1	Ten simple rules to follow when cleaning					
2	occurrence data in palaeobiology					
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23 corresponding author with any queries. We welcome any feedback.

ABSTRACT

25 Large datasets of fossil occurrences, often downloaded from online community-maintained databases, are a 26 vital resource for understanding broad-scale evolutionary patterns, such as how biodiversity has changed 27 through time and space. Such datasets, however, are not infallible and must be 'cleaned' of inaccurate, 28 incomplete, or duplicate data prior to analysis. Researchers must decide upon the extent, feasibility, and value 29 of data cleaning steps to perform, but while guides are available for working with neontological occurrences, 30 there is currently no clear procedure for palaeobiological data despite its unique attributes. Here, we outline 31 ten rules that aim to aid the process of cleaning fossil occurrence data for downstream analysis. These rules 32 cover the major steps involved in processing data prior to analysis, including project setup, data exploration 33 and cleaning, and finalising and reporting work. We provide accompanying examples and a vignette covering 34 the entire data cleaning process to demonstrate the application of each rule. We believe that these rules will 35 serve as a useful guideline to support data cleaning and foster new standards for the palaeobiological 36 community.

37 Keywords: palaeontology, fossils, biodiversity, reproducibility, data cleaning

24

38 INTRODUCTION

39 Large-scale fossil occurrence datasets have revolutionised our understanding of the evolution of biodiversity 40 on Earth (e.g. Alroy et al., 2008; Alroy, 2010; Close et al., 2020a, 2020b) and enabled a diverse range of studies 41 across palaeobiology, palaeoecology, and conservation (e.g. Powell et al., 2015; Pimiento et al., 2017; Dean 42 et al., 2019; Jones et al., 2019; Allen et al., 2020; Mathes et al., 2021; Boag et al., 2021; Chiarenza et al., 2023). 43 Such datasets provide information about the temporal and spatial distribution of organisms through geological 44 time, along with associated stratigraphic, environmental and biological data (e.g. preservation, 45 palaeoenvironmental information, trait data). Over the last 30 years, palaeobiology has seen the introduction 46 of large-scale collaborative online databases (e.g. Neptune [Lazarus, 1994], the Paleobiology Database [Uhen 47 et al., 2023], Neotoma [Williams et al., 2018]) of fossil occurrences where data are entered (or uploaded) by 48 researchers from around the world with a range of goals, parameters, and collection methods. Using such 49 databases is now commonplace within the field, with the Paleobiology Database (PBDB) and Neotoma both 50 reporting over 500 associated official publications each at time of writing (March, 2025). The scale of these 51 databases has moved palaeontology into the age of 'big data' (Allmon et al., 2018), allowing for the 52 interrogation of Phanerozoic scale patterns that would have been impossible to implement previously.

53 Despite their value, the use of large-scale databases can be hindered by data quality issues such as variable 54 data curation efforts (e.g. resolving and updating taxonomic opinions, updating geochronological ages), 55 inconsistencies during data entry, general error from those inputting data, ambiguity in the original published documents, and lack of familiarity with the underlying data. Resolving these data issues at the source can be 56 57 challenging; such databases can contain millions of records but only maintained by a small group of volunteers 58 who lack the necessary resources (e.g. time, funding, or relevant expertise) to identify and resolve incorrect 59 records at pace. These issues can be non-random and consequently lead to bias in downstream analysis (Panter 60 et al., 2020). Unfortunately, issues related to data quality are commonplace within all large datasets (Cai and 61 Zhu, 2015; Isaac and Pocock, 2015), and palaeobiological resources are no exception. A recent estimate based 62 on flowering plants (~19,000 records) from the PBDB suggested at least ~6% of records could be viewed as 63 potentially 'problematic' (Zizka et al., 2019), while another estimate based on fossil occurrences from the Hell 64 Creek Formation suggested an error rate up to 92.6% in taxonomic data (Schroeder et al., 2022). Cleaning 65 occurrence data is therefore critical to ensure accurate, reliable, and up-to-date data analysis. However, it is by

no means a trivial task, particularly for complex datasets where values may change over time (e.g. due toupdates in taxonomy or nomenclature).

68 Here, we offer ten simple rules as guidance to follow when cleaning fossil occurrence data in preparation for 69 palaeobiological analysis (Fig. 1). Many of these guidelines are equally applicable for neontological 70 occurrence data and have previously been advocated for by ecologists (e.g. Chapman, 2005; Zizka et al., 2019; 71 Panter et al., 2020; Ribeiro et al., 2022). We expand upon these guidelines and present them within a 72 specifically palaeobiological context. The rules are structured broadly in chronological order to aid in carrying 73 out an individual research project, covering project setup (Rules 1-3), data exploration and cleaning (Rules 4-74 8), and finalising and reporting work (Rules 9–10). For each rule, we provide guidance on the value of its 75 implementation and, where appropriate, highlight useful resources. Additionally, we demonstrate how each 76 rule can be put into practice within the in-text boxes and in an accompanying vignette on crocodylian 77 biogeography, available within the supplementary material and at https://tenrules.palaeoverse.org/. We hope 78 this guidance acts as a helpful checklist for researchers to follow when cleaning their data, and highlights the 79 extensive skill and knowledge often required to prepare datasets in preparation for palaeobiological analysis. 80 While the rules presented here aim to be of use to the broader community, our intention is to specifically 81 support researchers getting started with analyses using fossil occurrence data. As such, we assume no former 82 knowledge on the subject, and start by defining fossil occurrence data and data cleaning.

83 WHAT IS FOSSIL OCCURRENCE DATA?

84 Fossil occurrence data comprise records of the presence of a particular taxon at a unique location in space and 85 geological time. This is distinct from specimen-level data, which provides information about a specific fossil 86 specimen. For example, if three specimens of Tyrannosaurus rex are present in the same geological bed at a 87 single location, an occurrence-level dataset would record just one occurrence of T. rex. Typically, occurrence 88 data will include information about the observed organisms such as detailed taxonomy (e.g. scientific name 89 and taxonomic affiliation), location (e.g. modern and/or palaeo-geographic coordinates), geological context 90 (e.g. bed, member, formation) and age (e.g. age, epoch, period, era, eon), and may also contain various 91 associated metadata (e.g. references). From a user perspective, fossil occurrence data are most frequently 92 organised as a single wide-format data table (Box 1) where each column represents a unique field and each

- 93 row represents a unique occurrence record. From a user-perspective this is a common structure, but fossil
- 94 occurrence data are regularly hosted in online databases as a set of relational data tables, linked through unique
- 95 identifiers.
- 96 Fossil occurrence data can be sourced from a variety of online databases such as the Paleobiology Database
- 97 (<u>https://paleobiodb.org/#/</u>) (Uhen et al., 2023), Neotoma (<u>https://www.neotomadb.org/</u>) (Williams et al., 2018),
- 98 Triton (Fenton et al., 2021), Global Biodiversity Information System (<u>https://www.gbif.org/</u>), and the
- 99 Geobiodiversity Database (<u>http://geobiodiversity.com</u>) (Fan et al., 2013). An exhaustive list of other data
- 100 sources can be found in Supplementary Table 1 in Dillon et al. (2023).
- **101 Table 1:** A list of terms used in this article and their respective definitions.

Term	Definition				
Data cleaning	The process of fixing or removing incorrect, duplicate, or incomplete data present within a dataset (e.g. incomplete locality information, misspellings).				
Data filtering	The process of removing data present within a dataset that is beyond the scope of the study (e.g. taxonomically, geographically, temporally, etc.).				
Data imputation	The process of replacing missing values within a dataset with modelled values based on the existing observed values.				
Data preparation	The process of preparing and transforming raw data so it is suitable for analysis and processing.				
Duplicate data	Non-unique data records.				
Data outlier	A data record value that notably deviates from other comparable data records.				
Inconsistent data	Non-uniform or non-standardised data record values.				
Metadata	Structured information that describes, explains, locates, or makes it easier to retrieve, use, or manage data.				
Reproducibility	The ability to obtain consistent results using the same data and analyses.				
Reusability	The ability to reapply data or code for purposes other than their original purpose.				

