

BOOM! Tephrochronological dataset and exploration tool of the Southern $(33-46^{\circ} \text{ S})$ and Austral $(49-55^{\circ} \text{ S})$ volcanic zones of the Andes

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1	BOOM! Tephrochronological dataset and exploration tool of the
2	Southern (33–46° S) and Austral (49–55° S) Volcanic Zones of the
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17 Abstract

18 Tephrochronology studies the deposits of explosive volcanic eruptions in the stratigraphic record. The Southern (SVZ, 33–46° S) and Austral (AVZ, 49–55° S) Volcanic Zones of the Andes are two very active 19 20 volcanic zones where tephrochronology is of great use. There, it can be used to improve chronologies of 21 paleoenvironmental records in Patagonia, an area providing valuable records at global scale; as well as 22 to identify areas likely to be affected by volcanic eruptions in the future, essential for producing volcanic 23 hazard maps. The close proximity of many volcanic centers with recurrent explosive activity, which have 24 very similar geochemical compositions, and very often poor age constraints, represent a challenge for the 25 study of tephrochronology in the region. In addition to this, the ever-growing amount of 26 tephrochronological information in the area, dispersed in different types of publications which vary 27 greatly in format, makes the integration of the data produced by different actors, and consecutively its 28 interpretation, increasingly difficult. Here we address this issue by compiling the BOOM! dataset, which 29 integrates \sim 30 years of research on 32 active volcanic centers and 132 different eruptions, which took 30 place during the last 20,000 years. To help users find and reuse data in the large dataset, we developed 31 an online platform which provides user-friendly tools for exploring it, and helps users download subsets 32 of it. To integrate this very heterogeneous information, special attention was given to include information 33 which allows users to evaluate data quality and comparability, as well as to provide tools in the explorer 34 for users to filter data by different criteria. The integration of this dataset opens new perspectives for the 35 development of novel visualizations of tephrochronological data, for example, to better understand the 36 multidimensional uncertainties associated with it. For example, uncertainties associated with analytical 37 precision, with age estimates of both tephra deposits and volcanic eruptions, and of tephra classification. 38 Additionally, it allows for the use of robust statistical tools to correlate tephra deposits, including those 39 based on machine learning algorithms, which are here explored.

40 **Keywords:** Tephrochronology, Southern Volcanic Zone of the Andes, Austral Volcanic Zone of the Andes,

41 Geochemistry, Radiocarbon, Machine learning

42

43 **1 Introduction**

Tephrochronology is a discipline of geosciences which uses the deposits of explosive volcanic eruptions 44 45 as stratigraphic and chronological markers. These deposits are called tephras, and by studying them, 46 researchers can reconstruct the eruptive history of volcanic centers: how often volcanic activity occurs, 47 the magnitude of the eruptions, and the dispersion of the volcanic products. The Southern (SVZ, 33-46° S) and Austral (AVZ, 49–55° S) Volcanic Zones of the Andes are two very active volcanic zones, where 48 49 \sim 65 volcanic centers have been identified. Many of these centers have had recurrent explosive activity in 50 historical times, e.g., Llaima (Naranjo & Moreno, 2005), Puyehue-Cordón Caulle (Naranjo et al., 2017), 51 Calbuco (Sellés & Moreno, 2011), Hudson (Naranjo et al., 1993) and Lautaro volcanic centers (Mayr et al., 52 2019). While for others, evidence of recurrent explosive activity during the last ~20,000 years has also 53 been identified, e.g., Mocho-Choshuenco (Rawson et al., 2015), Michinmahuida (Amigo et al., 2013) and 54 Mount Burney volcanic centers (Smith et al., 2019). More so, some of these volcanic centers are very 55 explosive, with distal dispersion of tephras being registered hundreds of kilometers from their source, as 56 the H1 eruption from Hudson volcanic center (Naranjo & Stern, 1998; Kilian et al., 2003; Stern, 2008; Del 57 Carlo et al., 2018; Smith et al., 2019). Because of the latter, one important concern in these areas is 58 protecting surrounding villages and other important infrastructure (e.g., power plants or dams) from 59 potentially dangerous eruptions. Part of this work is done by the Chilean Geology and Mining agency 60 SERNAGEOMIN, which produces volcanic hazard maps of the different volcanic centers and regions in 61 the country and distributes them to the population (e.g., Bertin et al., 2018). In order to produce these 62 maps, SERNAGEOMIN relies on tephrochronological and volcanological information from their own 63 surveys as well as from peer-reviewed scientific publications (e.g., Sellés & Moreno, 2011; Bertin et al., 64 2018), which helps them identify areas likely to be affected by future eruptions. Besides this very important application, and because of the recurrent explosive activity of the SVZ and AVZ, there is great 65 66 potential of using tephrochronology to improve the chronologies of paleoenvironmental records in Patagonia (Fontijn et al., 2014). If tephras deposited during the same eruptive event are identified in 67 68 different sedimentary archives (e.g., lake sediment cores, marine sediment cores, peat cores, or

69 archaeological sites), the chronologies of different records paleoclimatological, (e.g., 70 paleoceanographical, or archaeological records) can be synchronized. Paleoenvironmental records in 71 Patagonia provide valuable climatic records, such as the variations in the Southerly Westerly Winds (e.g., 72 Moreno et al., 2018); valuable oceanographic records, such as changes in oceanic circulation in the 73 Southern Ocean (e.g., Siani et al., 2013); as well as unique records describing interactions between human 74 populations, climate change and volcanic activity at high latitudes (e.g., Villarosa et al., 2006; Prieto et al., 75 2013). In order to correctly integrate these records, having good chronologies is essential, thus 76 highlighting the potential of using tephrochronology in the area.

77 In the last four decades, tephrochronology together with volcanology have increased our understanding 78 of the eruptive history of the SVZ and AVZ, revealing higher than previously thought recurrence rates and 79 explosivity of many of the volcanic centers in the area (e.g., Chaitén and Michinmahuida volcanoes (Amigo 80 et al., 2013; Watt et al., 2013; Moreno et al., 2015; Alloway et al., 2017a, b; Martínez Fontaine et al., 2021)). 81 This work, and especially the study of sedimentary archives which favor the preservation of tephras 82 (such as lake cores (e.g., Bertrand et al., 2014)), has revealed a very intricate tephrostratigraphic record 83 in the area, given by the close proximity of the volcanic centers together with their high eruptive 84 recurrence rates. In order to disentangle this record, tephrochronologists try to fingerprint tephras using 85 their physical characteristics, geochemical composition, stratigraphic position, and age (e.g., Lowe, 2011). 86 By doing this, they can correlate tephras deposited in different locations and ideally identify their volcanic 87 source and the specific eruption during which they were deposited. In the SVZ and AVZ, doing this is not 88 trivial. For example, many volcanic centers and eruptions have very similar geochemical compositions, 89 or in other cases, the age estimates of tephra deposits have high uncertainties, or they do not exist at all, 90 making it hard to distinguish tephras based on these criteria. This issue is enhanced by the unFAIRness of 91 the tephrochronological data (e.g., physical characteristics, geochemical composition, stratigraphic 92 position, and age of tephras) in the area, i.e., data is not readily Findable, Accessible, Interoperable, or 93 Reusable (Wilkinson et al., 2016; Abbott et al., 2022). At present, the available tephrochronological and 94 volcanological information of the SVZ and AVZ can be found dispersed in journals, undergraduate or 95 doctoral theses, publications from government institutions (SERNAGEOMIN), and personal collections,

96 which vary greatly in format, and with some information sometimes very difficult to find. This, together 97 with the increased data stream associated with the development of analytical techniques (such as Electro 98 Probe microanalysis (EMPA, also referred to as EMP), typically used for analyzing glass (or mineral) 99 major element composition of volcanic ash shards, e.g., Lowe (2011)), makes the integration of the data 100 produced by different actors (researchers and practitioners from government institutions), and 101 consecutively its interpretation, more and more difficult. The increasing need for organization of the vast 102 and growing amount of tephrochronological and volcanological data in the region, is an issue that has 103 already been addressed in previous publications (Fontijn et al., 2014, 2016; Alloway et al., 2017a, 2017b). 104 Here we address it by making two main contributions. First, by compiling a dataset which standardizes 105 and integrates ~30 years of research mainly in tephrochronology (complemented with volcanological 106 information), on 32 active volcanic centers and 132 different eruptions of the SVZ and AVZ during the 107 last 20,000 years. Additionally, we developed an online platform¹ which provides user-friendly tools for 108 the exploration of the large dataset, and helps users download subsets of it. Both contributions aim to be 109 a step towards making these data FAIR (Wilkinson et al., 2016).

110 2 Methods

111 **2.1 Understanding the problem: Interviews with domain experts**

In order to characterize the work and needs of people using tephrochronology in the SVZ and AVZ, we 112 113 conducted a series of interviews with researchers and practitioners who are part of this community, 114 including volcanologists, tephrochronologists, palaeoclimatologists, among others. This information was 115 then used as input to design the dataset structure and the exploration tool. Between June and August 116 2020, we interviewed 19 people: two researchers in volcanology, one researcher in paleoceanography 117 and a team of 16 people from the Chilean National Volcanic Vigilance Network, part of SERNAGEOMIN. 118 However small, the interviewed sample represents to some extent the diversity of the 119 tephrochronological community in the area. Each interview lasted between one and three hours and was

¹ https://boom-vis.lisn.upsaclay.fr/

120 divided in two main phases. In the first phase, we asked them about their demographic information (age, 121 research area, position) and their daily work using tephrochronological data. More specifically, we 122 focused on understanding what scientific questions they try to answer, which data they use to do so, how they acquire, organize and analyze these data, and what problems they commonly encounter in this 123 124 process. In the second phase, we asked them to show us a concrete example from their work in order to 125 confirm or complement the answers given during phase one, and particularly to understand how they 126 use visualizations to organize data and answer their scientific questions. Finally, we showed them an 127 early prototype of the exploration tool in order to get initial feedback to iterate its design. All interviews 128 were audio recorded with the participants' consent (available in section S1 of the supplementary 129 material). A summary of the answers from the interviews can be found in Table S1 in the supplementary 130 material.

131 The interviews had two main results. On the one hand, we confirmed that the unFAIRness of the data was 132 an important issue for the participants. All of them expressed how difficult and time-costly it was for 133 them to collect, organize and analyze tephrochronological data given the dispersion of data sources and 134 the lack of common publication standards. On the other hand, the interviews allowed us to list the 135 information more routinely used by tephrochronologists working in the area, as well as pinpointing the 136 problems they encounter when using these data (Table S1). Then, we designed a structure that contains 137 this information in a way that, together with the explorer, addresses those issues. In particular, the main 138 problems we addressed were: difficulties organizing the bulk of data, ignoring the existence of data, not 139 understanding a priori if data from different sources are comparable or not, and problems visualizing 140 data in its multidimensionality (e.g., visualizing at once the geographical position of the tephra deposits, 141 their geochemical composition, stratigraphy and chronology). More detailed descriptions on the design 142 of the BOOM! dataset and explorer, and how they address these issues, are presented in sections 3 and 4, 143 respectively. The information from the interviews substantially aided the development of the structure 144 of the dataset and the exploration tool.

