Promoting analysis reproducibility with accessibility: An example in evolutionary biology

Abstract

Reproducibility is essential for scientific development. Efforts to increase scientific reproducibility have focused on increasing availability of code and data. However, availability does not imply accessibility, and the latter is infrequently addressed, even if it is key to achieve full workflow automatization and reproducibility. Using an example in evolutionary biology, we identify factors that have specifically affected accessibility in the natural sciences, and ways researchers can address this to ensure reproducible and automatic workflows. The Open Tree of Life project (OpenTree) has developed a platform that facilitates availability of results from evolutionary biology research. However, baseline computational knowledge and skills required to access scientific results are often not found among target users. While documentation is available, it is often written using highly specialized language that is also inaccessible for the average target user. We identified a set of principles to improve accessibility of OpenTree scientific data, implement them in a tutorial, and elaborate on their general application to code and documentation of scientific workflows.

Keywords: open science, education, R, phylogenetics, tutorials

Introduction

Reproducibility –the extent to which consistent results are obtained when a scientific research experiment is repeated (Curating for Reproducibility Consortium (2021))– is a key aspect for the advancement of science, as it constitutes a minimum standard that allows understanding scientific products (methods, analysis, results), to determine their reliability and generality, and eventually build up scientific knowledge and applications based on those products (King (1995), Peng (2011), Powers & Hampton (2019)). In the natural sciences, rates of reproducibility are low (Ioannidis (2005), Prinz et al. (2011)), prompting concerns about a reproducibility crisis in the field (Baker (2016)). In response, the scientific community has been generating standards and incentivizing cultural changes in an effort to improve reproducibility rates long term (Peng (2015), Wilkinson et al. (2016)). One standard that has received much attention is scientific availability, which we define as the property of research objects to be acquired, copied, analyzed, processed and/or reused, at no financial, legal or technical cost (Arnold et al. (2019)), and with no geographic, demographic or temporal barriers (Fecher & Friesike (2014)). In this paper, we argue that availability can not be fully achieved without accessibility (Box 1) We identify factors that have particularly affected accessibility in the natural sciences, and ways researchers can address them to ensure reproducible and automatic scientific workflows.

Box 1. The role of accessibility to achieve full availability. Availability is generally defined as the ability or potential of something to be used and accessed (”Availability”, (2022)). Following this definition, accessibility is generally considered a synonym of availability. Yet, in practice, availability does not imply accessibility. One example we find really useful to practically differentiate the concepts of availability and accessibility is the ”marshmallows in an office” story, which goes like this. A couple of brand new marshmallow bags remained in a common office area after a social gathering. The marshmallows were not claimed by anybody, so they were left in the common are, freely available to be taken or eaten by anyone in the office. Yet, the marshmallow bags stayed in the common area, unopened for days and even weeks. It was not until someone decided to open the bags and placed the marshmallows on a tray, that people started actually eating them. They were gone in a matter of hours. Scientific products are not sweet as marshmallows, but they are a coveted resource. While sharing, describing and documenting makes scientific products available, it does not necessarily makes them accessible. For example, documentation of an available scientific workflow might be written using expert language that is too foreign for a general audience to successfully reproduce the workflow. While some individuals might be able to invest the time to learn the expert language to successfully reproduce the workflow, this will not be the case for the majority, even if it is something that would be useful long term, the short term time investment is often too high for individuals to engage with it, making the workflow and its results effectively inaccessible and hence unavailable to the majority of the community.