102 WHAT IS AND IS NOT DATA CLEANING?

103 Data cleaning is the process of fixing or removing incorrect, duplicate, or incomplete data present within a

104 dataset (Chapman, 2005). This process typically involves checking that essential fields like taxonomic names,

105 location, and stratigraphic information contain accurate, consistent, and complete information. Common steps 106 for palaeobiological datasets may involve correcting spelling errors in taxonomic names, updating ages of 107 geological formations, or investigating and resolving occurrences suspected to contain inaccurate information. 108 Within our definition of data cleaning, we exclude the use of filtering to remove data outside the scope of the 109 study, whether that be temporally, spatially, environmentally, taxonomically, or by other criteria (see Table 1). 110 For instance, if investigating the evolution of Phanerozoic terrestrial biodiversity, removing marine organisms 111 from the occurrence dataset would constitute data filtering. However, if a fossil occurrence or taxon had been 112 mistakenly coded as a marine organism (e.g. with crocodylomorphs) when it was in fact terrestrial, fixing this 113 issue would constitute data cleaning (e.g. Mannion et al., 2015, 2019).



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Figure 1: Graphic summary of the proposed ten rules and steps to follow when cleaning occurrence data for palaeobiological analysis. The rules are grouped within their respective theme: project setup (Rules 1–3); data exploration and cleaning (Rules 4–8); and reporting and archiving (Rules 9 and 10).

118 RULE 1: CHOOSE THE RIGHT DATA FOR YOUR QUESTION

119 Selecting the right data is a crucial first step in addressing your research question. Failure to do so can lead to 120 wasted effort in data cleaning, biased results, or misleading conclusions. The data required to address a research 121 question depends on the scope of the study, whether it involves taxonomic diversity, biogeographic patterns, 122 evolutionary rates, ecological reconstructions, or some other thematic area. Before gathering data, whether 123 through fieldwork or using existing databases, researchers must determine what fields, resolution (e.g. 124 taxonomic rank, chronostratigraphic level), and coverage (e.g. temporal, spatial, environmental) are required 125 for their specific inquiry. During this process, researchers should consider whether flexibility related to data 126 resolution and coverage (e.g. taxonomic, temporal, or geographic sampling) may be useful, or introduce 127 unnecessary biases and/or analytical noise. For example, are the same macroevolutionary or ecological trends 128 still identifiable at coarser taxonomic levels or temporal resolutions (e.g. Sepkoski, 1997; Pandolfi, 2001; 129 Hendricks et al., 2014)? Can macroecological trends be reliably reconstructed given the available spatial 130 sampling (e.g. Darroch et al., 2020; Jones et al., 2021; Maidment et al., 2021)? Is sufficient granularity 131 available to determine which environments favour high diversification (e.g. Kiessling et al., 2010)? While 132 data-specific questions are important, defining a research question can be an iterative process and can be 133 refined to meet what data is available, rather than abandoning a project altogether. This refinement may be 134 necessary to ensure analyses are both robust and relevant, as well as to reduce bias and increase the reliability 135 of palaeobiological interpretations.

136 Many steps exist in identifying the right data to address a research question, and often vary between research 137 questions. Nevertheless, some are shared across palaeobiological studies. The initial steps for data selection 138 often include defining the target group (be that taxonomic, geographical, temporal, etc.) and the level of data 139 resolution required. Including data at inappropriate resolutions can either dilute meaningful signals (if too 140 broad) or introduce unnecessary noise (if too fine-grained), particularly if taxonomic or temporal assignments 141 are uncertain or in flux (e.g. Paterson, 2020). For example, studies on species-specific ecological interactions 142 or evolutionary trends require species-level data resolution (e.g. Kempf et al., 2020; Raja et al., 2021; Godbold 143 et al., 2025), whereas broader macroevolutionary patterns may be addressed at the genus or family level (e.g. 144 Sahney and Benton, 2008; Kiessling and Kocsis, 2015; Mannion et al., 2015; Dimitrijević et al., 2020; Drage

145 and Pates, 2024). This can be dependent on the taxonomic group of choice; for instance, there may be 146 insufficient occurrences identified at the species level to enable analysis at this resolution, such as commonly 147 the case with fossil pollen (e.g. Goring et al., 2013). When considering taxonomic resolution, researchers might 148 also assess whether their study will benefit from incorporating multiple taxonomic groups. While focusing on 149 a single clade may allow for taxon-specific trends to be identified, integrating data from multiple lineages can 150 provide insights into ecosystem-wide responses and provide higher data coverage (e.g. Song et al., 2020). 151 Nevertheless, increasing taxonomic breadth should be done deliberately, as different groups may have distinct 152 preservation biases or ecological niches, complicating direct comparisons (e.g. Fernández-Jalvo et al., 2011; 153 Kiessling and Kocsis, 2015; Dean et al., 2019; Shaw et al., 2020, 2021). Studies conducted at wide taxonomic 154 breadth may therefore provide a large-scale picture of the clade included, but risk averaging across the nuanced 155 trends of the individual subclades within it.

Temporal resolution is equally important as taxonomic resolution. Overly broad temporal bins can obscure evolutionary or ecological signals, while excessively fine bins may introduce sampling noise and/or empty bins if observed fossil occurrences are sparse (Olszewski, 1999; Dean et al., 2020; Fan et al., 2020). For example, analysing faunal turnover leading up to the end-Cretaceous mass extinction within a regional setting requires well-constrained stratigraphic placements, rather than general assignments to the Late Cretaceous (Dean et al., 2020). Consequently, researchers should consider whether increasing temporal precision is truly necessary for their study or whether it will introduce more noise than clarity.

163 Geographic resolution and coverage should also align with the research question. A global-scale study on 164 biodiversity change must incorporate data from diverse regions rather than being limited to well-sampled areas 165 like North America and Europe (Vilhena and Smith, 2013). If data from key regions are unavailable due to 166 sampling biases (e.g. poor fossil records or insufficient sampling effort), researchers should reconsider whether 167 their question can still be adequately addressed, then explicitly acknowledge this limitation if so. This 168 assessment should be made before cleaning data, ensuring that all necessary regions are included and that 169 limitations are acknowledged in the study design. Failure to do so can result in global signals being obfuscated 170 by regional trends, or highlight apparent 'global' trends that are actually sampling artefacts (Allison and

171 Briggs, 1993; Vilhena and Smith, 2013; Brusatte et al., 2015; Jablonski and Shubin, 2015; Antell et al., 2020;

172 Close et al., 2020b; Flannery-Sutherland et al., 2022b).

173 If the planned study uses existing data rather than collecting new data (e.g. from a publication or online 174 database), then selecting the right data source is a critical step. Different databases serve different purposes, 175 and the choice depends on the research question and required resolution and coverage. The PBDB is a widely 176 used resource for fossil occurrences, providing broad-scale taxonomic, geographic, and stratigraphic data 177 (Uhen et al., 2023) that is best suited for large-scale palaeobiogeographic and macroevolutionary studies. The 178 Neotoma Paleoecology Database specialises in Quaternary palaeoecological data, including pollen, 179 vertebrates, and geochemistry, making it ideal for studies on more recent environmental changes (Williams et 180 al., 2018). The Geobiodiversity Database (GBDB) is a taxonomic, stratigraphic, and geographic database 181 providing occurrence, collection, and strata data within geological sections (Fan et al., 2013) that is well-suited 182 to high-resolution temporal analyses (Fan et al., 2020). The Global Biodiversity Information Facility (GBIF) 183 and Ocean Biodiversity Information System (OBIS) include modern and fossil occurrences/specimens, which 184 can be leveraged to integrate information from palaeontological and neontological datasets (e.g. Kiessling et 185 al., 2012; Lima-Ribeiro et al., 2017; Jones et al., 2019; Pilotto et al., 2021; Chiarenza et al., 2023; Hodgson et 186 al., 2025). Many other potential data sources exist and a comprehensive list can be found in Supplementary 187 Table 1 in Dillon et al. (2023). Finally, cross-referencing and combining data from multiple databases can be 188 important for enhancing data reliability and completeness, although particular care is needed to ensure datasets 189 and collection approaches are compatible, and that this does not create duplicates. Researchers should consider 190 the full range of data sources available and their data quality, accessibility, resolution and coverage before 191 committing to a dataset.