145 **2.2 Data collection**

146 We collected tephrochronological and volcanological information on 32 active volcanic centers belonging 147 to the SVZ and AVZ, between volcanoes Llaima (~38.7° S) and Mount Burney (~52.3° S). Here, volcanic 148 centers are considered active if evidence of volcanic activity occurring during the last ~20,000 years has 149 been identified. This time frame is relevant for volcanology as it captures the volcanic centers that are 150 likely to still erupt in the future. However, it is also informed by practical limitations due to the presence 151 of the Patagonian Ice Sheet (PIS) in the area during the last glacial period (~20,000–60,000 years Before 152 Present; (Davies et al., 2020)). During the last glacial period, the PIS covered most of the Andes south of 153 \sim 38° S, and thus, unconsolidated tephra deposits older than \sim 20,000 years have been largely eroded.

154 Three types of data were collected:

i. Physical characteristics and geochemical analyses (e.g., EMPA) of **pyroclastic material** (tephras

156 themselves). A full list of the geochemical analyses included in the dataset is detailed in Table S2.

157 ii. Radiocarbon (¹⁴C) ages of organic matter *associated* with the tephras, typically recovered from
158 within the deposits or from palaeosols immediately underlying them (used to estimate when
159 tephras were deposited).

160 iii. Geochemical composition and ⁴⁰Ar/³⁹Ar ages of effusive material (e.g., lava, breccia, 161 prismatically joint blocks).

162 Even though this dataset is aimed to help the tephrochronological community, volcanological data (i.e., 163 data of effusive material) was also collected to complement the tephrochronological information. 164 Because effusive material builds the volcanic edifice itself, there is little uncertainty regarding its volcanic 165 source. On the contrary, tephra deposits can be identified thousands of kilometers away from any 166 volcanic center, and often their source has not been robustly identified yet. Thus, the geochemical 167 composition of effusive materials was included in the dataset as a geochemical "ground truth", to which 168 to compare the geochemical composition of tephra deposits for which the volcanic source has not been 169 yet identified. This information is particularly useful for volcanic centers for which little 170 tephrochronological information is available. On the other hand, ⁴⁰Ar/³⁹Ar ages provide age constraints

171 when no ¹⁴C ages or other stratigraphic constraints are available. Errors associated to ⁴⁰Ar/³⁹Ar ages are 172 usually one order of magnitude larger than those of ¹⁴C ages and generally do not allow to differentiate 173 between eruptions in the SVZ and AVZ. However, in recent years ⁴⁰Ar/³⁹Ar errors are getting smaller 174 thanks to the development of more precise analytical techniques.

175 From the publications in the literature, we prioritized those which included analyses of the geochemical 176 composition of tephras, together with age or stratigraphic constraints, as long as the composition 177 reported was magmatic (in this particular geologic setting, this corresponds to $\sim 40-80$ wt.% SiO₂). 178 Otherwise, and because of the data scarcity for many volcanic centers, we included all publications we 179 could find in the literature which met these criteria. However, we always tried to include information 180 necessary for users to evaluate the quality and comparability of the data (sections 4 and S5) and flagged 181 the data when some issue was identified (section S5.4, Table S4). In total, we collected data from 72 182 scientific publications published in peer-reviewed journals, five publications from SERNAGEOMIN, and 183 two doctoral theses (the whole list of publications can be found below). These publications included 184 works on tephrochronology (31), volcanology (28), geological mapping (6), palynology (6), glaciology 185 (2), volcanic hazard mapping (1), archaeology (1), limnology (1), pedology (1) and paleoceanography (1). 186 The information included in the dataset was extracted either directly from the publication tables, text 187 and supplementary material, or alternatively through private requests to the authors when the data 188 discussed in the publication was not readily available. The authors were informed of the purpose of the 189 data request beforehand. From this process, ~16,800 sample analyses were included in the dataset, 190 identified as sourced in 132 different eruptive events, from 32 different volcanic centers. Tephra deposits 191 described in the literature for which the volcanic source has not been identified yet were also included in 192 the dataset, which correspond to $\sim 11\%$ of the sample analyses.

193 Publications in peer reviewed journals:

Abarzúa & Moreno, 2008; Abarzúa et al., 2004; Alloway et al., 2015; Alloway et al., 2017a; Alloway et al.,
2017b; Amigo et al., 2013; Bertrand et al., 2008a; Bitschene et al., 1993; Bouvet de Maisonneuve et al.,

196 2012; Brahm et al., 2018; Bucchi et al., 2015; Carel et al., 2011; Casati et al., 2019; Clapperton et al., 1995;

197 Constantini et al., 2011; Del Carlo et al., 2018; D'Orazio et al., 2003; Fontijn et al., 2016; Futa & Stern, 198 1988; Geoffroy et al., 2018; Gerlach et al., 1988; Haberle & Lumley, 1998; Harambour, 1988; Heusser et 199 al., 1989 Heusser et al., 2000; Hickey-Vargas et al., 1989; Jacques et al., 2014; Kilian et al., 2003; 200 Kratzmann et al., 2008; Lara et al., 2004; Lara et al., 2006; Lohmar et al., 2012; López-Escobar et al., 1992; 201 López-Escobar et al., 1993; López-Escobar et al., 1995; Martínez Fontaine et al., 2021; Mayr et al., 2019; 202 Miranda et al., 2013; Weller et al., 2014; Moreno & León, 2003; Moreno et al., 2015; Moreno, 2004; 203 Morgado et al., 2015; Morgado et al., 2019; Motoki et al., 2006; Naranjo & Moreno, 1991; Naranjo et al., 204 1993; Naranjo & Stern, 2004; Naranjo & Moreno, 2005; Naranjo & Stern, 1998; Naranjo et al., 2017; Pesce 205 & Moreno, 2014; Rawson et al., 2015; Rawson et al., 2016; Reubi et al., 2011; Schindlbeck et al., 2014; 206 Simmons et al., 2020; Singer et al., 2008; Smith et al., 2019; Stern et al., 2011; Stern et al., 2015; Stern, 207 1992; Stern, 2008; Tagiri et al., 1993; Villarosa et al., 2006; Wastegård et al., 2013; Watt et al., 2011a; 208 Watt et al., 2011b; Watt et al., 2013; Weller et al., 2014; Weller et al., 2015; Weller et al., 2017; Weller et 209 al., 2019.

210 Publications from SERNAGEOMIN :

211 Naranjo & Stern, 1998; Naranjo & Moreno, 2005; Lara et al., 2006; Moreno et al., 2010; Sellés & Moreno,
2011; Bertin et al., 2018.

213 Doctoral theses: Lohmar, 2008; Mella, 2008.

214 **2.3 Data Visualization: Development of the BOOM! explorer**

215 The BOOM! explorer is complementary to the dataset itself and aims to provide tools for users to make 216 the most of it. As mentioned before, we designed the explorer to address the main problems participants 217 expressed during the interviews (section 2.1, Table S1). In turn, this helped us better understand the 218 dataset we were collecting and modify its structure in order to better answer to community requests. For 219 example, when looking for ways to visualize if data from different sources were comparable or not, we 220 realized that important information to evaluate this was missing in the dataset, such as the type of 221 register the sample corresponds to (pyroclastic material, organic matter, or effusive material) or the type 222 of analysis performed in the sample (bulk versus micro analytical). Taking this into consideration, this

223 information was included in the dataset and users can choose which type of register and analysis to 224 visualize in the explorer. This process led an iterative redesign of the explorer, which included: modifying 225 the visual representation of the data, including additional User Interface interactions (e.g., filtering data 226 by different criteria), and reorganizing the visual elements in the explorer. This iterative redesign was 227 also supported by informal meetings with practitioners, some of them from the same group we had previously interviewed, where they told us their impressions of the tool, expressed their need for 228 229 additional features, and gave us general feedback. The development of the explorer additionally helped 230 us identify gaps in the dataset; include additional information, for example, a particular type of data of a 231 particular volcanic center or eruptive event in order to better characterize them; as well as identify 232 outliers and flag data. A detailed description of how the explorer can be used to explore the dataset is 233 exemplified in section S6 by a use case.

234 Given the above process, we decided to build a light visualization tool, which can be easily installed in a 235 local environment. In this way, other researchers can make modifications/improvements to the explorer. 236 The BOOM! explorer is published under an MIT License², which allows to reproduce it and build from it, 237 under the same license as the original one. The tool was developed in Javascript, using node.js³ as the 238 back-end environment. For the visualization components, we used the Leaflet library⁴ for the map, D3.js⁵ 239 for the timelines, and dc.js⁶ with Crossfilter⁷ for the geochemical composition scatterplots. The dataset is 240 delivered as a CSV file (see section 3 for more details), but in order to allow fast queries in the 241 visualization, we exported it to a SQLite⁸ dataset that is accessed from node.js. This transformation also includes precomputed queries that help with the performance of the tool. The BOOM! explorer 242 243 (https://boom-vis.lisn.upsaclay.fr/) is hosted by the Laboratoire Interdisplinaire des Sciences du

² https://mit-license.org/

³ https://nodejs.org/

⁴ https://leafletjs.com/

⁵ https://d3js.org/

⁶ https://dc-js.github.io/dc.js/

⁷ https://crossfilter.github.io/crossfilter/

⁸ https://www.sqlite.org

Numérique, LISN (Université Paris-Saclay, CNRS & Inria), France, which guarantees its hosting and access
as long as the server exists.

246 **3 BOOM! Dataset structure**

247 Tephrochronology identifies deposits from explosive volcanic eruptions in the stratigraphic record, 248 samples, and characterizes them based on their physical characteristics, geochemical composition, 249 stratigraphy and age. Then, based on this characterization and the comparison with available 250 tephrochronological (and volcanological) information in the area, tephrochronologists ideally identify 251 the volcanic source and the specific eruption during which the tephra was deposited, i.e., they *classify* it. 252 The BOOM! dataset follows this structure. It is composed of a collection of descriptions and laboratory 253 analyses of tephra deposits identified in the SVZ and AVZ (complemented with data on some lava flows). 254 In the BOOM! dataset, each of these descriptions or analyses is called a "sample observation", and one 255 sample of a tephra deposit may be described by one or many sample observations. For example, in order 256 to characterize a tephra deposit, researchers can describe the physical characteristics of the deposit as a 257 whole (e.g., its color, grain size, and thickness) and at the same time analyze the geochemical composition 258 of dozens of individual volcanic glass shards obtained in just one sample. Then, one sample observation 259 corresponds to the analyzed geochemical composition of one individual glass shard (as exemplified in 260 Figure 1). The sample as a whole, on the other hand, is described by the physical characteristics of the 261 tephra deposit and the geochemical composition of all the analyzed glass shards. Additionally, tephra 262 deposits are ideally not described isolated, but as part of a stratigraphic column, and their relative 263 stratigraphic position is used to identify their volcanic source. In the BOOM! dataset, each stratigraphic 264 column is called a "section", and each interval of that column is called a "sub section". In total, 1,303 265 sections are contained in the BOOM! dataset. However, it is important to note that for 876 sections, only 266 one tephra deposit is described, and no name is given for the section by the authors. The remaining 427 267 sections are given a name in the original publication and are described by between one and 46 sub 268 sections, characterized by between one and ten samples, each described by between one and 105 sample 269 observations, corresponding to a total of 2,899 samples and 16,768 sample observations.