To elaborate on our thesis, we use an example in evolutionary biology that focuses on understanding the shared ancestry of organisms through phylogenetic trees, which provide the basis to study and understand biological processes in an evolutionary context (Dobzhansky (1973)). As such, improving reproducibility rates in phylogenetic research is relevant for many aspects of biological research. The Open Tree of Life project (OpenTree) has developed a computational platform that provides availability of results from phylogenetic research, by creating a standardized database of phylogenetic data that is used to synthesize a single phylogenetic tree encompassing all life (OpenTreeOfLife et al. (2019)). The OpenTree database Phylesystem () is open access and available programmatically through its many Application Programming Interface (API) services (OpenTreeOfLife et al. (2021)). Additionally, R packages (Michonneau et al. (2016)) and Python libraries (Mctavish et al. (2021)) have been developed as wrappers for OpenTree API services to make them available to a wider programming audience. The R and Python OpenTree wrappers have been utilized by computer-literate individuals, to seamlessly establish reproducible workflows to use and reuse expert phylogenetic knowledge for biological research (Sánchez-Reyes & O'Meara (2019)) and education (Nguyen et al. (2020), Jodie Wiggins and Phylotastic Team (2021), Matt Wilkins and Galactic Polymath (2021)).

The OpenTree project demonstrates that efforts to increase availability for reproducibility in phylogenetics have also increased baseline computational knowledge and skills required in the field. "Computers are playing an increasingly important role in many scientific disciplines" (Piccolo & Frampton (2016)). Baseline computational skill requirements are increasing across all natural sciences. Yet, computing is not traditionally a core skill taught to biologists and naturalists (Sayres et al. (2018), Wright et al. (2019), Williams et al. (2019)). Still, many students are now being trained in R programming language as a statistics and data analysis environment. In order for reproducible computational tools to be adopted for research, they need to be much more accessible for present and future researchers. Data and code availability is a core requirement for reproducibility research (Peng (2011), Sandve et al. (2013), Powers & Hampton (2019)). However, the utility of data resources is limited by the technical challenges of accessing the data. In order to motivate reproducible research, that gap needs to be bridged. In this work we focus on improving accessibility of code examples and documentation. In particular, we identify the necessity for documentation that is written down using language that is common to the target audience to facilitate examination, application, and adoption of code by the wider audience.

We present a set of principles to generate documentation that improves accessibility of code and documentation. We applied these principles to a series of tutorials and vignettes developed for the OpenTree project.

Identifying hurdles to accessibility

Good primary documentation for code describes general usage of individual functions, the components and variables a function can take, and it should be accompanied with function usage examples on how to apply it. As opposed to code, primary documentation is written in natural language (i.e., any known human language, e.g., English, Spanish, Chinese) and usually makes use of highly specialized computational jargon (computationally specific concepts, words, and phrases) as well as formal language, which often slows down or even obstructs examination, application, and adoption of code by external individuals. Because primary documentation is considered a professional document, acceptance of the research by the scientific community could diminish if a more informal language is used. Vignettes and tutorials work as secondary pieces of documentation, that help to demonstrate additional cases of individual function usage, and showcase function associations that work for specific analysis workflows in more detail. As secondary documentation has become more common practice, we identify and propose a series of principles to support improved accessibility for secondary documentation.

Addressing hurdles to accessibility: some principles

a. Literate programming: Demonstrate code usage with integrative examples

Programming languages are abstract and usually hard to remember without an obvious link to an application (Knuth (1984)). A story or narrative that links pieces of code together can greatly support users/students to remember the code and its usage. The "literate programming" paradigm (**?**knuth1984literate)) integrates narratives with computer code in the same document, to support users in following the code usage, improving reproducibility of scientific analyses (**?**piccolo2016tools)).

We examined available primary documentation for the OpenTree API R wrapper (the package 'rotl'), and designed a workflow that visits as many functions as possible, and demonstrate uses commonly requested by OpenTree users that are not demonstrated elsewhere. By framing the function workflow using highly requested uses, the documentation acquires a narrative arc that is easier to follow and remember by users. This facilitates the translation of functions to specific use cases in biology.

For the tutorial demonstrated here, we used the commonly requested use case of obtaining a phylogenetic tree for all lineages within a specific taxonomic rank.