Box 1. Rule 1: Choose the right data for your question

Robin is starting a project looking at the palaeodiversity of crocodiles through time, assessing their biogeographic patterns during the Paleogene. They decide to download the necessary data from the Paleobiology Database, where Crocodylia are reasonably well represented for this time interval and where relevant information (e.g. taxonomic, geographic, age) are available. When downloading these data, Robin

sets the time interval as "Paleogene" and the taxa to include as "Crocodylia", also making sure to only include body fossils in the download and therefore avoiding the potential for ichnotaxa or ootaxa in the dataset. As they are interested in biogeographic patterns, Robin also makes sure to include information related to geographic coordinates, such as both modern and palaeo- latitude and longitude. They also want to assess the association between Crocodylia occurrences and the number of Crocodylia-bearing geologic formations through time, so they make sure that geological information is included within the download.

 Table 2: Example occurrence dataframe of "Crocodylia" fossil occurrences from the Paleobiology Database

 (https://paleobiodb.org/) demonstrating the structure of a wide-format dataframe.

occurrence_no	collection_no	accepted_name	max_ma	min_ma	lng	lat	
40163	3113	Crocodylia	59.2	56	-74.68	39.97	
40167	3113	Gavialoidea	59.2	56	-74.68	39.97	
40168	3113	Gavialoidea	59.2	56	-74.68	39.97	

192 RULE 2: KEEP RAW DATA RAW

193 Once you have identified or collected appropriate occurrence data for the desired research question, a digital 194 copy must be obtained. This digital copy is defined as raw data and remains so if it does not undergo any form 195 of transformation, leaving the structure and composition of its fields and records identical to the data at the 196 point of acquisition. As such, raw data represents the information available to the researcher at that moment in 197 time (see Box 2). Although data cleaning is likely necessary prior to analyses, it is essential to keep a raw copy 198 alongside any cleaned data. Keeping raw data raw is crucial for two reasons. The first is to allow identification 199 of errors inadvertently introduced during data transformation, by ensuring that the original data remains 200 available for cross-reference. The second is to enable scientific reproducibility, by ensuring that exactly the 201 same data that informed an analysis is available for scrutiny and reuse by future researchers.

Raw data is not necessarily primary data. For example, a fossil occurrence dataset sourced from the supplementary information of a published article, or a static data repository (e.g. Zenodo), may constitute firsthand field observations, or a compilation from previous literature (as is usually the case for large online databases). What matters here is that the raw data are new and unedited with respect to the project currentlybeing conducted.

Upon acquisition, raw data files should be immediately stored locally in a dedicated directory using a simple, descriptive file name, and in a format that preserves its structure and integrity (Borer et al., 2009). If a dataset contains entries with non-ASCII-printable text, such as accented characters (e.g. Candelária Formation), then it may also be appropriate to ensure that the file encoding will preserve this text as accurately as possible (e.g. a .csv file with UTF-8 encoding). If compression is required to meet memory restrictions, then a lossless format should also be used to avoid degradation of the raw data (e.g. a zip folder), although this is unlikely to be an issue for fossil occurrence datasets, which are frequently less than 1 GB in size.

214 Manually opening raw data files should be avoided where possible; different software programs and versions 215 may—and often do—perform automatic formatting upon opening, potentially resulting in mass data alteration 216 (Perkel, 2019). A file may be stored in a read-only format to prevent inadvertent alteration of the raw data 217 (Broman and Woo, 2018), with backups stored in other locations to further guard against future losses or 218 alterations (Wilson et al., 2017). To avoid editing raw data, a researcher can perform manual edits on a working 219 copy of the static file, or by reading the file data into a programming environment where scripted edits can be 220 made to the temporary copy in the computer's memory using a programming language (e.g. R or Python). In 221 the latter case, the script then also functions as a precise log of any alterations to that dataset (see Rule 3; 222 vignette) (Borer et al., 2009).

Understandably, a researcher may wish to make small, practical alterations to the raw data itself (e.g. renaming column headers, manual correction of singular or overwhelmingly rare typographical errors) or performing simple reformatting (e.g. extraction of relevant columns or data sheets) to improve ease of downstream use. In most cases, such procedures can be scripted and manual manipulation of the raw data should still be avoided (Borer et al., 2009). If manual editing of the raw data is essential, this should be kept to the minimum possible, and a comprehensive description of these changes should be documented (e.g. as a plain text file) and kept alongside the static raw data file.

Every effort should be made to ensure that any raw data acquired for analyses remains static and accessiblefor future users. New data are constantly being added to online community databases (e.g. PBDB and

232 Neotoma), while existing entries can be revised, merged, or deleted for a range of reasons including—but by 233 no means limited to-human error, changes in taxonomic opinion, and refined age dating. As such, online 234 community databases are not strictly static repositories, as a future user may obtain a different dataset from 235 that of a past user, even with identical download parameters. Some databases provide a service to archive a 236 copy of a raw data download on request (e.g. PBDB; Uhen et al., 2023), and others automatically do so (e.g. 237 GBIF), providing a citable unique digital object identifier (DOI). However, it should not be taken for granted 238 that raw data being archived at the source will always be available, whether that be an online database or the 239 supplementary files of a journal article. Raw data may become unavailable in the future due to the loss of 240 funding and maintainers, file corruption, and journals becoming non-operational. To further guarantee the 241 long-term availability of raw data, raw data should be archived in a suitable open-access repository whenever 242 possible (see Rule 10).

Box 2. Rule 2: Keep raw data raw

Robin downloads the occurrence data as a '.csv' file to their computer, checking the option to "include metadata at the beginning of the output" to preserve information about the download. They then immediately copy the downloaded dataset to a separate raw data folder, and save it as 'read-only' to make sure that it can't be accidentally manipulated. The raw data file has a total of 886 occurrences.

243 RULE 3: DOCUMENT YOUR WORKFLOW

244 In almost every data-oriented project, researchers carry out some form of filtering, cleaning, formatting, or 245 other operations to transform raw data into a workable and appropriate state for analysis (see Rules 4–8). 246 Documenting these steps is essential to ensure transparency, reproducibility, and a clear understanding of how 247 data have been processed (Stoudt et al., 2021). Together, these steps can be described as a 'workflow', which 248 represents a sequence of tasks or processes that are systematically organised to achieve a specific purpose (Box 249 3). In a workflow, each step often depends on the previous one, and tasks are completed in a particular order 250 to maintain efficiency, consistency, and accuracy. Workflows can be simple, involving just a few steps (e.g. 251 restructuring of data), or complex (e.g. data cleaning and imputation), encompassing multiple transformations.

Having a clearly defined workflow can help streamline data processing steps, reduce errors, and enhancereproducibility by providing a clear, repeatable structure for completing work.

Documenting your workflow improves the transparency, reproducibility, and overall value of your research by serving as a reference or guide for repeat, follow-up, or new analyses; whether by the individual who documented the workflow, a collaborator, or any member of the research community. This can be particularly vital when going through the review process or onboarding new team members and collaborators. Documented workflows can also serve as a key avenue for transferring knowledge about data processing decisions through preserving the 'what' (i.e. what data is being transformed), 'why' (i.e. why is the data being transformed), and 'how' (i.e. how is the data being transformed).

261 Workflows for cleaning occurrence data in palaeobiology fall into two categories that can be used 262 independently or in combination: (1) manual transformation (e.g. hand-typed step-by-step actions in 263 spreadsheet software) and (2) programmatic transformation (e.g. use of automated functions or pipelines within 264 a script of a programming language). Manual manipulation of occurrence data often takes place in spreadsheet 265 software such as Microsoft Excel, Google Sheets, or Apple Numbers, but can also be implemented in text 266 editors. While transforming data in such software can often be more intuitive and user friendly than through 267 programmatic solutions (e.g. in R or Python), the process of documenting the exact steps taken when 268 transforming raw data can be laborious and prone to a lack of clarity. Conversely, programmatic data cleaning 269 provides a clear and traceable workflow, recording the steps taken to clean the data. Through commenting 270 code, additional context for specific data cleaning steps can also be provided to justify decisions made (e.g. 271 taxonomic updates, exclusion of a specific data point), or simply to guide future users. In addition, several 272 formal workflow tools exist that can be leveraged to support data cleaning and workflow documentation (e.g. 273 SnakeMake [Köster and Rahmann, 2012; Mölder et al., 2021] and Galaxy [Giardine et al., 2005; The Galaxy 274 Community, 2024]). To achieve sufficient code proficiency to the extent that a fully programmatic workflow 275 can be developed, however, is not necessarily easy or efficient, and can be a steep learning curve (Brousil et 276 al., 2023). While we generally advocate for a code-based approach to occurrence data cleaning herein, 277 succinctly described manual data cleaning steps can be of equal value and may even be more accessible to the 278 broader community. For researchers with less familiarity with programmatic data transformation (e.g. regex,

text parsing), resources are also available for generating a reproducible script of manual data transformation (e.g. OpenRefine). Notably, even in workflows which are entirely code-based, some elements may still require a degree of manual notation. For instance, when acquiring secondary data (e.g. downloading a dataset), it can be important to document the date of download, which may not inherently be obvious within an entirely codebased pipeline. Through the implementation of Rule 2 and Rule 10, the exact data cleaning that has taken place can be inferred through file comparison software (even with manual workflows).