270 These descriptions of tephra deposits in the BOOM! dataset have been, for the most part, already 271 classified, i.e., their volcanic source and the specific eruptive event during which they were deposited 272 have been identified by the authors. Thus, they can be used to characterize different volcanic centers and 273 individual eruptive events in the SVZ and AVZ and serve as a reference to compare unclassified samples 274 to. In the BOOM! dataset, an eruptive event is characterized by all the samples (and respective sample 275 observations) which have been correlated with that eruptive event (Figure 1). Since these samples have 276 been collected in different locations, in different types of sedimentary archives, and provide different 277 types of information (physical characteristics, geochemical composition, age), together they can be used 278 to provide a more complete characterization of an eruption. For example, when did the eruption occur, 279 what was its explosivity, the dispersion of its products, and the type of the eruption it corresponded to. 280 In the same way, all the samples attributed to a particular volcanic center can be used to describe it. These 281 samples may or may not be attributed to a particular eruptive event yet, in which case they are labeled 282 as unknown eruptions. Nevertheless, all the samples attributed to a volcanic center can be used to 283 describe it, though grouping them by eruption provides more information to understand their eruptive 284 history: the recurrence of volcanic activity, its general explosivity, if temporal changes in volcanic activity 285 have been registered, etc.

In practice, the BOOM! dataset is distributed as two .CSV files: a main file named BOOMDataset, and a secondary file named MeasurementRuns. In the BOOMDataset file, each sample observation corresponds to a row, which can be characterized by a maximum of 80 attributes (columns), which in turn can be grouped by the type of information they provide (Figure 1, Figure 2, Table S3):

Identification attributes: these attributes correspond to information used to identify the
 sample observation, but which do not further describe the tephra deposit itself. They can be
 subdivided into ID attributes, Position attributes, Reference attributes, and Analysis attributes.

Characterization attributes: they correspond to the actual observations (data) of the samples,
 which are used to characterize – and ideally fingerprint– tephra deposits. These attributes can be
 further subdivided into: Stratigraphy attributes (the stratigraphic position of the tephra deposit

and age estimate(s)); Physical characteristics attributes (color, thickness, and grain size of the tephra deposit); and Geochemical composition attributes (major elements (both *raw* and normalized), trace elements and isotope ratios compositions of either pyroclastic or effusive material).

300 3. Interpretation attributes: They correspond to information that is inferred based on the 301 characterization of the tephra deposit (together with previous tephrochronological information). 302 In particular: the volcanic source of the deposit (Volcano); the specific eruptive event during 303 which the volcanic products (tephra or lava) were deposited (Event); and the Magnitude and 304 Volcanic Explosivity Index (VEI) of the eruptive event. The fact that these are interpretation 305 attributes is very relevant in tephrochronology. On the one hand, because tephra can be deposited 306 far away from their volcanic source (e.g., H1 eruption from Hudson volcano has been identified 307 ~700–900 km away from its source (Naranjo & Stern, 1998; Kilian et al., 2003; Stern, 2008; Del 308 Carlo et al., 2018; Smith et al., 2019)), identifying which volcanic center and during which 309 eruption a tephra was deposited is not always trivial. Additionally, the tephrochronological 310 record is incomplete and biased towards the stratigraphic sections that are best preserved or 311 more easily accesible. Thus, the interpretation of the eruptive event, volcanic center, magnitude 312 and VEI may be updated as new information becomes available. In fact, the volcanic source of 313 some of the tephra samples in the BOOM! dataset have been questioned and re-interpreted over 314 time. For example, the volcanic source of MIC2 and COR1 tephra deposits identified by Naranjo & 315 Stern (2004) as sourced from the Michinmahuida and Corcovado volcanic centers, have been 316 questioned in later publications, such as Watt et al., (2009, 2013), Amigo et al. (2013) and Alloway 317 et al. (2017a, b). In these cases, the reinterpretation of the samples is indicated by a flag (see 318 below).

Metadata: A final group of attributes corresponds to Flags and Comments, which give additional
information to interpret the data. On the one hand, the Flag attribute is used to communicate
issues identified when including the data in the BOOM! dataset. Sample observations can be
flagged for seven types of reasons (detailed in Table S4): problems with the sample ID

323 (SampleID_Issue), its position (Position_Issue), the Digital Object Identifier (DOI) of the 324 publication where the data was obtained from (DOI_Issue), its age (Age_Issue), its geochemical 325 composition (Geochemistry Issue), the volcanic source it is attributed to (VolcanicSource Issue), 326 or the name given to the eruptive event (EventName_Issue). In every case, the type of flag is 327 indicated under the Flag attribute, and the particular reason why the sample observation is flagged is detailed under the Flag Description attribute. On the other hand, the Comments 328 329 attribute corresponds to additional information that can help users interpret the data, which is 330 not described by any other attribute.

331 As mentioned before, in total ~16,800 sample observations are included in the BOOM! dataset, 332 interpreted as sourced from 32 volcanic centers and 132 different eruptive events. The amount of 333 information related to each volcanic center varies from a total of less than 20 sample observations for 334 volcanic centers such as Huequi, Corcovado, Yanteles, or Cay, to thousands of sample observations for 335 volcanic centers such as Llaima, Quetrupillán, Mocho-Choshuenco, Puyehue-Cordón Caulle and Chaitén. 336 For each volcanic center, sample observations attributed to between one (Aguilera volcano) and twenty-337 six (Mocho-Choshuenco) different eruptive events are included in the dataset. Because of the 338 heterogeneity of the information included in the BOOM! dataset (the different types of sedimentary 339 archives, sources of the information, dates of publication, and of uses of the tephrochronological 340 information), not every sample observation is described by all of the 80 attributes previously described. 341 In fact, in the BOOMDataset file, 58.3% of the attribute information is "missing" (Figure 2).

BOOM! DATASET

SAMPLE OBSERVATION



342

- 343 **Figure 1** BOOM! dataset structure. To the left are shown the attributes in the BOOMDataset and MeasurementRuns files, grouped by the type of
- 344 information they provide, as described in the text. Attributes from the MeasurementRuns file correspond to the information below "Quality of analysis".
- 345 The metadata attributes are not illustrated. The information shown corresponds to sample LAZ-T7A (Alloway et al. 2017b). The full description of the
- 346 attributes and units is described in Table S3.



353 In addition to the main BOOMDataset file, a second CSV file named MeasurementRuns is also distributed (Figure 3). This file contains information which is part of the Geochemical composition attributes 354 355 previously described (attributes under "Quality of analysis" in Figure 1). It corresponds to information used by geochemists to evaluate the quality and comparability of the geochemical analyses performed by 356 357 different laboratories. We decided to store this information in a different file because of the way the 358 geochemical composition of most of the samples in the BOOM! dataset were analyzed. Most of the data in 359 the dataset corresponds to analyses of the geochemical composition of individual volcanic glass shards 360 (~88% of the sample observations in the BOOMDataset file), which were analyzed either by EMPA (for 361 major elements) or by Laser Ablation - Inductively Coupled Plasma - Mass Spectrometry LA-ICP-MS, for 362 trace elements. Individual glass shards are analyzed in "batches", and during one batch (called a 363 "measurement run" in the BOOM! dataset), dozens or hundreds of individual glass shards from different 364 samples can be analyzed. To evaluate the accuracy and precision of the analyses performed during one

⁹ https://github.com/ResidentMario/missingno

Figure 3 Representation of the "missing" values in the MeasurementRuns file. Dark grey cells represent
filled values and white cells represent missing values. The figure was created using the Python library
Missigno.

369 measurement run, geochemists repeatedly analyze the composition of different secondary standards along with the glass shards to be studied. These secondary standards ideally have certified reference 370 371 values (e.g., Jochum et al., 2006, 2011, 2016) which can be compared with the analyzed values during each measurement run to estimate their accuracy and precision. In particular, by comparing the mean 372 value of each analyzed element of each secondary standard to the certified values, the accuracy of the 373 374 analysis of each element during that particular measurement run can be estimated (more details on how to do this with the BOOM! dataset is explained in section 4.2.2). In a similar way, the precision can be 375 376 estimated as the standard deviation of the analyzed composition of each element on each secondary 377 standard analyzed during a particular measurement run. Taking this into consideration, in order to 378 provide information for other researchers to evaluate the comparability of their geochemical analyses, 379 researchers generally publish: the label given by them to a particular measurement run; which samples 380 and sample observations were analyzed during that run; which secondary standards were analyzed; the number of analyses of each secondary standard in that run; the mean value and the standard deviation 381 382 of each analyzed element of each secondary standard; as well as the analytical totals if major elements

383 were analyzed. In the MeasurementRuns file, each row corresponds to the information of one secondary 384 standard during a particular run, thus one run can correspond to several rows. The reason for analyzing 385 different secondary standards during one measurement run is that they have different geochemical 386 compositions (e.g., GOR132-G (~46 wt.% SiO₂), StHs6/80-G (~63.7 wt.% SiO₂), ATHO-G (~75.6 wt.% 387 SiO_2 (Jochum et al., 2006)), and the performance of an analytical technique is associated with that 388 composition. Taking the latter into consideration, to assess the quality of the analyses, geochemists 389 usually consider the accuracy and precision of the secondary standard or multiple secondary standards 390 with a geochemical composition relatively similar to that of the analyzed sample. In addition, in order to 391 evaluate the comparability of EMPA analyses, the analytical conditions during each measurement run are 392 also considered (e.g., beam size, accelerating voltage, and beam current). Thus, this information is also 393 stored in the MeasurementRuns file. In both the MeasurementRuns and BoomDataset files, each batch 394 analysis label is indicated under the measurement run attribute, which links both files. The 395 MeasurementRuns file contains 81 different measurement runs where between one and seven secondary 396 standards were analyzed. The measurement runs described in the MeasurementRuns file corresponds to 397 10,891 of the sample observations in the BOOMDataset, attributed to 26 volcanic centers and 61 eruptive 398 events. In the same way as with the BOOMDataset file, because of the heterogeneity of the data, \sim 69% of 399 the cells in the MeasurementRuns file are "missing" (Figure 3).

The two files of the dataset are hosted on the ESPRI server of the IPSL, France, which guarantees its hosting and access as long as the server exists. Both sets can be downloaded directly from the IPSL catalog¹⁰ as a Web Map service (WMS), Web Feature service (WFS) or as a CSV file; or using the BOOM! explorer to download subsets of it (see section S6 for more details).