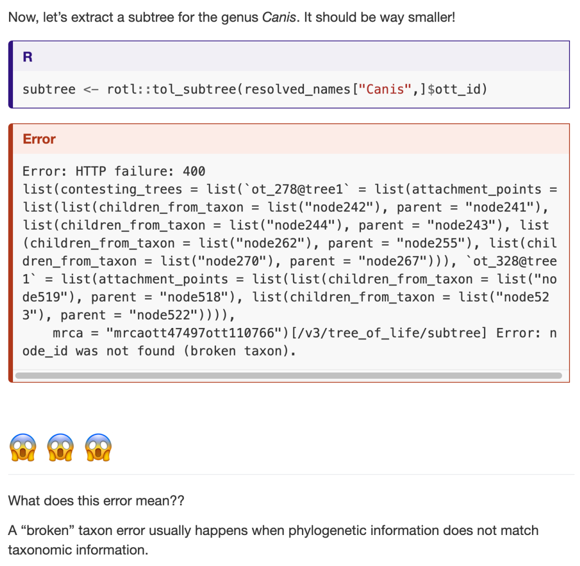
b. Demonstrate errors and warnings thoroughly

A practice that has become more and more widespread in programming languages pedagogical practices is the use of typos and mistakes to normalize them for learners and show them how to solve them when they are outside the classroom (Shannon & Summet (2015)). Yet, this is rarely done for written pedagogical materials. Primary documentation focuses on demonstrating usage function with examples that work seamlessly, without errors. We argue that the opposite is needed to support adoption of reproducible workflows and support long term independence in learners (Gaspar & Langevin (2007)). We demonstrate examples that do not work as expected and exemplify ways to address them (Figure 1).

We identify inputs that would give a wide range of warnings and errors, focusing on demonstrating these cases. This helps users to not be afraid of errors and warnings, but instead to use them to their advantage. We also identify effects of warnings and errors downstream of the workflow.

We identify ways to evaluate inputs to know if they will produce an error, and design alternatives on what to do when faced with an error or warning, and demonstrate these alternatives. One of the most essential skills in programming is interpreting and moving forward from errors. Many finely honed tutorials do not trigger errors, which precludes helping students to develop the tools to understand and address errors when they do encounter them, as they inevitably will. On our tutorial, we focus on explaining the meaning and downstream of warnings and errors, and showcase ways to detect them before they are triggered (i.e., before using an input that would elicit a warning or error). This has two pedagogical benefits: 1) it provides users/students with the means to troubleshoot their own warnings and erros, and 2) it allows users/students to understand with more depth what the function is doing.

We designed ways to access the different elements of the outputs.


Now, let's extract a subtree for the genus *Canis*. It should be way smaller!

R

```
subtree <- rotl::tol_subtree(resolved_names["Canis",]$ott_id)
```

Error

```
Error: HTTP failure: 400
list(contesting_trees = list(`ot_278@tree1` = list(attachment_points =
list(list(children_from_taxon = list("node242"), parent = "node241"),
list(children_from_taxon = list("node244"), parent = "node243"), list
(children_from_taxon = list("node262"), parent = "node255"), list(chil
dren_from_taxon = list("node270"), parent = "node267"))), `ot_328@tree
1` = list(attachment_points = list(list(children_from_taxon = list("no
de519"), parent = "node518"), list(children_from_taxon = list("node52
3"), parent = "node522")))),
    mrca = "mrcaott47497ott110766")[/v3/tree_of_life/subtree] Error: n
ode_id was not found (broken taxon).
```

😱 😱 😱

What does this error mean??

A "broken" taxon error usually happens when phylogenetic information does not match taxonomic information.

Figure 1: Snapshot of a section of the tutorial website, where we demonstrate a common error.