Box 3. Rule 3: Document your workflow

Robin then begins to set up their project. They make a new project in RStudio, which they also link to their GitHub account to ensure that they have version control and therefore a record of all the steps taken when developing their code and assessing their data. They begin to set up their R workflow, making sure to have a clear overarching structure in their project, making use of section labels. Robin also begins to set up their manuscript file, documenting the steps taken so far in the "Methods" section. They will continue to update this with relevant information as they carry out their analysis, and will make sure to add inline comments to the R script explaining what they're doing and why.

285 RULE 4: EXPLORE YOUR DATA

286 After obtaining the raw data to address your research question and deciding how to document your workflow 287 (see Rules 1–3), a practical next step is to explore your data. Exploratory data analysis (EDA) involves using 288 graphical tools and basic statistical techniques to better understand the characteristics of your dataset, identify 289 anomalies, and uncover patterns (Tukey, 1977; Quinn and Keough, 2002). This step is important for a variety 290 of reasons. First, EDA can reveal the structure and attributes of your dataset, such as variable types and 291 distributions, numbers of observations, and spatial or temporal dependencies between observations. Second, it 292 can highlight relationships between variables to guide future analyses and maximise statistical insights. Third, 293 EDA can help you select appropriate statistical tools and verify their assumptions to avoid type I (false positive) 294 and II (false negative) errors that might lead to incorrect conclusions (Zuur et al., 2010). In doing so, EDA can 295 illuminate aspects of your data that should be accounted for when constructing models, such as non-normality, 296 collinearity or interactions between covariates, and spurious correlations. EDA can also flag systematic biases 297 (e.g. taphonomic or sampling biases) that warrant careful consideration when interpreting your results. Lastly,

EDA can reveal missing values (see Rule 5), outliers (see Rule 6), inconsistencies (see Rule 7), duplication (see Rule 8), and other unusual or erroneous values that require cleaning. Together, EDA is used to assess the quality and completeness of your dataset and gauge whether it can provide a meaningful and representative sample to address your research question. Without this step, you run the risk of applying inappropriate statistical techniques or making faulty inferences.

EDA is a creative and iterative process that is driven by asking questions about your dataset. As such, EDA workflows will inherently be dataset dependent. Nonetheless, the core data exploration steps often include the following: (1) creating data summaries, (2) visualising distributions of individual variables, and (3) visualising relationships between variables. These data exploration steps, together with data cleaning, will often take up the majority of the time you spend analysing your data (Zuur et al., 2010). However, starting simple and being thorough upfront can ultimately produce a more robust and insightful data analysis.

309 A first step when becoming familiar with your dataset is to produce descriptive summary statistics of the 310 central tendencies and variances of groups in the data. Histograms are typically used to plot the distributions 311 of individual variables, flag outliers, determine whether there are high numbers of zeros, and assess normality 312 (along with QQ-plots and formal tests like Shapiro-Wilk). A combination of scatterplots, correlation matrices, 313 box plots, ordinations (e.g. principal component analysis), and cluster analyses should then be used to visualise 314 bivariate and multivariate relationships between variables, depending on the data types present (see Zuur et 315 al., 2010). These graphical tools can reveal interesting patterns between variables and highlight covariates that 316 might be important to include as predictors in more complex models. This process can also help refine the 317 hypotheses being tested, especially given the observational nature of palaeobiological data, yet caution should 318 be exercised to avoid circularity (Hammer and Harper, 2024). Circular reasoning can arise when the same 319 variable is used to both define and test for differences between groups, such that the outcome is guaranteed by 320 the analytical approach (Makin and Orban de Xivry, 2019). For example, you might notice during EDA that 321 your occurrences cluster in a particular way. If you then use those clusters to filter your data and define groups 322 (e.g. clades that either increase or decrease in richness through time), you run into issues if you then examine 323 differences in diversity across those groups because the statistic inference is tied to your grouping criteria; it's

- a self-fulfilling prophecy. For more in-depth treatment of these tools, Zuur et al. (2010) outlines protocols for
- 325 EDA in ecology, which can readily be adapted to palaeobiological data (see Birks et al., 2012).

326 Each of these steps can be scripted in R, other computer programming languages, or even in spreadsheet 327 software, and used to create a transparent and reproducible log of the EDA workflow (see Rule 3), what was 328 discovered, and how these initial inferences shaped the final analysis. To wrangle data and generate basic 329 summary statistics, the *dplyr* (Wickham et al., 2023b) and *tidyr* (Wickham et al., 2024) packages (part of the 330 tidyverse; Wickham et al., 2019) as well as *skimr* (Waring et al., 2022) are particularly helpful. These packages 331 can be used in tandem with *palaeoverse* (Jones et al., 2023), which contains functions designed for working 332 with fossil occurrence data such as temporal or spatial binning, range calculations, identifying unique taxa, 333 and flagging misspellings of taxonomic names. For example, you might want to assess how many bins you 334 have data available for. To visualise relationships between variables, ggplot2 (Wickham, 2016), psych (e.g. 335 'pairs.panels' function; Revelle, 2024), GGally (e.g. 'ggpairs' function; Schloerke et al., 2024), corrplot (Wei 336 and Simko, 2024), and DataExplorer (Cui, 2024) offer useful graphical functions. A multitude of online 337 resources exist to help build competency in programming as you explore your data, including R for Data 338 Science (Wickham et al., 2023a), R Graphics Cookbook (Chang, 2018), and Posit cheat sheets 339 (https://posit.co/resources/cheatsheets/). Importantly, we recommend commenting code and keeping a record 340 of EDA results and visualisations to refer back to as you develop analyses and communicate findings (see Rule 341 9).

Box 4. Rule 4: Explore your data

To get an idea for how their data is distributed and its various characteristics, Robin first decides to generate some basic summary statistics and plots. As they are interested in assessing palaeodiversity, Robin checks the proportions of the different taxonomic ranks in the dataset. They find that ~28% of the occurrences— about 250 in total—are assigned to the species level, and that a further ~28% are assigned to genera. Because of this, they think it might be wise to carry out palaeodiversity analysis at the rank of genus to ensure that they have enough data to find meaningful patterns. However, they will decide upon this after doing a more thorough assessment of the data. They also look at the geographic distribution of occurrences by looking at their associated country codes, finding that Paleogene crocodiles are found in a total of 46 countries.

However, after sorting these data, they find this number drops to 45 countries. Something odd has happened that they will have to investigate during future data cleaning steps.

342 RULE 5: IDENTIFY AND HANDLE INCOMPLETE DATA RECORDS

343 When exploring your dataset by carrying out EDA (see Rule 4), you may encounter ambiguous, incomplete, 344 or missing data entries. These incomplete or missing data records can occur due to various reasons. In some 345 cases, the data truly do not exist or cannot be estimated due to issues relating to taphonomy, collection 346 approaches, or biases in the fossil record (e.g. information derived from highly fragmentary fossils, historical 347 collections without associated geological or chronological information, or underrepresentation of certain 348 taxonomic groups). In other cases, discrepancies may arise because data were collected when definitions or 349 contexts differed, such as shifts in geopolitical boundaries and country names over time (e.g. an occurrence 350 that only has "Czechoslovakia" listed as the country of origin cannot be precisely located today). Additionally, 351 data may be incomplete for some records, but can be inferred through other available data (e.g. inferring 352 country of origin through geographic coordinates). Although an intuitively common issue in palaeobiology 353 given the uneven and incomplete nature of the fossil record (Raup, 1972; Allison and Briggs, 1993; Cherns 354 and Wright, 2000; Vilhena and Smith, 2013; Dean et al., 2019), missing information can bias the results of 355 palaeobiological studies (e.g. Norell and Wheeler, 2003; Kearney and Clark, 2003; Wiens, 2003; Marshall et 356 al., 2018; Jones et al., 2021; Dean and Thompson, 2025). Occurrence data are inherently based on the existence 357 of a particular fossil, but missing data associated with that fossil occurrence can also affect analyses that rely 358 on that associated data (e.g. studies examining environmental associations will be impacted by missing 359 environmental data).