¹⁰<u>https://doi.org/10.14768/47b4525f-ff39-4940-a963-4d2673f2362e</u>

404 **4 Data comparability**

405 As already mentioned, the BOOM! dataset integrates tephrochronological (and volcanological) 406 information extracted from 79 different publications. Even though all these publications provide relevant 407 information for tephrochronology, they can be very heterogeneous: they correspond to different types of 408 publications (scientific publications, government reports, and doctoral theses); from different disciplines 409 (tephrochronology, volcanology, archaeology, limnology, geological mapping, palynology, glaciology, 410 pedology, and paleoceanography); which were published through 30 years of research (1988-2021 C.E.); and which additionally can have very different research goals (e.g., produce volcanic hazard maps, do 411 412 research on volcanology and tephrochronology, and improve chronologies of sedimentary archives for 413 paleoclimate, palynology or paleoceanography studies). The idea behind collecting the BOOM! dataset, is 414 that all this information together can be used to better describe eruptive events and volcanic centers in 415 the SVZ and AVZ and help disentangle the tephrochronological record there. However, because of the 416 heterogeneities in the source of the information, different publications might study the same 417 phenomenon in a slightly different way. This does not necessarily mean that the information cannot be 418 integrated, but it is necessary to understand what the information actually represents in order to 419 correctly interpret it. Taking this into account, several of the attributes included in the dataset, 420 correspond to information for the user to evaluate the comparability of the data. In the following we focus 421 on attributes associated with age estimates and geochemical composition comparability. For further 422 description of other relevant attributes, such as type of register, type of section, and flags, the reader is 423 referred to the supplementary material (section S5).

424 **4.1 Age estimate comparability**

A very important part of fingerprinting tephra deposited during different eruptive events in a very active volcanic region, such as the SVZ and AVZ, is estimating the age of the eruption. In the timeframe comprehended in the dataset (last 20,000 years), the age of a tephra is generally estimated by ¹⁴C dating organic matter which has been identified *associated* to the tephra deposits. This is done because the pyroclastic material itself generally cannot be directly dated with enough precision to differentiate

430 between eruptions (for example, by the ⁴⁰Ar/³⁹Ar method, for which errors are generally on the order of 431 thousands of years, whereas eruptions can occur every as little as tens of years (e.g., Singer et al., 2008)). 432 Because of this, researchers try to identify organic matter which is ideally embedded within the tephra 433 deposit itself, and alternatively immediately above or below it. This organic matter can be ¹⁴C dated with 434 a precision of tens of years, and in that way, provide a more precise reference for when the eruption 435 occurred. Both the stratigraphic position of the organic matter with respect to the tephra (above, within, 436 or below), and the specific material that has been dated, are important aspects to consider when 437 evaluating the comparability of the different age estimates. For instance, if a piece of charcoal is found 438 within a tephra deposit, it is assumed that the charcoal is the result of hot pyroclastic material burning 439 living trees during an explosive eruption. Thus, by dating the charcoal, a more or less precise age of when 440 the eruptive event happened, can be obtained. Alternatively, if no organic matter is found within the 441 tephra deposit itself, soil that has formed either above or below the deposit, might be dated. 442 Unfortunately, the ¹⁴C age of the soil might not represent the *true* age of the tephra deposit. Soil is formed, 443 among others, by the degradation of organic matter, and during its formation it incorporates organic 444 matter that is contemporary to the soil formation process, but it can also incorporate older organic matter 445 that was already present when soil formed; as well as younger organic matter which can infiltrate from 446 above, for example through a permeable tephra layer. Thus, soil ¹⁴C ages or bulk organic sediment ¹⁴C 447 ages, correspond to a mean value of organic matter of different ages. Additionally, soil can be found either 448 below or above the tephra deposit, and thus, it might have formed long before the eruption, or it might 449 have taken years to develop after the tephra deposition. In these cases, the ¹⁴C ages from the soil are 450 generally interpreted as maximum and minimum ages of the tephra deposit, respectively. In a similar 451 way, if organic macro remnants, such as charcoal or wood, are found below or above the tephra deposit 452 and dated, those ages are also considered as maximum and minimum ages. Because of the latter, a good 453 practice, which can help reduce the age estimate uncertainties is replicates, i.e., dating more than once a 454 determined sample. In the BOOM! dataset, however, most ¹⁴C ages have not been replicated, which can 455 be associated with increased expenses, but also with material availability.

456 Another important aspect to consider when estimating the age of eruptive events, is the type of 457 sedimentary archive where the tephra -and associated organic matter- were identified. Depending on the 458 depositional environment, different types of organic matter for ¹⁴C dating will be available. For example, 459 in the ocean, generally wood or charcoal are not identified and planktic foraminifera are dated instead to 460 provide an age estimate of tephras. However, these ages cannot be directly compared with on land ages, 461 as the concentration of ¹⁴C in the ocean and the atmosphere are not in equilibrium. Because of this, a 462 correction must be applied to marine ages in order to compare them with atmospheric ages. This 463 correction changes in time and space, and is a subject of ongoing research (e.g., Siani et al., 2013; Merino-464 Campos et al., 2019). A similar situation occurs with ¹⁴C ages in lake sediment cores. In this case, ideally 465 terrestrial macrofossils found within the lake sediment cores are dated, which represent the atmospheric ¹⁴C age, as long as the sediment has not been reworked. In many cases, however, these are not available 466 467 and bulk sediments are date instead. Because of different processes occurring in lakes, bulk sediment ¹⁴C 468 content is generally not in equilibrium with the atmosphere. Among these processes: terrestrial input of 469 *old* organic matter by river inflow, groundwater ¹⁴C content, dissolution of aged carbonate or variations 470 in biological activity in the lake (e.g., Geyh et al., 1998; Yu et al., 2007). Because of this, the difference 471 between the contemporary atmosphere and lacustrine sediment ¹⁴C age can change both in time and 472 space and is characteristic of each lake. Thus, marine ¹⁴C ages and bulk sediment ¹⁴C ages in lake sediment 473 cores, provide a loose reference of the time of deposition of tephra deposits, but should in no case be 474 directly compared with on land ages without a proper correction.

Taking the latter into consideration, in order to correctly interpret the 14C ages in the BOOM! dataset in terms of time of deposition of tephras, in addition to the 14C age and respective analytical error, users should also consider the analyzed material (e.g., charcoal, wood, soil, organic macro remnants, planktic foraminifera), the type of analysis (micro analytical (e.g., charcoal, wood) or bulk (e.g., soil, bulk sediment)), the stratigraphic position of the analyzed material (e.g., X cm above or below the tephra), the type of section (e.g., marine core, lake core, outcrop), and whether or not replicates for the sample have been published.

482 **4.2 Geochemical composition comparability**

483 An important aspect when fingerprinting tephras is assessing their geochemical composition. Because 484 many volcanic centers and eruptive events have distinct compositions, by analyzing the geochemical composition of tephras, researchers can discriminate between potential sources. To do this, 485 486 tephrochronologists most often analyze the major element composition of volcanic products (~82% of 487 the sample observations in the BOOM! dataset). However, especially in the SVZ, many volcanic centers 488 and different eruptive events have overlapping major element compositions, thus additional information 489 is needed to discriminate the volcanic source of tephras. Because of the latter, in some cases trace 490 elements are also analyzed (~23% of the sample observations in the BOOM! dataset), and less frequently, 491 isotopic ratios (for example ⁸⁷Sr/⁸⁶Sr and ¹⁴³Nd/¹⁴⁴Nd), which provide a good discrimination tool, 492 however are less routinely analyzed (0.1% of the sample observations in the BOOM! dataset). When 493 comparing the geochemical composition of different volcanic products, there are several aspects to 494 consider to understand if data from different publications are comparable or not. In the first place, it is 495 important to understand what kind of volcanic product (pyroclastic or effusive material), and particular 496 material (e.g., individual glass shards, bulk tephra, melt inclusions, etc.) has been analyzed. Different 497 materials can represent different processes associated with eruptive activity, and as such, can have 498 different geochemical compositions, even if they correspond to the same eruptive event (for more details, 499 see section 4.2.1). Secondly, it is important to check if the data interpreted meet community quality 500 criteria and if not, filter the data accordingly (section 4.2.2). Finally, when comparing the major element 501 composition of different sample observations, it is important that the major element compositions are 502 normalized to a volatile-free composition in order to compare them. Additionally, as different major 503 elements are analyzed in different publications (for example FeO_T versus Fe₂O_{3T}), it is also important to 504 check that the normalizations are comparable (section 4.2.3). In the following sections we describe these 505 three aspects in detail.

506 4.2.1 Analyzed volcanic products

507 Pyroclastic and effusive material represent different expressions of eruptive activity, and because of that,
508 even if they correspond to the same eruptive event, they will not necessarily have the same geochemical

509 composition. In addition, different materials can be analyzed within the same type of register, which 510 should also be taken into consideration when interpreting the data. For example, in a pyroclastic deposit, 511 generally individual glass shards or crystals are analyzed, which represent different magmatic processes 512 and thus they will have very different geochemical compositions, even though they correspond to the 513 same tephra deposit (e.g., Morgado et al., 2015). In the BOOM! dataset, the analyzed materials were 514 entered as they were presented in the publications not to lose the raw information and as a way to make 515 explicit the heterogeneity on how data is published. Analyzed materials within pyroclastic deposits 516 include: tephra, bulk tephra, pumice, bulk pumice, scoria, bulk scoria, lapilli, accretionary lapilli, 517 individual accretionary lapilli, bulk ash, bulk glass, glass shards, matrix glass, melt inclusions, closed melt 518 inclusions, open melt inclusions, and juvenile lithics; whereas for effusive material, analyzed material 519 comprehend: lava, prismatically jointed blocks (PJB), and breccia.

520 Another important aspect to note when using the geochemical composition of volcanic products for 521 fingerprinting tephras, is what in the BOOM! dataset is called the "type of analysis". Pyroclastic deposits 522 and effusive material can be analyzed either micro-analytically (e.g., individual glass shards or minerals) 523 or instead, the sample can be crushed and analyzed as a whole. The latter case is called a "bulk" analysis, 524 and it represents a mean value of minerals, glass shards and even lithics, and most often they display 525 narrow trends in bivariate plots. When available, micro-analytical analyses are preferred to bulk analyses 526 because the glass (melt) composition might be more sensitive to small amounts of fractional 527 crystallization and thus may reflect a more variable geochemical composition. Thus, providing more options for fingerprinting tephras, for example, of different eruptions from the same volcanic source 528 529 (Lowe, 2011). When bulk analyses are performed, on the other hand, the composition of different 530 eruptive events and even different volcanic centers can be very similar and does not always allow to 531 discriminate the source of volcanic products.

In order to correctly interpret the geochemical composition of eruptive events and volcanic centers in the BOOM! dataset, the user should take into consideration: the type of register (effusive material, pyroclastic material), type of analysis (micro-analytical, bulk) and the analyzed material (e.g., lava,

pumice, wood). These qualitative attributes can help users understand if the geochemical compositions
they are interpreting represent similar processes or not, and thus if they can be directly compared.

537 4.2.2 Quality control of analyses

538 Generally, when researchers obtain the results from the geochemical analyses they perform (but also 539 when collecting information to compare their samples with), they check if the data meets some 540 community criteria, to understand if the analyses are *good* analyses. Among these: if the analysis was 541 correctly performed, if what is said to be analyzed was in fact analyzed, and if the accuracy and precision 542 of the analysis is within an acceptable range. In most cases, researchers will publish only the data that 543 meet these criteria. However, different researchers, disciplines, or fields of application, can follow slightly 544 different criteria. Thus, it is important for the users to have access to the information necessary for them 545 to evaluate the latter, so they can filter data according to their own criteria. In the BOOM! dataset, we 546 have included several attributes for users to evaluate this, which we describe in the following.