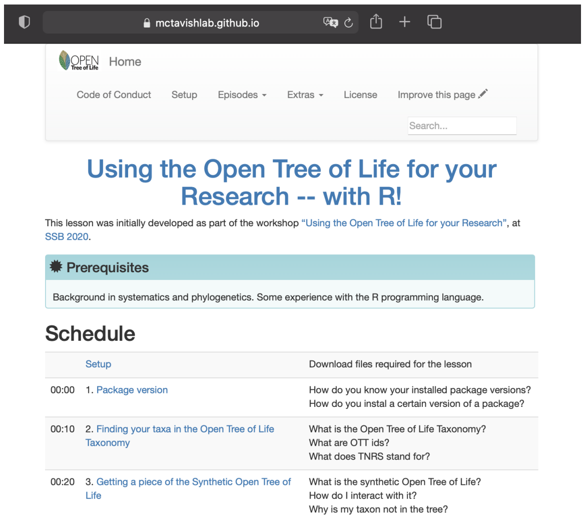
c. Avoid jargon and expert language

Besides avoiding formal language, and incorporating elements of pop culture, such as picture character icons known as ”emojis”, to make the language more familiar to a broader target audience (see Figure 1), we made an effort to specifically complement the primary documentation by identifying computational concepts that were assumed or were not explained in depth. We vetted the tutorials with an audience on workshops as well as individual user. We choose examples that are charismatic for the audience. For example, when we presented the tutorial for a team specialized in Amphibians, we tailored the examples using frogs and their allies.

d. Make it stable through time

We published the tutorials on a public, free license, free of cost, and free for use and reuse repository and persistent website (Sanchez-Reyes, Luna L and McTavish, Emily Jane and Holder, Mark T (2021*a*,*b*)). The tutorial is available for the users to go back to it any time they need it, and to be passed on to other users (Figure 2).

Following the carpentries, we created a main version of the tutorial that is updated.



Using the Open Tree of Life for your Research -- with R!

This lesson was initially developed as part of the workshop "Using the Open Tree of Life for your Research", at SSB 2020.

Prerequisites

Background in systematics and phylogenetics. Some experience with the R programming language.

Schedule

	Setup	Download files required for the lesson
00:00	1. Package version	How do you know your installed package versions? How do you instal a certain version of a package?
00:10	2. Finding your taxa in the Open Tree of Life Taxonomy	What is the Open Tree of Life Taxonomy? What are OTT ids? What does TNRS stand for?
00:20	3. Getting a piece of the Synthetic Open Tree of Life	What is the synthetic Open Tree of Life? How do I interact with it? Why is my taxon not in the tree?

Figure 2: Snapshot of the home to our tutorial website, showing part of the schedule.

Versions presented on workshops are a copy from the original repository, and represent a stable and temporal snapshot of the functions and workflows presented in the tutorial.

Conclusion

Ultimately, the improvement of reproducibility rates in science long term depends on our ability to intentionally integrate the subject of reproducibility in the the curriculum for college students and aspiring researchers to develop the skills necessary to create reproducible scientific workflows and materials.

Some universities have been incorporating the subject in their classes (see University of Washington and The National Institute for General Medical Sciences). The focus has been on students to develop skills to document their work. The principles identified and outlined here can be used to set learning goals and outcomes on new reproducibility syllabus.

We have received emails from senior researchers thanking us for this materials, and students have been able to engage using the packages with less hep from the PIs.

The principles to create tutorials described here facilitate adoption of software and analysis workflows among researchers at different academic levels, from undergrads to established researchers. It will also help closing the gap between students that had access to computational resources (and computational training) from an early age and students that did not. Late access to computational resources and training can occur due to lack of economic resources, often occurring in households from underrepresented communities and minorities. It can also be due to gender-biased parental and community pressures, in which male individuals are more often encouraged to perform activities related to computers, while female individuals are discouraged. These principles can be used to aide not only in improving reproducibility practices, but also software adoption in the natural sciences.

Making accessible reproducible workflows has several advantages: save explanation/training time when analyses are run again by students and collaborators. save research time for yourself when analyses are run again with more data, a different dataset, a different organism or biological model. scientific efforts can build off of each other

SUPPLEMENTARY MATERIAL

Title: Website and GitHub repository containing the complete teaching materials developed and demonstrated here.

GitHub repository link: `https://github.com/McTavishLab/R_OpenTree_tutorials`

Website link: `https://mctavishlab.github.io/R_OpenTree_tutorials`

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