Depending on your research goals and the data required to address your questions, incomplete entries may either be removed through filtering or addressed through imputation techniques. Data imputation approaches can be used to replace missing data with values modelled on the observed data using various methods (Gendre et al., 2024). These can range from simple approaches, like replacing missing values with the mean for continuous variables (e.g. morphometric measurements or associated climatic variables), to more advanced statistical or machine learning techniques (Demirtas, 2018; see Van Buuren, 2018; Haghish, 2022). If you do 366 decide to impute missing data, it is essential that this process and its effects on the dataset are clearly justified 367 and documented (see Rule 3) so that future users of the dataset or analytical results are aware of these decisions. 368 Although missing data can reduce the statistical power of analyses and bias the results, imputing missing values 369 can introduce new biases, potentially also skewing results and interpretations of the examined data (Newman, 370 2014). Therefore, if a dataset has sufficient data to test the desired hypotheses, or if incomplete data entries 371 cannot be imputed reliably, these entries should be deleted in their entirety during the data cleaning process, 372 while clearly documenting how entries were chosen for exclusion (see Rule 3). Alternatively, some data 373 analyses allow for incomplete data entries (e.g. non-metric multidimensional scaling), and so where these 374 methods are appropriate, you may choose to retain your incomplete data entries as-is.

375 To decide how to handle missing data, start by identifying the gaps in your dataset, which are often represented 376 by empty entries or 'NA' (meaning "not available" or "not applicable"). For imputing missing values, 377 numerous methods and tools are available in your coding language of choice, such as *missForest* (Stekhoven 378 and Buehlmann, 2012), mice (Van Buuren and Groothuis-Oudshoorn, 2011), and kNN (Kowarik and Templ, 379 2016). Additionally, the R packages TDIP (Gendre et al., 2024) and mlim (Haghish, 2022) integrate various 380 imputation and error identification methods, facilitating method comparison. Many detailed open-access 381 references exist with which to compare the underlying methodologies of imputation approaches, and which 382 provide guidance on the different missing data types and how to choose imputation methods and parameters 383 (e.g. see Van Buuren, 2018).

384 Removing missing data can be straightforward when working with small datasets. For manual removal, tools 385 such as spreadsheet software can be sufficient (although see Rule 3). In R, built-in functions such as 386 complete.cases() and na.omit() quickly identify and remove missing values. The tidyr package also provides 387 the drop na() function for this purpose (Wickham et al., 2024). However, incomplete data entries can also be 388 of use without imputation or removal; for example, the tax unique() function from the *palaeoverse* R package 389 (Jones et al., 2023) can flag 'cryptic diversity' that arises due to taxa not assigned to a specific species or genus, 390 but which represent the only appearance of that clade in the geographic region or time period of choice (e.g. 391 Mannion et al., 2011).

18

Box 5. Rule 5: Handling incomplete data records

Robin next begins to systematically explore their data in more detail, first making sure that the occurrences aren't missing vital information. As they are assessing biogeography, they first find any occurrences that are missing palaeocoordinates and decide to remove them from the dataset rather than trying to estimate new palaeocoordinates using available tools. After removing these data, they check to make sure that all of the occurrences have both modern and palaeo- coordinates, then decide to revisit the issue of missing data within the 'country code' field. They find that there are two occurrences which have a value of 'NA'; normally this would mean missing data, on further checking their geographic position using modern coordinates, Robin finds that they are actually from Namibia (i.e. NA!). It seems R has misconstrued these records!

392 RULE 6: IDENTIFY AND HANDLE OUTLIERS

393 Outliers, data points which lie to the extremes of the distribution of all data or otherwise deviate from 394 comparable data points, will become readily apparent when applying EDA to your dataset (see Rule 4). 395 Outliers may arise from a mistake in data entry, or because the value represents a genuine anomaly compared 396 to the other available data. Identifying outliers is therefore doubly useful: it is a way of highlighting potentially 397 suspect data for subsequent checking, and also allows us to better understand the range of values our data 398 holds. Outliers are particularly important when an analysis investigates the maximum and minimum values of 399 a field, or for calculations involving confidence intervals, as unusually small or large values can influence such 400 analyses more strongly than other data points.

401 Most data types are amenable to some form of outlier analysis. For numerical data, this usually involves 402 identifying the points lying at the extremes of the range of values. A simple example of this is creating a box 403 plot, where typically the 'whiskers' are quantified based on some range of values describing the data, and any 404 points lying outside of this range are plotted as individual outliers. Here, the choice of cut-off is very important, 405 and many different methods exist for setting outlier cut-off points that might be applicable in different 406 situations (Aggarwal 2017). The shape of the distribution of the data also matters. Many methods of generating 407 confidence intervals assume that data are normally distributed, but this is often not the case for real-world 408 biological or palaeobiological datasets, and should be borne in mind when selecting a method. For categorical

data, a more appropriate method of identifying outliers might be examining abundance counts for the different
categories to identify those with only a few instances. On such topics, we recommend referring to classic
textbooks on statistics for (palaeo-)ecologists (e.g. Hammer & Harper 2024).

412 The types of data commonly present in occurrence datasets can be checked for outliers in a multitude of ways. 413 Checking age data for outliers can be very important: if we wish to quantify the temporal or stratigraphic range 414 of a taxon, then a misplaced data point could falsely prolong our inferred range by millions of years. This is 415 true for both numerical (e.g. '250 Ma') and categorical (e.g. 'Triassic') forms of age data. Collecting tip or 416 node age priors for phylogenetic inference is a common use of such data for which identifying outliers can be 417 particularly important for downstream analyses (Mulvey et al. In Press). For such questions, the data resolution 418 at which outliers are quantified should be carefully considered: for example, the age of an occurrence may 419 appear anomalous for a specific species, but not within the context of the wider genus. This difference may 420 alter the appropriate course of action for dealing with such data points. An example of a palaeontology-specific 421 outlier detection method is the "Pacman" method (Lazarus et al. 2012), which uses 'known' age distributions 422 for biostratigraphic markers to identify outliers in numerical stratigraphic data. This approach, and other 423 relevant functions, are available in the *fossilbrush* R package (Flannery-Sutherland *et al.* 2022b).

424 Exploring data to search for taxonomic outliers can also be a helpful way of identifying mistakes. In the case 425 that a collection of fossils is stated to contain nine species of bivalve and one species of shark, it is worth 426 checking that the shark occurrence is correct. Otherwise, for example, it could be that the shark species actually 427 has the same name as a bivalve species and has been miscategorised, or that the shark species is a misspelling 428 (an example of this being the genus Megalodon, a bivalve from the Jurassic, being confused with Otodus 429 megalodon, the giant shark from the Neogene). For multivariate data (e.g. geographic coordinates), convex 430 hulls can be generated to identify points that form the corners of the hull, and therefore lie at the extremes of 431 the data. The distance of these points from the rest of the data can then be quantified, with those at the greatest 432 distance highlighted for further checking. However, it is worth considering that geographic coordinates are 433 often subject to limits which can artificially create clumpiness in the data. At a global scale, the distribution of 434 the continents serves as a major control on the potential spread of both species and fossil preservation, and an 435 apparently large distance between any two data points may simply represent an area of ocean between two

436 continents. *CoordinateCleaner* (Zizka *et al.* 2019) is an R package designed specifically for cleaning the
437 geographic coordinates of occurrence data, including via outlier detection.

It is also possible to design downstream analytical workflows with outliers in mind, which may be particularly appropriate when it is unclear whether outliers should be removed from a dataset or not. For example, a simple strategy is to calculate and use the 90th or 95th percentile of the data instead of maximum values, or median values over mean values. More complex alternatives include bootstrapping, jackknifing, and related methods implement repeated subsampling of a dataset; this has the overall effect of amplifying the signal of common data values, and diminishing the signal of rare data values (which typically include any outliers). This can reduce the influence of outliers on the results without completely excluding these values from analysis.