A first order quality control of analyses of geochemical composition is a check of the analytical conditions in which they were performed. Depending on the technique employed, this information is more or less routinely communicated. Because most of the BOOM! dataset corresponds to EMPA analyses of glass shards (~76% of sample observations), we have included only the analytical conditions for analyses performed by EMPA, which correspond to beam size, accelerating voltage, beam current of a particular measurement run, stored in the MeasurementRuns file. Common values are described in Table S3.

553 An additional important aspect to evaluate when assessing the quality of a geochemical analysis, 554 particularly of major element analyses, is that the analytical total is within accepted values. Major (and 555 minor) elements correspond to the geochemical elements found more abundantly in igneous rocks, and 556 their abundances are typically expressed in weight percentage (wt.%) of oxides: SiO₂, TiO₂, Al₂O₃, FeO 557 and/or Fe₂O₃, MnO, MgO, CaO, Na₂O, K₂O, P₂O₅. Additionally, in some cases Cl and F are also analyzed and 558 considered with minor elements. The sum of the analyzed major (and minor) elements composition is 559 called the "analytical total" ("Total" in the BOOM! dataset), and typically is between 90-100 wt.%. The 560 difference between the analytical total and a 100 wt.% can derive from different situations, among them:

561 analytical error (including due to surface roughness of the samples, poor sample positioning, and loss of 562 alkalis during the analysis), from post-depositional hydration (e.g., alteration of the volcanic products), 563 or from the presence of non-degassed volatiles in the groundmass of the volcanic products. For a more 564 detailed discussion on *acceptable* analytical totals depending on the volatile content of the volcanic 565 products, the reader is referred to Pearce et al. (2008). The value of the analytical total that is considered 566 as a *good* analysis also depends on the analytical technique employed, which is associated with the type 567 of analysis performed (bulk or micro analytical). On the one hand, when bulk samples are analyzed, for 568 example, by X-ray fluorescence (XRF), Atomic Absorption Spectroscopy (AAS), or Inductively Coupled 569 Plasma Emission Spectrometry (ICP-AES), in addition to the major element composition, a value called 570 Loss on ignition (LOI) is sometimes estimated. The LOI corresponds to the volatile content of the sample, 571 for example H₂O, CO₂, SO₂, which can derive from different degrees of post-depositional hydration or syn-572 eruptive characteristics of the volcanic products. In this case, the analytical total plus the LOI should approach 100 ± 2 wt.%, otherwise it is considered a *bad* analysis. In the dataset, ~1.9% of the sample 573 574 observations corresponding to bulk analyses of major elements of pyroclastic or effusive material, are 575 outside this range, which corresponds to ~ 0.2 % of the sample observations in the whole BOOM! dataset. 576 On the other hand, when glass shards are analyzed by EMPA, the volatile content is usually not directly 577 analyzed. In this case, analytical totals lower than 100 ± 2 wt.% do not necessarily reflect poor quality 578 analyses or alteration of the samples, but more often reflect characteristics of the volcanic deposit and 579 environment, which are not accounted for by the major elements alone. Because of the latter, there is no 580 consensus regarding acceptable totals for EMPA glass data, and thus, in the dataset this value is stored 581 when presented in the literature (\sim 86% of the sample observations analyzed for major elements in the 582 BOOM! dataset have been published along with their analytical totals) for the user to judge for 583 themselves. For ~95% of the sample observations analyzed for major elements with EMPA, the analytical 584 total is between 95 and 102 wt%. Samples with analytical totals lower than 90 wt% were not included in 585 the dataset.

586 Another important quality control researchers perform is making sure that what was intended to be 587 analyzed, actually was. To do this, they generally check that the geochemical composition is within

588 plausible ranges. In the case of bulk analyses, this means that the composition is magmatic, i.e., that SiO₂ 589 is between \sim 40–80 wt.%. In the case of micro-analytical analyses, it depends on what it is analyzed, 590 generally glass or mineral crystals. Sometimes, the groundmass in pumice, scoria, individual glass shards, 591 etc., can be very microlite-rich, particularly for relatively mafic samples (e.g., of basaltic andesite 592 composition) and so it can be difficult to analyze the glass phase using a defocused beam by EMPA or LA-593 ICP-MS; on the other hand, when crystals are analyzed, if they are very small ($<20 \,\mu$ m) it might be difficult 594 to analyze their composition at specific locations (e.g., core vs. rim). In order to check if the analyses were 595 performed on the desired material, researchers check the composition of major elements and evaluate 596 whether it is feasible for the expected phase (e.g., glass vs. a mineral phase). In the BOOM! dataset, data 597 was included as long as it was magmatic and indicated as either bulk tephra or individual glass shards in 598 the original publication. The user can choose to filter the information based on their own criteria.

599 One of the most robust ways of reducing the uncertainties in correlations based on the geochemical 600 composition of tephras is side-by-side analysis. This means, analyzing in the same laboratory and with 601 the same methodology unknown and reference tephras (Lowe et al., 2017). In the BOOM! dataset, this 602 has strictly been done in only publication (Smith et al., 2019). Smith et al. (2019) reanalyzed reference 603 tephras previously identified on land by Stern (1992, 2008) and by Weller et al. (2015), to check for 604 potential correlations with the tephras identified by them in a lake sediment core. On the contrary, most 605 publications a side-by-side analysis is not done. However, in many publications unknown tephras 606 identified in several sections are analyzed which allow authors to robustly correlate them and 607 characterize eruptions methodologies (e.g., Rawson et al., 2015; Fontijn et al., 2016; Alloway et al., 2017a, 608 b). These analyses are done in the same laboratory and following the same methodologies, reducing the 609 uncertainty in their correlation. In general though, samples which have been analyzed in previous 610 publications are not reanalyzed, probably because of the increase in expenses or complications obtaining 611 the samples. Alternatively, one important way of evaluating if analyses performed in different 612 laboratories are comparable, as well as of evaluating their accuracy and precision (see below), is 613 analyzing secondary standards along with the unknown samples and reporting the results.

614 An important evaluation to make to correctly interpret the available geochemical information, is 615 assessing the accuracy and precision of the analyses. In the case of isotope ratios included in the BOOM! 616 dataset (87Sr/86Sr and 143Nd/144Nd), an analytical error (generally 2o) is directly provided by the 617 laboratories and is included in the dataset, which allows users to understand the analytical precision of 618 that data. In the case of major and trace elements, however, assessing this is less straightforward. The 619 most appropriate way to assess the accuracy and precision of these analyses, is to consider the 620 composition of the secondary standards analyzed along with the samples, as described in section 3. From 621 the total of sample observations analyzed for major and trace elements, for $\sim 64\%$ (10,438 of the sample 622 observations), it was possible to obtain the full secondary standard information (i.e., name of the 623 standards analyzed in each measurement run, number of analyses performed during each measurement 624 run, analyzed mean value and standard deviation for each analyzed element for each standard). In $\sim 2.8\%$ 625 of the cases (453 sample observations) only the mean analyzed values were published. Thus, for \sim 33.2% 626 of the sample observations analyzed it is not possible to evaluate the accuracy and precision of the 627 analyses. Additionally, from the 33 secondary standards analyzed in the publications included in the BOOM! dataset, certified values are available for only 19 of them, which corresponds to \sim 55% of the 628 629 sample observations, from which \sim 53% has the full information (mean, standard deviation and n). Eight 630 of the certified secondary standards correspond to glass: GOR128-G, GOR132-G, KL2-G, ML3B-G, T1-G, 631 StHs6/80-G, ATHO-G (Jochum et al., 2006), NIST SRM 610 (Jochum et al., 2011), and eleven to whole rock 632 powders AGV-2, BCR-2, BHVO-1, BHVO-2, BIR-1, JA-1, JA-2, W-2 (Jochum et al., 2016), S-Y¹¹, OREAS184¹², OREAS700¹³. For the whole rock analyses included in the dataset, only the mean values were published. 633

In order to provide a broad idea of the accuracy and precision of the analyses included in the BOOM! dataset, we have estimated the accuracy and precision of the analyses for which the authors provided the full information, and the certified values are available online. The accuracy is estimated as the mean analyzed value versus the certified value of each element analyzed on each secondary standard during

¹¹ Certified values available at: https://www.nrcan.gc.ca/our-natural-resources/minerals-mining/mining-resources/sy-4-diorite-gneiss/8025

¹² Certified values available at: https://www.oreas.com/crm/oreas-700/

¹³ Certified values available here: https://www.oreas.com/crm/oreas-184/

each measurement run, and the precision as the relative standard deviation (RSD) of the *n* analyzed 638 639 values of each element on each secondary standard during each measurement run (RSD = 640 (1SD/mean)*100). Figure 4a and b show the results of these estimations, grouped by secondary standard. 641 Jupyter notebooks written in Python are available in the github repository¹⁴ of the project for users to 642 explore the overall dataset accuracy and precision, as well as for each measurement run or sample. Overall, the highest accuracies and precisions are observed for SiO₂, which range between ~0.96 and 643 644 ~1.02, and ~0.09% and 1.54%, respectively; and the lowest accuracies and precisions are observed for 645 P_2O_5 , which range between ~0.16 and ~2.00, and between 3% and 206%, respectively.

646 As mentioned in section 3, more than one secondary standard is generally analyzed by run, which are 647 intended to represent the geochemical composition of the studied samples. Because of that, more than 648 one value for accuracy and precision for each analyzed element is associated to each batch (for example 649 as in Figure 5a and b). In this case, researchers will generally evaluate the accuracy and precision of a 650 sample observation by comparing it with the secondary standard(s) with the geochemical composition 651 closest to that of the unknown sample. Thus, the precise analytical error is not calculated, rather it is 652 generally estimated as the highest value of precision and accuracy for each element. For example, along 653 with sample CLD025A (~55–57 wt.% SiO₂), analyzed during measurement run 11112 by Fontijn et al. 654 (2016), secondary standards GOR132-G (45.5 wt.% SiO₂), KL2-G (50.3 wt.% SiO₂), T1-G (58.6 wt.% SiO₂), 655 StHs6/80-G (63.7 wt.% SiO₂) and ATHO-G (75.6 wt.% SiO₂) were analyzed. In this case, standards KL2-G 656 and T1-G have the composition closest to the sample. During that run, the analysis of TiO₂, for example, is estimated as ~5% for standard KL2-G, and ~3% for standard T1-G, whereas precisions are 2% and 5%, 657 658 respectively. Thus, the estimated accuracy and precision for the analysis of TiO_2 are both ~5%.

Users should take into consideration all of the above when interpreting the data and the dataset, and filterregarding their own criteria.

