020, ZhangZhou et al. 2024), Orange-Volcanoes distinguishes itself by offering an interactive, expandable, and collaborative visual programming environment. It combines multiple statistical and machine learning algorithms with many analytical and visualization tools already available in Orange. These features, together with explainable artificial intelligence and cross-validation widgets, make Orange and Orange-Volcanoes a powerful and robust framework for future petro-volcanological research on large data sets (e.g., volcano plumbing system dynamics, petrological monitoring, and tephra investigations).

While Orange-Volcanoes facilitates data-driven exploration, its application should always be guided by expert knowledge and understanding of the geological and physical context of the data. Although Orange-Volcanoes does not yet include every tool needed for advanced petrological and geochemical investigations, it is designed for easy expansion. This design allows external research groups to develop and integrate their own tools, further broadening their use within the geoscientific community.

Overall, Orange-Volcanoes provides a collaborative, open-source environment that bridges modern data analysis techniques and the needs of geoscientists. Future developments will incorporate additional geochemical and petrological tools and data sets. This will enhance the platform's capabilities and expand its applications to a wider range of volcanological, geochemical, and petrological problems.

CRediT authorship contribution statement

Alessandro Musu: Writing – review & editing, Writing – original draft, Validation, Methodology, Formal analysis, Data curation, Software. **Valerio Parodi:** Writing – review & editing, Writing – original draft, Software, Investigation, Formal analysis, Data curation. **Marko Toplak:** Writing – review & editing, Validation, Supervision, Software. **Alessandro Carfì:** Writing – review & editing, Validation. **Mónica Ágreda-López:** Writing – review & editing, Writing – original draft, Validation, Methodology, Formal analysis. **Fulvio Mastrogiovanni:** Writing – review & editing, Validation. **J. ZhangZhou:** Writing – review & editing, Validation, Investigation. **Diego Perugini:** Writing – review & editing, Validation, Funding acquisition. **Donato Belmonte:** Writing – review & editing, Validation. **Penny E. Wieser:** Formal analysis, Software, Validation, Writing – review & editing. **Blaž Zupan:** Writing – review & editing, Validation, Software. **Maurizio Petrelli:** Writing – review & editing, Writing – original draft, Supervision, Investigation, Conceptualization, Software.

Code availability section

All the codes, data, and apps used in this manuscript are open source and distributed under the GNU General Public License v3.0 license. Source codes are available on GitHub for downloading and collaboration at the link: https://git.new/orange-volcanoes.

The Orange-Volcanoes documentation is available at: https://orange3-volcanoes.readthedocs.io.

Declaration of competing interest

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

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.acags.2025.100270.

Data availability

Data and codes are available at https://github.com/AIVolcanoLab/orange3-volcanoes.

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