Box 6. Rule 6: Identify and handle outliers

Happy that the dataset contains the information needed, Robin sets out to identify potential outliers that might affect the specific variables that relate to their research question. To do this, Robin first plots a map of where crocodiles have been found across the globe to see if any fall in places that we would not expect. They find several occurrences that appear within Antarctica, which is outside the expected climate tolerances of the group. By checking these occurrences against the associated references, it turns out that the collections associated with these anomalous occurrences appear to be legitimate, but the occurrences themselves are only listed as "Crocodylia indet.". Robin could consider removing these occurrences due to this lack of certainty, but they would have to be consistent in their approach across the data, and make sure that a record of this is documented so that future researchers can follow their approach (see Rule 3).

445 RULE 7: IDENTIFY AND HANDLE INCONSISTENCIES

When carrying out EDA on your dataset (see Rule 4), it is also likely that inconsistencies will become apparent. Inconsistencies refer to deviations in the format, structure, or definitions of data values in a dataset, and they can occur in all types of variables (e.g. numerical, categorical, etc.). Inconsistencies can represent information that is definitively incorrect (e.g. a taxonomic name spelt both correctly and incorrectly in different records) but can also arise from variation of input into a dataset. This could be due to inconsistencies in standards or unclear definitions of variables (e.g. alternative, but correct, spellings of the same geological formation or 452 different date formats being used in the same column), standards which have changed over time (e.g. a stage 453 being given new age boundaries as a result of increased accuracy of new radiometric dates) or conflicting 454 scientific opinions (e.g. two fossils of the same species input under different taxonomic names by researchers 455 holding differing opinions). Although it is common for inconsistencies to apply across different rows within a 456 single column of variables, they can also apply across multiple related columns. For example, columns for the 457 earliest and latest ages of a fossil occurrence may have different data formats, or there could be a discrepancy 458 between the named chronological interval for an occurrence in one column and its numerical age in a separate 459 column. Inconsistencies may not inherently represent errors in data values, but their inclusion in a dataset can 460 lead to a variety of downstream issues during data analysis, including skewing of summarised values, or the 461 incorrect parsing of data by software. These issues can have serious knock-on effects for the interpretation of 462 results, so it is essential that they are rectified prior to further data analysis. Given the variety of ways that 463 inconsistencies can arise in a dataset, identifying them is challenging and can require high familiarity with the 464 dataset. EDA should therefore be performed iteratively (see Rule 4) to minimise their risk of inclusion.

465 When searching for inconsistencies in your data, it is essential to first set definitions and standards for the data, 466 which may be different from those associated with the original format of the dataset. This involves ensuring 467 that you have made clear and consistent decisions on value formats, structures, and classes (e.g. are dates listed 468 as DD-MM-YYYY or MM-DD-YYYY?), variable definitions (e.g. the column 'min ma' is referring to the 469 minimum possible numerical age of the fossil occurrence in millions of years; see Box 1), and the necessary 470 precision of your values (e.g. all measurements in a column will be in centimeters rather than millimetres). 471 When making decisions regarding the formatting of a column, it is always advisable to make edits in a copy 472 of that column to retain the original information (see Rules 2 and 3). Similarly, adding new columns and 473 comments that contextualise your decisions or concerns about a column's accuracy can help avoid the pitfalls 474 of manual workflows (see Rule 3) and aid future users of your data.

475 Many inconsistencies will become apparent as you familiarise yourself with the spread of data within a 476 particular column (see Rule 4). When using R, the 'table()' function can highlight the frequency of categorical 477 values within a column, which can quickly reveal inconsistent data. Additionally, systematically checking 478 within and between columns for formatting and spelling discrepancies will flag data values which appear 479 problematic. Some inconsistencies may relate to facets of your data that you are less familiar with. This could 480 result in incorrectly identifying values as inconsistencies which are actually separate data points (e.g. close 481 taxonomic spellings, which represent different taxonomic units rather than spelling mistakes. For instance, 482 Varanops is a genus of early Permian carnivorous synapsid, whereas Varanopus is an ichnogenus of tetrapod 483 footprints also from the Permian), or missing inconsistencies due to a lack of knowledge (e.g. two geological 484 formation names that have now been united under one name). In these cases, we recommend flagging potential 485 issues and obtaining assistance from the literature or other researchers who have expertise in that particular 486 area, rather than making decisions which may result in inaccurate data.

487 Because inconsistencies are inherently related to the values of the data that you are working on, the ultimate 488 resource for resolving issues is the literature for the corresponding geographic region, taxonomic group or time 489 period of study. Additionally, there are a variety of packages in R that can help identify potential 490 inconsistencies in your dataset. The fossilbrush package (Flannery-Sutherland et al. 2022b) aims to assist with 491 chronostratigraphic and taxonomic harmonisation within a dataset. Similarly, the 'tax check()' function of the 492 palaeoverse package (Jones et al. 2023) can help to check for and tally potential spelling variations of the same 493 taxon. The previously mentioned CoordinateCleaner package (Zizka et al. 2019) is also widely used to 494 automatically and systematically flag common spatial and temporal errors in biological and palaeobiological 495 collection datasets in a way that is systematic, transparent and easily built into personal workflows. However, 496 packages such as these automatically flag records based on predetermined mathematical rules and so are blind 497 to the context of the data that they are assessing. Consequently, such approaches should be used as a 498 complement to, rather than a replacement for, decision making by the researcher.

Box 7. Rule 7: Identify and handle inconsistencies

It's then time for Robin to do a thorough check for inconsistencies in the dataset. They check whether the class types of the fields in the dataset make sense (e.g. the 'max_ma' and 'min_ma' variables are listed as 'numeric'), and makes sure that there aren't inconsistencies between columns in the dataset (e.g. making sure that occurrences with the same value in the 'max_ma' column all have the same value for 'early_interval'). Robin then uses several automatic check functions in different R packages to flag any taxonomic or formation names that might have several different spellings. They quickly find that there are

several formations which have suspiciously similar names, one obvious pair being "San Sebastián" and "San Sebastian". After checking the literature to make sure that these are indeed the same formation, Robin corrects the spelling to ensure consistency across the dataset.

499 RULE 8: IDENTIFY AND HANDLE DUPLICATES

500 Duplicate appearances of data entries are also a common issue with occurrence datasets. The identification of 501 duplicate fossil occurrences is an essential step in data cleaning, as neglecting them can directly impact the 502 accuracy of analyses in a non-random way, i.e. by increasing the signal of repeated data points in the dataset 503 (see Rules 6 and 7). There are several ways in which the same occurrence might be recorded in a dataset 504 multiple times. The first is identical duplicates, where the exact same record appears twice or more within a 505 dataset. This is unlikely, as occurrences within large databases are often assigned consecutive unique 506 identifiers and by definition cannot appear twice. However, there are several circumstances where this can 507 occur. For example, when two previously taxonomically unique occurrences are synonymised under the same 508 taxonomic name, when merging occurrences sourced from different databases (e.g. the same fossil specimen 509 could be independently entered into both GBIF and the PBDB), or from user error when manually manipulating 510 a dataset (although this should be minimal if following Rules 2 and 3). A more common form of data 511 duplication is the entry of the same fossil or collection of fossils as two separate occurrences or collections by 512 different contributors to the database in question.

513 The first step for resolving duplicate occurrences in your dataset is choosing the criteria for identifying 514 duplicates. Identical duplicates should be inherently easy to spot, as they will consist of exactly the same values 515 across all variables (after inconsistencies have been addressed). Duplicate occurrences arising from multiple 516 entries of the same fossil are more challenging, as user variation during data entry will mean that not all 517 variables are likely to be identical. When this is the case, one potential way to identify duplicates is to use 518 columns in the dataset related to the reference (e.g. original descriptive publication) from which the occurrence 519 was acquired; though consideration of what constitutes a duplicate should be established for your specific 520 project (e.g. if we are interested in the total number of localities, multiple references may refer to the same 521 locality and therefore could be defined as duplicates). Multiple occurrences of the same taxon from the same

reference might indicate that data duplication has taken place; checking the original reference will help resolve
this. Other columns that are likely to have obvious duplicate values include those that tie a data record to a
particular geographic or temporal position (e.g. two records with similar/identical geographical coordinates)
(Pires *et al.* 2015; Zizka *et al.* 2020; Bonnet-Lebrun *et al.* 2023).