¹⁴ https://github.com/consuelola/BOOM/Notebooks

Figure 4. Accuracies (a) and precisions (b) of the geochemical composition analyses included in the 662 663 BOOM! dataset, estimated as described in the text. When the same secondary standard was analyzed in more than three measurement runs, the 1σ range are plotted as a vertical line and the number of 664 measurement runs considered is indicated in the legend as #MRs. When a secondary standard was 665 analyzed during three or less measurement runs, accuracy and precision are plotted as a dot. Bold grey 666 horizontal lines correspond to 0.95 and 1.05 values for the accuracy and 5 and 10% for the precision. 667 668 Only secondary standards with certified values are shown, analyzed during measurement runs for which the name of the secondary standard for which the full information is published (as described in the text): 669 670 ATHO-G, GOR128-G, GOR132-G, KL2-G, ML3B-G, T1-G, StHs6/80-G, (Jochum et al., 2006), NIST SRM 610 (Jochum et al., 2011). 671

672 Figure 5 Accuracies and precisions of the geochemical composition analyses of each secondary standard analyzed during measurement run 11112 (Fontijn et al., 2016), as an example. a: Accuracy for major 673 674 elements, calculated as mean analyzed value of each element of each secondary standard analyzed during 675 measurement run 11112, versus the certified values (Jochum et al., 2006). b: Precision of the geochemical analyses, calculated as mean analyzed value of each element of each secondary standard analyzed during 676 677 measurement run 11112, divided by the standard deviation of the n analyses during that measurement run. Bold grey horizontal lines correspond to 0.95 and 1.05 values for the accuracy and 5 and 10% for the 678 679 precision.

680 **4.2.3 Major element normalization**

As already mentioned, the major element composition of volcanic products is expressed in wt.%, and ideally the sum of all the major oxides and LOI (when analyzed) should approach 100 wt.%. However, because of post-depositional alteration, variable volatile contents in magmas, and analytical errors, the analytical totals are generally not exactly 100 wt.%. In order to eliminate the effects of these processes in the composition of oxides, researchers normalize the major element composition to a 100% volatile-free (also named anhydrous) basis, i.e., by the sum of the major oxides without LOI (when analyzed). In order for users to be able to directly compare the major element compositions of sample observations in the

BOOM! dataset, both the *raw* and normalized major elements are stored. Because of the heterogeneities in the data sources in the dataset, when normalizing major elements two aspects should be taken into consideration, which we describe in the following.

691 In the first place, in order to normalize the major element compositions of samples by a comparable 692 amount, special attention must be paid to how iron (Fe) was reported. Fe can exist in volcanic rocks in 693 two states of oxidation (Fe²⁺, as FeO; and Fe³⁺, as Fe₂O₃), which exist in different proportions in different 694 types of rocks. Most analytical techniques employed to analyze volcanic rocks are not able to distinguish 695 between these two states of Fe, and thus it is presented in most publications as a *total* Fe content. For 696 example, when individual volcanic glass shards are analyzed by EMPA, Fe is usually reported as total Fe 697 as FeO, which might be communicated by authors as FeO, FeO_T or FeO*. In contrast, when bulk samples 698 are analyzed, for example by XRF or Inductively Coupled Plasma - Optical Emission Spectrometry (ICP-699 OES), Fe is typically reported as total Fe as Fe_2O_3 , and it might be presented in the publication either as 700 Fe₂O₃ or Fe₂O_{3T}. Additionally, other techniques such as AAS and wet chemical analysis (titration) can 701 discriminate between Fe²⁺ and Fe³⁺, however they are not commonly used. In this case, publications 702 calculate the total Fe as $FeO_T = FeO + 0.899*Fe_2O_3$, or as $Fe_2O_3T = 1.1*FeO + Fe_2O_3$. Thus, when normalizing 703 major element compositions of heterogeneous sources, it is important to calculate the analytical total 704 using the same expression for Fe, as using one or the other will result in different normalized 705 compositions. In the BOOM! dataset, ~90% of the major element compositions were analyzed by EMPA. 706 Because of this, the normalization in the dataset is done considering Fe as FeO_T for calculating the 707 analytical total. When FeO_T was not directly presented in the original publication, it was calculated either 708 as: FeO + $0.899*Fe_2O_3$, when both FeO and Fe₂O₃ were analyzed (~3% of major element observations); 709 or as $0.899*Fe_2O_{3T}$, when Fe was analyzed as Fe_2O_{3T} (~5% of major element observations). To save the 710 original data and its heterogeneity, Fe is described in the dataset by four attributes: FeO, Fe₂O₃, FeO_T and 711 Fe₂O_{3T}, and only the original data is filled in the non-normalized (raw) version of the dataset.

Second, different publications might analyze different sets of major elements and thus, samples might not
be normalized by a comparable analytical total. In particular, elements found in lower concentrations

714 (such as P₂O₅, MnO or Cl) are not always analyzed (Figure 6), because of the increased amount of time 715 required to analyze them with reasonable precision, versus the information they provide (when using 716 EMPA). However, because of their low concentrations, whether these elements are analyzed or not, will 717 have a small influence on normalizations. We have performed a small test in order to check if the 718 normalized values of samples where different major elements have been analyzed are still comparable. 719 We re-normalized the major element compositions of sample observations where all major elements 720 included in the BOOM! dataset were analyzed by a new analytical total, calculated as the sum of all major 721 elements analyzed, excluding Cl, P₂O₅ and MnO. Then, we calculated the variation between the 722 normalized and the re-normalized compositions of each element (e.g., SiO_{2 renormalized} – SiO_{2 normalized}) for 723 each sample observation and compared it to the maximum achievable precision for that element. For the latter, we considered the 95% CL of the certified values of the secondary standards analyzed along with 724 725 the samples (Figure 7). We only tested sample observations for which both the analytical total are included in the BOOM! dataset and the secondary standards analyzed have certified values (~61% of 726 727 sample observations analyzed for major elements). Because the secondary standards used for whole-728 rock and glass analyses are different, we compare the sample observations with their respective 729 secondary standards. In all cases, except for SiO_2 , Al_2O_3 , and FeO, the difference of the analyzed 730 composition between the normalizations is lower than the 95%CL of the geostandards analyzed along 731 with the samples (Figure 7, S1, S2). Nevertheless, in the case of SiO₂, Al₂O₃, and FeO, ~99% of the sample 732 observations the difference is within or lower than the 95% CL of the standards for the range of 733 compositions of the sample observations. For Al₂O₃, the difference between the two normalizations is 734 lower than 0.13 wt.% in \sim 99% of the cases, which is lower than the 0.2 wt.% analytical error of Al₂O₃ for most secondary standards analyzed along with the samples, except for BHVO-2G, for which it is 0.1 wt.%. 735 736 Thus, even though in the BOOM! dataset sample observations are included for which different major 737 elements where analyzed, their normalized compositions are still comparable.

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Figure 6 Heterogeneity of the analyzed major elements contained in the BOOM! dataset. The rows
 correspond to the sample observations. Dark grey cells represent "filled" values and white cells represent

⁷⁴¹ "missing" values. In this case, 13,791 sample observations have major element data, but not all elements

have been analyzed for each sample. The figure was created using the Python library Missigno.

743

744 Figure 7. Impact of normalizing major element compositions of sample observations in the BOOM! 745 dataset by different analytical totals. Δ: Normalized value considering the analytical total as the sum of all analyzed major elements - Normalized value considering the analytical total withouth Mn0, P_2O_5 and 746 747 Cl. a, c, e: glass shard analyses; b, d, f: whole-rock analyses. Only samples for which the anaytical total is 748 published in the original publication are plotted. The 95% CL of the certified secondary standards 749 analyzed along with the samples are plotted as a reference of the highest achievable precision of the analyses. GOR128-G, GOR132-G, KL2-G, ML3B-G, T1-G, StHs6/80-G, ATHO-G and T1-G (Jochum et al., 750 751 BCR-2, BHVO-1, BHVO-2, W-2 2006), BIR-1, JA-2, (Jochum et al., 2016), SY-4 752 (https://www.nrcan.gc.ca/our-natural-resources/minerals-mining/mining-resources/sy-4-diorite-753 gneiss/8025), OREAS184 (https://www.oreas.com/crm/oreas-184/), OREAS700 754 (https://www.oreas.com/crm/oreas-700/).

5 Using the BOOM! Dataset to explore potential correlations

756 The BOOM! dataset and explorer were developed to help in the difficult task of disentangling the 757 tephrochronological record in the SVZ and AVZ, which in practice means robustly correlating tephras 758 deposited during the same eruptive event. The latter is generally done by fingerprinting them, i.e., 759 identifying unique characteristics that distinguish tephra deposits. Doing this is often quite difficult, 760 because of the multidimensionality of the tephrochronological information, as communicated during the 761 interviews (Table S1). Because of this, researchers often use different tools to explore and visualize 762 different type of data (GIS software, Excel, R, Adobe Illustrator, etc.), and so, characterizing each volcanic 763 center and eruptive event can become very tedious, especially when dealing with large amounts of data, 764 such as in the BOOM! dataset. With this in mind, the BOOM! explorer (https://boom-vis.lisn.upsaclay.fr/) 765 was created as a complementary tool to the dataset. By using it, users can visualize at the same time the geographical distribution of volcanic centers and the volcanic products originated during specific 766 767 eruptive events, as well as their geochemical composition, and the available information to assess the 768 chronologies of the eruptive events (Figure 8). The BOOM! explorer can at the same time be used to 769 compare the available data for each volcanic center and known eruptive event and evaluate the "finger-770 printability" of the tephras. In section S6 of the supplementary material we exemplify how the BOOM! 771 explorer can help users in correlations with an example. It is important to note that the BOOM! explorer 772 is not meant to be a comprehensive tool, and users can always download the dataset, add supplementary 773 information, and produce different visualizations fitted to their specific needs; as well as download the 774 source code of the explorer and make changes fitted to their needs. In this regard, the explorer can also 775 be used as a catalog of the data in the BOOM! dataset. By using it, users can perform a first inspection of 776 the dataset, understand the amount and type of information available for each volcanic center and 777 eruptive event, and chose which information to download. Additionally, we have produced a Jupyter 778 notebook called Correlations, available in the github¹⁵ repository, which users can use to plot their own 779 unknowns and compare them with the BOOM! dataset.

¹⁵ https://github.com/consuelola/BOOM/assets/Notebooks

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Figure 8 Screenshots of the sections of the exploration tool (https://boom-vis.lisn.upsaclay.fr), showing different visualizations of the data in the dataset. In the figure,
 volcanic centers Llaima, Quetrupillán, Mocho-Choshuenco have been selected. For more details on how to use the explorer, the reader is referred to section S6.

784 Even though being able to visually compare tephrochronological data in its multidimensionality is very 785 helpful, sometimes it is not enough to robustly distinguish tephras. The latter is especially true in areas 786 where the geochemical composition of many volcanic centers and eruptive events is very similar, as is 787 often the case in the SVZ and AVZ. This is worsened by having large amounts of data from different 788 eruptive events. The latter is not uncommon, and because of it, statistical tools are sometimes used by 789 tephrochronologists to find ways to more robustly fingerprint tephras (Lowe et al., 2011; 2017). In 790 section 5.1, we briefly evaluate the use of geochemical composition together with machine learning 791 algorithms to classify samples in the dataset labeled as *unknown* volcano. This exploration is not aimed 792 to be exhaustive either, but rather to provide a starting point and encourage the use of the BOOM! dataset 793 to explore the application of machine learning for tephra classification.