526 Once the criteria for removing duplicates are established, only one occurrence record should be retained in the 527 processed dataset if multiple share the same taxonomy, geological age, and coordinates. It is ultimately the 528 researcher's decision whether to exclude potential duplicates from the dataset, and the reasons for doing so 529 should be documented (see Rules 3 and 9). However, accidental removal of non-duplicate data can also bias 530 the results of a study, and so it is advisable to be conservative when removing entire occurrence entries. Data 531 duplicates can be more difficult to identify if inconsistencies (see Rule 7) are present in the dataset, such as if 532 the same taxon has an entry for two different ages or geological localities, where the age/location names have 533 been redefined or have different regional names. This means that identification of inconsistencies and 534 duplications (see Rule 8) should often be performed iteratively.

535 Identification and removal of duplicates can be done manually, but this approach has a high time-cost with 536 large datasets, particularly when identifying them can be challenging in the first place. Alternatively, different 537 softwares can help streamline this process. Duplicates can be removed using Excel by filtering the different 538 columns of your dataset, though this can be too time intensive. In Python, this can be achieved using Pandas 539 (McKinney 2011), a library developed specifically for data manipulation. Scripting in R offers quick and 540 effective alternatives; unique() or distinct() from the *dplyr* package (Wickham *et al.* 2023*b*) can be used to 541 return a dataset with any direct duplicates removed. More complex approaches, such as CoordinateCleaner 542 (Zizka et al. 2019) and fossilbrush (Flannery-Sutherland et al. 2022b), can flag spatial, temporal, and 543 taxonomic errors in occurrence data. As discussed in Rule 7 and above, thorough literature and repository 544 searches, or external expertise on variables/groups you are less familiar with, should also be used in tandem 545 with the above analytical approaches to resolve data duplications.

Box 8. Rule 8: Identify and handle duplicates

For the last step of data cleaning, Robin needs to remove any duplicates that might have crept into the dataset,

as these could impact further analyses. Robin makes a new dataset including only the fields 'collection_no' and 'accepted_name', and then retains only the unique rows. By comparing the number of rows between this dataset and the total dataset, they find that 24 occurrences were absolute duplicates. Robin then double checks these, and removes them from the original dataset. After finishing this step, Robin now has a pretty good idea of how this dataset looks. They therefore decide to go back and re-run their initial summary statistics as well as adding some additional tests, before going back and further refining the dataset.

546 RULE 9: REPORT YOUR DATA AND CLEANING EFFORTS

547 After cleaning your data and ensuring that it is fit for purpose, it's crucial to report on the cleaning steps you 548 took and the overall state of your data. Reporting includes detailing how you carried out the cleaning steps (see 549 Rules 5–8, using the workflow from Rule 3), why these were taken, the impact cleaning had on dataset 550 composition (such as the pre- and post-cleaning occurrence counts; see Rule 4), and dataset summary statistics. 551 Reporting these steps enables reproducibility: without knowing how the data were cleaned, it is impossible to 552 understand the dataset in its processed form or reproduce the downstream analyses. This also increases 553 transparency, such that other researchers will understand how and why the cleaning steps were performed, as 554 well as the time investment on pre-analysis steps that is not otherwise well documented. Reporting on data 555 cleaning also provides a venue for furthering acknowledgement; we can take this space to document other data 556 sources and software (e.g. R packages) that contributed to the dataset in question before or during the cleaning 557 process.

558 Reporting should involve carefully documenting at minimum: (1) how the data were chosen to be collected 559 (see Rule 1); (2) the data exploration performed (see Rule 4); (3) how outliers, inconsistencies, and duplicates 560 were identified, their counts, and how they were dealt with (e.g. removed, corrected, resampled; see Rules 5-561 8); and (4) the pre- and post-cleaning dataset summary statistics. The summary statistics should cover, for both 562 the original raw dataset and the final cleaned dataset: the overall counts of occurrences, sampling units, or any 563 other variables of interest; if applicable to the data, aspects like means and standard deviations or ranges of 564 variables of interest; the degree of uncertainty regarding pertinent variables (e.g. how certain are the taxonomic 565 assignments or stratigraphic occurrences, and to what granularity are these recorded?); the impact of any

566 filtering (i.e. *n* occurrences were excluded by cleaning step *n*); and any imputation in the dataset. Reporting 567 your data cleaning should be clearly documented in the methods section, in the supplementary material, or 568 accompanying the dataset (see Rule 3).

569 Dataset reporting should also cover any cleaning cases specific to your data or difficulties in data processing 570 that would be of interest to future data users or relevant specialists. This might include removing any 571 occurrences of specific taxa due to a debate over synonymisation or higher group assignment, or removing 572 occurrences from specific geographical regions or localities due to uncertain age assignment. For example, a 573 study on global trilobite evolutionary trends might choose to identify and exclude entries in their occurrence 574 dataset of families that recent assignments place within the poorly defined (i.e. 'waste-basket') order 575 'Ptychopariida' (by following a published taxonomic list, such as Adrain 2011). A global study on Cambrian 576 palaeobiogeography might explain that they chose to time-bin their dataset differently because the Cambrian 577 Stage 10 (Cohen et al. 2013) has an as-yet undefined base. In both examples, these data cleaning decisions 578 require direct explanation because they are not obvious to non-specialists (or future researchers) on the 579 taxonomic group or time period, and will have extensive impacts on the analysis results, which might influence 580 how other researchers view or use the data or results in the future.

581 Several resources exist to aid the reporting process. When downloading raw occurrence data, such as from the 582 PBDB, you can often download a supplementary reference list citing all the contributors to the data you 583 downloaded. These should then be incorporated into publication reference lists (preferably) or supplemental 584 references (see Smith et al. 2024 for discussion). If you gathered data from the primary literature, or used 585 literature to verify potentially erroneous entries in your dataset (e.g. Rules 7 or 8), then you should compile a 586 list of references manually or using bibliographic software (e.g. Zotero). Similarly, you can download package 587 version citations in R or Python for those used during cleaning. Additionally, pre-formatted reporting templates 588 exist, such as those by PRISMA (Page et al. 2021), which could be included in the supplementary information 589 of an article.

Box 9. Rule 9: Report your data and cleaning

Robin now has a cleaned dataset that they use to run some analyses, and they find some results which are

worthy of publication. When Robin writes up their manuscript, they make sure to report all the steps that they took to clean the data in their 'methods' section and in the associated supplementary materials, drawing attention to the decisions that they made on particular occurrences (e.g. what Robin decided to do with the 'Crocodylia indet.' specimens from Antarctica). Robin makes sure their code is clean, structured, and legible, and sufficiently commented such that it can be followed by someone who is less familiar with the approaches that they took.

590 RULE 10: DEPOSIT YOUR DATA AND WORKFLOW

591 Once you have documented and reported how you have followed Rules 1-8 (see Rule 9), it is critical that you 592 deposit all of your data and workflow files in a reliable archival repository, preferably prior to review. This 593 enables transparency, data accessibility, and reusability as well as research reproducibility (see Table 1) for 594 the foreseeable future. Further, by uploading your workflow, you allow others to apply your cleaning and 595 filtering steps to their own data, reinforcing standard practices and preventing duplicated effort. At the 596 minimum, your archived files should include your raw data file(s) (see Rule 2) and your data processing 597 documentation (see Rule 3). However, you should aim to archive as much of your entire research workflow as 598 possible (see Rule 9). For example, such an archive would ideally include the scripts that you wrote to perform 599 cleaning and filtering operations (see Rule 3) and/or analysis and visualisation of your cleaned data, including 600 any figures in the accompanying paper (see Rule 4). It should also include modified versions of the data file 601 created before or after manual and/or automated cleaning and filtering steps have been performed, and your 602 reporting on how the data was changed by cleaning (see Rule 9). Finally, in addition to depositing these files 603 (preferably in non-proprietary formats, e.g. .csv or .txt), you should also include a metadata file which 604 describes the attributes of your various files, including their source, purpose, and, in the case of data files, 605 column definitions (Baca 2016). In the case of occurrence data, the standards set forth and resources created 606 by Darwin Core (https://dwc.tdwg.org/) may be useful (see https://fairsharing.org/ for other data and metadata 607 standards). In addition to increasing the accessibility and reusability of your data, accurate and descriptive 608 metadata is also vital for improving the discoverability of your data (Löffler et al. 2021).