794 **5.1 Machine learning application**

795 The BOOM! dataset offers a great opportunity for the application of machine learning in the discipline of 796 tephrochronology. To demonstrate this potential, we trained models on the BOOM! dataset to perform 797 automatic tephra correlation. In machine learning terminology, this corresponds to a classification task, 798 where the input are sample observations describing the geochemical composition of tephras, and the 799 outcome to predict is the volcanic system which originated the tephra deposit. For simplicity, in this 800 experiment we classified each sample observation rather than the sample as a whole, which can be done, 801 for example, by a majority vote (e.g., Bolton et al., 2020). In practice, when the geochemical composition 802 of more than one sample observation is available for one tephra deposit, researchers consider the 803 geochemical trend described by all the sample observations to classify the sample. Thus, future 804 applications should take this into consideration.

805 **5.1.1 Preprocessing**

Prior to training the models, a few preprocessing steps are necessary. First of all, only sample
observations for which the volcanic source has been identified were considered, which corresponds to
~89% of the dataset. This is necessary because the volcanic source "labels" are needed both for training
the models and for evaluating their performances. From the latter, we discarded sample observations for

810 which the volcanic source is debated in different publications (sample observations with a 811 VolcanicSource_Issue flag, corresponding to 86 sample observations). Additionally, we only considered 812 sample observations for which the major or trace elements composition of the volcanic products were 813 analyzed, i.e., sample observations which correspond to ¹⁴C ages of organic matter were ignored. From 814 these, we discarded sample observation which are geochemical composition outliers (31 sample observations), those which have analytical totals lower than 95 wt.%, and those with LOI higher than 5 815 816 wt.%, as they might correspond to altered samples (3,242 sample observations, for more details the 817 reader is referred to section 4.2.2). After this treatment, we only kept sample observations from volcanic 818 centers left with more than 10 sample observations, from at least two different samples. This is required 819 in order to have sufficient data for training and testing the models. The latter left a total of 13,925 sample 820 observations from 2,167 samples from 27 different volcanic centers. As a result of the preprocessing, the 821 volcanic centers Cay, Macá, Yanteles, Corcovado, Cordón Cabrera and Subsidiary Vcha dome were not 822 included in the dataset. The whole preprocessing is done in the preprocessing function in utils.py, 823 available in the github repository¹⁶. We call the resulting dataset the majors *or* traces dataset, as it 824 includes all sample observations for which either major elements, trace elements or both have been 825 measured.

826 **5.1.2 Methods**

827 We trained four machine learning classifiers or estimators: Logistic Regression, k-Nearest Neighbors 828 (kNN), Random Forest (RF) and Gradient Boosting (GB). These classifiers were trained with volcanic 829 centers as target values and major and trace element compositions as features. Because of the high percentage of missing data (~62 %), imputation of the missing values was performed prior to model 830 831 fitting for all models, except for Gradient Boosting which natively handles missing values. Four different 832 imputation methods were considered: mean imputation (with sklearn's SimpleImputer) which imputes 833 a constant value, in this case the mean value of each feature; k-Nearest Neighbors imputation (with 834 sklearn's KNNImputer) which imputes by the mean value of the nearest neighbors, in this case 15

¹⁶ https://github.com/consuelola/BOOM/Machine_learning/src

835 neighbors; iterative conditional imputation (with sklearn's IterativeImputer) relying on either a Bayesian 836 Ridge (BR) regressor or a Random Forest regressor. This method is related to the well-known imputation 837 method MICE (Multiple Imputation by Chained Equations, van Buuren, 2018). It consists in imputing 838 features iteratively, in a round-robin fashion, using a model (in our case one of BR or RF) that takes as 839 target the feature to impute, and as input data of all the other features. This results in a total of 13 840 imputer-estimator pairs tested. For all imputation algorithms and models, we used the scikit-learn¹⁷ 841 python library (Pedregosa et al., 2011). The code is available on the run_experiments.py function on 842 github.

843 The BOOM dataset is subject to class imbalance, i.e., the number of sample observations for each volcanic 844 center varies greatly. For example, six of the 27 volcanic centers are represented by less than 50 sample 845 observations in the dataset (Yate, Apagado, Hornopirén, Huequi, Lautaro and Aguilera), while five 846 volcanic centers are represented by more than 1,000 sample observations (Llaima, Quetrupillán, Mocho-847 Choshuenco, Puyehue-Cordón Caulle, and Chaitén). To account for this class imbalance, the performances 848 of the thirteen models were evaluated by comparing both their accuracies and balanced accuracies. The 849 accuracy indicates the proportion of correctly classified sample observations over the entire test set, 850 whereas the balanced accuracy weights sample observations according to the inverse prevalence of their 851 class (in this case, the volcanic center). Balanced accuracy therefore gives more weight to rarer classes 852 than accuracy, and allows a better understanding of whether these rarer classes tend to be well-classified 853 or not. It may, however, be affected by a higher variance: because of the little data available for some of 854 the volcanic centers (for example, 11 sample observations for Huequi) it can be more sensitive to changes 855 in the hyperparameters of the models chosen in each fold, to the randomness of the imputing mechanism, 856 and to the train-test divisions of the sample observations.

For model evaluation, we performed a 10-fold cross validation, which gives us 10 performance values (here accuracy and balanced accuracy) for each imputer-estimator pair tested. On each fold, a grid search is performed on the training set with an inner 5-fold cross-validation to select the best hyperparameters

¹⁷ https://scikit-learn.org

for the estimator. The model is then retrained with the hyperparameters identified on the whole train set
before being evaluated on the test set. Note that we optimized the hyperparameters of the estimators but
used default hyperparameters for the imputation algorithms to alleviate the computational burden.
As many samples are composed of several sample observations, special care was taken not to separate
sample observations belonging to the same sample in the train and test sets. This is very important, as in

865 practice, either the volcanic source is known for all sample observations in a sample, or unknown for all 866 of them. Moreover, sample observations coming from the same sample are most likely to be more similar 867 than sample observations coming from the same volcanic source in general. The failure to keep together 868 all sample observations from a given sample in the same set would thus not reflect a practical use case 869 and artificially inflate performances. To ensure that we do not split sample observations inappropriately, 870 we used a custom GridSearchCV_with_groups object as the usual GridSearchCV object from scikit-learn

does not allow yet to specify groups.

Model training was expensive in terms of memory (~228GB) and processing time (~24 hours on 30
cores), mainly due to the iterative conditional imputation with RF regressor which used a lot of memory
and took two orders of magnitude longer than all other imputation schemes.

875 **5.1.3 Results**

The mean, standard deviation (SD), and maximum error of the ten accuracies and balanced accuracies for each model are shown in Table 1 and Figure 9, and the detailed results for each fold can be accessed in the github repository in the results/major_or_traces folder. Additionally, the confusion matrix, feature importances, and bivariate plots to visualize the classifications were produced for each of the thirteen models and are also available in the github repository, in the figures/major_or_traces folder.

The BOOM! dataset allows the learning of successful models for tephra correlation - The best model obtained is the iterative conditional imputation with BR regressor and RF as prediction model. It achieves 92% (SD: 3) accuracy on average over the cross-validation folds, and 79% (SD: 6) balanced accuracy. This performance highlights a clear signal in the geochemical data. While the successful application of machine learning has been demonstrated in previous studies (Bolton et al., 2020; Pignatelli & Piochi, 2021; Uslular

et al., 2022), it is the first time that it is demonstrated at this scale (13,925 sample observations from 886 887 2,167 samples and 27 different volcanic centers) on heterogeneous data. Indeed, the geochemical 888 analyses were performed by many different laboratories, and many sample observations have been analyzed for either major or trace elements, which can affect the performance of machine learning 889 890 models. It is thus positive and encouraging that models good enough to be of practical interest (>90%) 891 accuracy) can be learned from this data set. Note that here we focused on a few classical and effective 892 models, without trying to obtain the best possible performances. It is thus very likely that improvements 893 are possible, for example by using ensembling techniques, or by improving the handling of missing values.

Table 1. Performances of the thirteen models tested in the major *or* traces set, i.e., the dataset containing
sample observations on which either major elements, trace elements or both have been measured. For
each of the imputer-estimator pairs, the mean accuracy and balanced accuracy of the 10-folds of the
cross-validation are presented. Imputers are indicated in the columns and estimators in the rows LR:
Logistic Regression; kNN: k-Nearest Neighbors; RF: Random Forest; GB: Gradient Boosting; BR: Bayesian
Ridge.

			Iterative conditional imputation with		
	Simple imputer with mean	kNN Imputer	BR regressor	RF regressor	
LR	0.74/0.71	0.75/0.69	0.76/0.72	0.70/0.67	
kNN	0.87/0.76	0.85/0.73	0.90/0.80	0.83/0.71	
RF	0.90/0.77	0.87/0.73	0.92/0.79	0.86/0.73	
GB					0.90/0.75

900 The imputation algorithm matters – Our results (Figure 9a and 9c) show that the choice of imputation 901 algorithm plays an important role in the performance of the models, both with regards to accuracy and 902 balanced accuracy. Interestingly, the ranking of imputation methods remains similar across models. The 903 kNN Imputer and iterative conditional imputation with RF led to the worst performances, while the mean 904 imputation and iterative conditional imputation with BR had the best performances. This is surprising as

iterative conditional imputation with RF is a state-of-the-art imputation method. This situation might be 905 906 related to the structure of the "missingness" patterns (Figure S5). The dataset has a block structure, with 907 10,305 sample observations for which only the major elements have been analyzed, 2,408 sample 908 observations for which only trace elements have been analyzed, and "only" 1,212 sample observations 909 for which both major and trace elements have been analyzed. In order to impute the major elements in 910 the "traces only" block and conversely, imputation algorithms need to learn the relationships between 911 the majors and traces from the sample observations for which both have been analyzed, which represent 912 here a relatively small fraction of the data. This is a rather difficult setting, which may explain that mean 913 imputation outperforms iterative conditional imputation with RF or the kNN imputer. In contrast, the 914 iterative conditional imputation with BR regression outperforms mean imputation for all models. 915 Previous work using machine learning for identifying the volcanic source of volcanic products have either 916 not had any missing values in their dataset (Bolton et al., 2020) or have solely used a simple imputation 917 with either the mean (Pignatelli et al., 2021) or with zero (Uslular et al., 2020). Our results highlight the 918 importance of having good imputation schemes to improve overall performances, especially with 919 datasets compiled from very heterogeneous data, such as the BOOM! dataset. In what follows, we 920 consider the accuracies and balanced accuracies obtained with the iterative conditional imputation with 921 BR regression.

922

923 Figure 9. Boxplots showing the performances of the thirteen imputation-estimator models tested. 924 Boxplots were obtained considering the performances on each of the 10 folds of the cross validation. a 925 and c correspond to the accuracy and balanced accuracy on the "major or traces" set, i.e., the dataset 926 containing sample observations on which either major elements, trace elements or both (13,925 sample 927 observations) have been measured. In the legend the different imputation mechanisms are indicated: 928 kNN: k-Nearest Neighbors; Iterative BR: iterative conditional imputation with Bayesian Ridge regressor; 929 Mean: Simple Imputer with the mean value of each element; Iterative RF: iterative conditional imputation 930 with Random Forest regressor. On the x axis, the different predictors tested are indicated: kNN: k-Nearest 931 Neighbors; LR: Logistic Regression; RF: Random Forest; GB: Gradient Boosting. b and d correspond to the 932 performances obtained on the "major and traces set", i.e., the dataset considering only sample 933 observations for which both major elements and at least one trace element have been measured. In b and 934 d, the comparison of the performances considering only the major elements of the major and traces set, 935 versus the performances considering major and trace elements of the major and traces set, are plotted.