609 There are different types of repositories for different purposes. The PBDB and Neotoma serve as ideal 610 repositories for individual occurrence data, and we strongly encourage you to input new occurrence and 611 taxonomic information in these repositories or other appropriate repositories. Nevertheless, these repositories 612 are not intended for storing your individual project materials such as raw data files and scripts. Further, while 613 the ever-growing and dynamic nature of these databases via community crowdsourcing is a clear benefit to 614 our field, this is also the same reason they are inappropriate for storing static versions of your raw data; they 615 may be edited by other users at some point in the future (see Rule 2). Therefore, you'll need to identify a 616 separate repository for your data archive. However, navigating the data repository landscape can be 617 challenging. For example, as of February 2025, the Registry of Research Data Repositories 618 (https://www.re3data.org/; Pampel et al. 2013) lists over 2,850 open repositories available for archiving data, 619 with over 85 of them covering 'Geology and Palaeontology'. Commonly used general repositories for 620 occurrence data and associated files include Dryad, Zenodo, FigShare, the Open Science Framework (OSF), 621 and Pangaea (Felden et al. 2023). Institutions (e.g. Yale University, University of Vienna) and national bodies 622 (e.g. UK National Geoscience Data Centre) may also offer their own in-house data archival services. When 623 choosing between repository options, you should consider several archival aspects, including longevity, 624 licensing, accessibility, discoverability, citability, version control, cost, and capacity.

625 First, you should confirm that your chosen repository will be able to store your files for a long time (i.e. 626 decades, at minimum). This information is often listed as 'longevity', 'persistence', or 'retention' within a 627 repository's policies. Most repositories aim to be sustainable and last indefinitely; however, uncertainties 628 around funding, future costs, and technological developments mean this may not hold true. Many repositories 629 will be clear about how much funding they currently have (usually in a number of years; e.g. OSF currently 630 states it has 50 years of funding for hosting data), with the potential for further funding in the future. If a 631 repository does not list a longevity of decades or guarantee permanent hosting, it should probably be avoided 632 (see Lin et al. 2020 for further discussion).

Next, your repository should either be clear of what copyright license your files are shared under or provide
you with a selection of copyright licenses to choose from. For data, the licenses developed by the Creative
Commons should be adequate, covering public domain, attribution, and non-commercial license types. In

636 general, datasets containing only new data are usually published under the CC0 license ("No Rights Reserved"; 637 https://creativecommons.org/public-domain/cc0/), which releases data into the public domain and makes the 638 data easy to reuse for other projects. For example, data in the PBDB are licensed under a CC0 license (Uhen 639 et al. 2023). On the other hand, data from the Neotoma database (Williams et al. 2018) are licensed under a 640 CC-BY license, meaning the data must be attributed accordingly. For sharing code, there is a wider variety of 641 licenses to choose from, with some of the most popular licenses including the MIT License, Apache License, 642 and GNU General Public License. If you find yourself having a hard time choosing between licenses, you can 643 find handy tools to choose a license from Creative Commons (https://creativecommons.org/choose/) and 644 GitHub (https://choosealicense.com/).

645 You should also ensure that your repository will make it easy to find and cite your data archive (Wilkinson et 646 al. 2016). The most common currency of academic scholarship is citation count, which is often used as one of 647 the determining factors for hiring, promotion, and funding decisions in academia, for better or worse 648 (Ravenscroft et al. 2017; Desrochers et al. 2018; Smith et al. 2024). For a long time, datasets, particularly 649 those of occurrence data, were not citable in the same way in which we cite publications (Payne et al. 2012; 650 Silvello 2018). Many repositories, such as Dryad, FigShare, and Zenodo, have introduced the automatic 651 assignment of permanent and unique identification numbers called Digital Object Identifiers (DOIs) to 652 archived datasets (Brown 2021). Theoretically, DOIs have brought data on par with standard publications with 653 regards to citability (although note that other restrictions may remain such as limits to the total number of 654 references imposed by journals [Payne et al. 2012] and the lack of inclusion of data citations in many common 655 citation indices [Silvello, 2018; Smith et al., 2024]). Some repositories may not automatically assign DOIs, 656 but may have other ways to provide unique identifiers. For example, GitHub (a common repository for 657 software and data files) does not assign DOIs and is therefore often not a citable repository in journal 658 publications. However, it does allow for integration with Zenodo which will archive each 'release' of a public 659 GitHub repository and assign each archive a DOI. This also ensures static versioning of the respective code 660 and data files. Similarly, OSF, which can optionally provide a DOI for a public repository, can be linked to 661 many other storage solutions such as Amazon S3, Dropbox, and OneDrive which are not otherwise citable. In 662 addition to citability, it is also important that the repository provides a way for other researchers to discover 663 your data. For example, Zenodo and FigShare provide simple search interfaces to search for datasets archived with their respective services. Note that Google Scholar historically has explicitly not indexed datasets, but
tools such as Google Dataset Search and Science Explorer (<u>https://scixplorer.org/</u>) support finding of archived
datasets across the web.

667 Finally, hosting files costs money, and therefore most repositories have limits to the amount of storage that 668 they provide to individual users or for individual repositories. For example, at the time of writing, free FigShare 669 accounts can only upload up to a total of 20 GB for free, whereas Zenodo and OSF limit each free public 670 repository to 50GB (with no account limits). Dryad similarly offers a storage limit of 50 GB per repository but 671 at a base cost of \$150 USD, though this cost can be covered by partnerships with journals or fee waivers. Most 672 repositories will have the option to increase these quotas for a cost. For example, Dryad charges \$50 USD for 673 every 10 GB of storage above the base 50 GB, whereas FigShare offers a paid premium service that enables 674 users to archive larger files and repositories with pricing based on the amount of storage required. Fortunately, 675 as mentioned previously, occurrence datasets tend to be relatively small (<1 GB), so these free storage quotas 676 should be sufficient for most occurrence data repositories.

Box 10. Rule 10: Deposit your data and workflow

When Robin submits the finished manuscript to *Palaeontology*, they make sure to upload their raw dataset, the cleaned dataset, and their R scripts to a data repository service. Robin then also makes sure to cite the dataset Digital Object Identifier (DOI) in the manuscript, drawing attention to where the data is kept. They can then sit back and wait for the (hopefully!) positive reviews on the manuscript, knowing that they have done their best to make sure that their research is accurate and easily reproducible.

677 CONCLUSIONS

Large fossil occurrence datasets have revolutionised the research questions that can be asked of the fossil record. However, a variety of decisions and processes must be carried out prior to conducting analyses that impact these data and subsequent conclusions, including how we set up projects (Rules 1–3), explore and clean data (Rules 4–8), and report our work (Rules 9–10). These steps can be further complicated by the specificities of palaeobiological data, particularly those collected over long time frames where collecting and reporting practices or broader geopolitical shifts may impact the quality and consistency of data being reported. 684 Consequently, despite data cleaning aiming to be an objective process, it is ultimately the product of 685 researchers who will make decisions based on their professional expertise. In this article, we provide general 686 guidelines to serve as a framework to follow for those working with and cleaning fossil occurrence data. Some 687 of these guidelines may or may not be relevant for individual projects, and they may not always be easy to 688 implement. However, we posit that each rule that can be followed will ultimately provide a clearer 689 understanding of the decisions made to process a dataset prior to analysis. This is an essential step to improve 690 the reproducibility of research; a necessary goal in the face of a broader reproducibility crisis within science 691 (Fidler *et al.* 2017). We hope that, in following these rules, we as a community can produce datasets that not 692 only benefit our own work in the present, but can assist future researchers for many years to come by providing 693 clear and consistent explanations for how we have carried out our work.

694 DATA ACCESSIBILITY

The data and code generated for this article have been included within a dedicated GitHub repository:
 https://github.com/palaeoverse/ten-rules. In addition, they have been uploaded to a Zenodo repository through
 integrated version control: https://doi.org/10.5281/zenodo.14938533.

698 AUTHORS' CONTRIBUTIONS

L.A.J. conceived the project; all authors contributed to the development of the project; all authors contributed
to the writing of the manuscript; C.D.D., H.B.D., and L.A.J. edited the manuscript with contributions from all
authors; B.M.F., J.S., and P.G. produced the manuscript figure; A.A.C., B.J.A, E.M.D., and W.G. produced
the vignette. All authors approved the final version of the manuscript.

703 COMPETING INTERESTS

704 We declare we have no competing interests.

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