936 Random Forest performs best, closely followed by KNN and Gradient Boosting - Overall, RF had the 937 best performances (acc. 92% / balanced acc. 79%), followed by kNN (90% / 80%), GB (90% / 75%), and 938 finally LR, whose performance was significantly lower (76% / 72%). These results are not surprising as 939 RF and GB have been shown to work well with a wide range of datasets (Fernández-Delgado et al., 2014). 940 In particular, RF is among the best performing algorithms in previous work assessing the use of machine 941 learning for identifying the volcanic source of volcanic products, (Bolton et al., 2020; Pignatelli & Piochi, 942 2021; Uslular et al., 2022). In contrast, GB was tested exclusively in the South Aegean Active Volcanic Arc, 943 with similar performances to that of RF (Uslular et al., 2022). kNN displays more variable results in the 944 literature. Good performances were observed in a study with Alaska tephras (Bolton et al., 2020) and 945 kNN had the best performance in the Neapolitan region (Pignatelli & Piochi, 2021), yet it obtained relatively bad performances in the South Aegean Active Volcanic Arc (Uslular et al., 2022). Finally, LR 946 947 displayed the worst performances considering both balanced and unbalanced accuracies, being lower 948 than all other models outside of 1SD. This reflects the fact that a linear model seems inappropriate on 949 such a dataset.

950 **Performances on rarer classes are satisfying –** Balanced accuracies are systematically lower than 951 accuracies, reflecting the fact that the learned classifiers are better on classes that have more sample 952 observations. This behavior is expected as the more samples we have of a class, the more accurately we 953 can characterize it. As can be observed in the confusion matrix for the model with the highest accuracy 954 (Figure 10), the five volcanic centers with more than 1000 sample observations are well classified by the 955 model. Only Llaima is sometimes classified as Villarrica or Mocho-Choshuenco, however it is relatively 956 well classified as well. Rarer classes are relatively well classified as well. In fact, from the five less 957 represented classes, Apagado, Hornopirén, and Huequi are very well classified. The few poorly classified 958 classes over the entire dataset (Sollipulli, Villarrica, Carrán-Los Venados, Osorno, Yate, and Aguilera), are 959 represented by a number of sample observations ranging from \sim 40 to 120, except for Villarrica with 858 960 sample observations. The latter indicates that classes that are less represented are more likely to be badly 961 classified. Thus, including more information in the future from the poorly classified samples could 962 increase the performances of the models.

963 Assessing the usefulness of traces in addition to major elements – In tephrochronology trace 964 elements are generally analyzed to increase the chances of fingerprinting tephras. However it is unclear 965 to which point measuring trace elements in addition to major elements can help better identify the 966 volcanic source of a deposit. To answer this question, we restricted our attention to sample observations 967 for which both major and trace elements are available, as both are needed to evaluate the effect of adding 968 traces in a model. As most samples have only a subset of trace elements measured, we included all 969 samples that have at least one trace element measured. It resulted in a dataset comprising 1,212 sample 970 observations, belonging to 908 samples and representing 25 volcanoes. On this dataset, we trained the 971 same models as above to predict the volcanic source, however, in this case, we first considered only the 972 major elements (in the github repository this experiment corresponds to major_and_traces_restricted), 973 and then, both the major and trace elements (major_and_traces in the github repository). All training 974 details are similar to above. When only major elements are considered, the dataset has few missing values 975 (0.1%) so we just imputed them by the mean. However, there are many missing values in the trace 976 elements (30%), therefore we compared the various imputation methods on the majors and traces 977 dataset. The results (Figure S6) show that mean imputation is one of the best methods for this dataset. 978 Thus, we chose to compare the results with majors only and with majors and traces when both datasets 979 are imputed by the mean (Figure 9b and 9d). Note that these results are affected by a higher variance 980 than previously as we are using a dataset with roughly 1,000 sample observations, compared to more 981 than 10,000 previously.

982

Figure 10. Confusion matrix showing the proportion of predicted sample observations by each volcanic
center. Rows with no data correspond to classes in which no sample observations were left in the train
set. The colored bar to the right of the figure indicates the proportion of classified sample observations,
yellow being 1, thus all sample observations were classified as that volcanic center; and purple being 0,
thus no sample observations were classified as that volcanic center.

988 Figure 9 (b, d) shows that using traces in addition to majors improves performances substantially across

all models. The accuracy of kNN, RF and GB rises by 10 percent from 80-85% to 90-95%, while that of LR

- 990 increases by 15 percent. The effect of adding traces as predictors is even stronger when looking at the
- 991 balanced accuracy, except for kNN. While the balanced accuracy greatly varies across models when using
- 992 majors elements only, it is roughly on par across models when adding traces. This may indicate that some
- 993 rarer classes may be better classified when traces are used in addition to majors. Surprisingly, in terms

of balanced accuracy, even LR performs almost as well as RF or kNN when traces are considered, reaching
83.4%. This is an interesting observation as LR is a simple and easy to inspect model which
tephrochronology experts might prefer over models that are more difficult to interpret. Overall, these
results highlight the potential of traces for better (automated) fingerprinting of tephras.

998 The results discussed here constitute a first exploration showing encouraging performances. With more 999 than 90% accuracy and around 80% balanced accuracy, the tests here performed highlight that machine 1000 learning with the BOOM! dataset has a great potential to improve correlations in the SVZ and AVZ. 1001 Nevertheless, models would benefit from an improvement in their balanced accuracy to help disentangle 1002 all tephrochronological records in the region, including the under-represented ones. As mentioned 1003 before, imputation algorithms have a noteworthy effect on performances when considering the whole 1004 dataset. Future work should thus focus on understanding the best imputation strategies, given the 1005 missigness structure of the dataset. In addition, it is important to include in the future a method to make 1006 pooled predictions, i.e., to predict the source not only for each sample observation independently, but for 1007 the whole sample at once. This question has been explored by Bolton et al. (2020) and performances of 1008 all models improved when considering the predictions at the sample level rather than at the sample 1009 observation level. Finally, using the BOOM! dataset, a more in-depth study can be developed to further 1010 the use of machine learning not only to identify the volcanic source of tephras, but to identify the exact 1011 eruption originating the tephra. In this sense, additional information included in the dataset could be 1012 included in the models, such as the ages, the type of volcanic product, and the location where they were 1013 identified. The code for the experiment here performed is available on github and can be used to improve 1014 our baselines.

1015 6 Conclusions and perspectives

1016 The BOOM! dataset here presented integrates an unprecedented amount of tephrochronological (and 1017 volcanological) information in the SVZ and AVZ in a machine-readable way. It contains information on 32 1018 different volcanic centers and 132 eruptive events that occurred during the last 20,000 years, extracted 1019 from 79 different scientific publications, in ten different disciplines, produced through \sim 30 years of 1020 research. The machine-readable dataset allowed for the development of the BOOM! explorer, which 1021 provides novel visualizations of the tephrochronological information in the area. In particular, the BOOM! 1022 explorer allows users to visualize data in its multidimensionality (geographical distribution, chronology, 1023 and geochemical composition), filter data according to different criteria of comparability, and easily 1024 compare the available information for a given volcanic center or eruption, as well as directly linking the 1025 information to the source publication. The development of the explorer in parallel to the dataset greatly 1026 aided the development of its structure, by providing clear ways to organize the bulk of data and identify 1027 information that was missing in order to meet community needs.

1028 In order to effectively integrate this heterogeneous data, it was key to incorporate information for users 1029 to evaluate its quality and comparability, which is a repeated request from the tephrochronological 1030 community. However, much of this information is not always communicated explicitly in publications, or 1031 in a way that is easily integrated with data from other publications, which impedes the reuse of data and 1032 can lead to misinterpretation of it. For example, in many publications it is not communicated in which 1033 state of oxidation of Fe is analyzed, rather it is deduced from the analytical technique. The latter can lead 1034 to confusion, especially when researchers from different disciplines reuse the information. In other cases, 1035 the position, type of register, analytical totals, or secondary standards analyzed along with the samples 1036 are not indicated in publications and could not be obtained when contacting the authors. Other types of 1037 information are not always communicated in a machine-readable way, making it very time consuming to 1038 integrate it with other data. In particular, including the stratigraphy of sections was a common request 1039 by the community, however in many publications this is communicated only in figures showing 1040 stratigraphic columns without the exact stratigraphic position and thickness of tephras. Future work in

tephrochronology would ideally publish these data in a machine-readable way to increase its re usabilityand the efficiency of tephrochronological work in the area.

1043 The dataset and explorer are not meant to be comprehensive, and the work here presented is expected 1044 to be regarded as a basis from which to build upon. Regarding the dataset, more information could be 1045 incorporated to better describe tephra deposits. For example, more information to describe the physical 1046 characteristics of the tephra deposits, such as macroscopic description of it and photos; a more thorough 1047 description of the stratigraphy of sedimentary archives and their isotopic stratigraphy, when existing; as 1048 well as schematic representations of stratigraphic columns; supplementary dating methods, e.g., from 1049 dendrochronology, and more information to describe ¹⁴C ages, for example reservoir ages and the choice 1050 of macrofossil dated, when suited, as well as the calibrated ages by the last published calibration curve; 1051 regarding the geochemical composition, analyses of mineral compositions or additional isotopic ratios 1052 such as δ^{18} O. Regarding the explorer, additional or alternative visualizations could be developed to better 1053 visualize the uncertainty of the geochemical composition analyses and ¹⁴C ages, the uncertainties related 1054 to age estimates of eruptive events. Additionally, an important request of the community to pursue in the 1055 future is finding ways to better communicate the uncertainty associated with the interpretation of the 1056 volcanic source of tephras, and how this is susceptible to change in the future, as new tephrochronological 1057 information becomes available. Finally, an important request which could not be met in this version of 1058 the dataset and the explorer, is that people can upload their own data and compare it to the dataset, which 1059 would be of great use for the community.

Even though compiling the BOOM! dataset and providing the explorer is a great contribution to the tephrochronological community in the area, an important challenge for the future is finding ways for the dataset to incorporate more information. In its current form as described here, the version of the dataset is static. Taking the latter into consideration, a collaboration with the National Volcanic Network (RNVV) of SERNAGEOMIN is already in place to look for ways of transferring the dataset and explorer to secure its maintenance and evolution in the future.

1066 **7 Data Availability**

The BOOM! dataset is hosted on the ESPRI server of the IPSL, France, which guarantees its hosting and access as long as the server exists. Both files of the dataset can be downloaded directly from the IPSL catalog (https://doi.org/10.14768/47b4525f-ff39-4940-a963-4d2673f2362e) as a Web Map service (WMS), Web Feature service (WFS) or as a CSV file. Additionally, either the entire dataset or subsets of it can be downloaded as a CSV file through the BOOM! explorer (https://boom-vis.lisn.upsaclay.fr).

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