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A review of computer tools for prediction of ecosystems and populations: We need more open-source software

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ABSTRACT

Computer programs have taken an important role in the prediction of future ecological trajectories. This study reviewed the existing computer programs that aim to predict future trajectories of ecosystems, biological populations, or ecological systems. Overall, 106 programs were examined. A rich set of programs exist and most of them are free. A substantial proportion (43%) are distributed open source. A majority (57%) of these programs took some form of uncertainty into account, although not always in a rigorous way. Programs considering uncertainty were preferentially implemented in a standard compiled language (C/Fortran) or a statistical language (R). The vast majority of the programs were delivered with recent, sometimes extensive, documentation. None of the reviewed programs used an open-source collaborative framework. Two points require future attention from developers of software for ecological prediction: greater care in the implementation of uncertainty, particularly with appropriate statistical methods, and adoption of an open-source, collaborative framework.

Keywords: biodiversity; ecosystem; forecasting; modelling; software

“Prediction is very difficult, especially about the future.”

(<https://quoteinvestigator.com/2013/10/20/no-predict/>)

1. Introduction

Computer programs and software systems have taken an increasingly important role in predicting the future trajectories of ecosystems and natural populations. The increasing impact of human activities on ecosystems has increased the need for predicting their consequences (positive or negative). In 2016, the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES) published a report on modelling and scenarios of biodiversity and ecosystem services stating, among other things, that “Scenarios and models can contribute significantly to policy support, even though several barriers have impeded their widespread use to date.” (IPBES, 2016, p. xii). However, a number of weaknesses in the use of models were pointed out in this report. For example, “Currently available scenarios [...] do not fully address the needs of Platform assessments due to incomplete consideration of relevant drivers, policy goals and intervention options [...]”. Another important point in this IPBES report relates to uncertainty of predictions: “Uncertainty associated with models is often poorly evaluated and reported in published studies, which may lead to serious misconceptions” (p. xxvi).

Computer simulations are a central part of assessing future responses of ecosystems or natural populations that face environmental changes (Botkin et al., 2007; Dawson et al., 2011; Bonnot et al., 2017; Dijak et al., 2017). Some specific applications of simulations include predicting future biodiversity responses to climate changes (Trisurat et al., 2010, 2014; Staudinger et al., 2013; Mantyka-Pringle et al., 2014; Baltensperger and Huettmann, 2015), mapping ecosystem services (Kong et al., 2018), life-cycle assessment (Chaplin-Kramer

et al., 2017), food security (Mason-D’Croz et al., 2016), or future land use (Lehsten et al., 2015; Requena-Mullor et al., 2017). Some attention has been paid on the development and validation of conceptual frameworks used to predict future trajectories of ecosystems (Drielsma et al., 2014; Oliver and Roy, 2015; Zasada et al., 2017b). However, it is not clear how “best practices” in the development and implementation of these computer programs can be enhanced to improve predictions as well as policy recommendations (Newman et al., 2017; Zasada et al., 2017a). For instance, IPBES (2016, p. 61) emphasized the lack of repeatability of approaches such as strategic environmental assessments. Clearly, computer programs have an important role to play here since uncertainty assessment is typically based on computer-intensive methods.

The rise of open source software and worldwide networks such as the Internet has been a formidable stimulus for the development and spread of computer resources. For instance, scientific fields such as bioinformatics have now adopted a “free and open source software” (FOSS) model for the publication of computer programs. Furthermore, the availability of freely distributed computer programs is a requirement for publication in journals such as *Bioinformatics*, *BMC Bioinformatics*, or *Methods in Ecology and Evolution*. FOSS is not only about the price of the computer programs, but also about portability, repeatability, and open knowledge (Wheeler, 2015).

The following definitions are used in this paper: an ‘ecological system’ is a set of interacting living entities that also interact with their environment which can itself be composed of living and/or non-living entities. An ‘ecosystem’ is an ecological system that is restricted to a geographically defined area (e.g., a lake, a forest). A ‘biological population’ is an ecological system whose entities are individuals belonging to the same species so their interactions are directed by some specific activities (e.g., mating, feeding). An ecological system is characterized by a number of variables (e.g., nutrients, species richness, number

of individuals, age structure). 'Prediction' aims at finding the predicted values of these variables in the future.

In this paper, I report the results of an investigation of the availability of computer programs aimed at predicting the future trajectories of ecosystems, ecological systems, or biological populations. The main objectives were firstly to provide a global picture of the "software ecosystem" (Manikas, 2016) available for ecological prediction, and secondly to identify the issues that require attention to improve this 'ecosystem' following the statements from IPBES. Some suggestions on future directions are given at the end of this paper.

2. Methods

Computer programs aimed at prediction of ecosystems, ecological systems, or biological populations were searched using Internet search engines and the literature. The programs selected for further analysis were those available for download or purchase. The programs available for purchase were considered to answer some of the questions below but were not purchased. All the investigated programs were downloaded and checked for some features. Programs were selected on the basis that they provide tools, models, or approaches that can be directly related to prediction of ecosystems, populations, or other ecological systems. Programs dedicated to human health or epidemiology were excluded.

Specifically, the following questions were addressed for each program:

1. What is (are) the computer language(s) used to implement the program?
2. Is the program freely distributed?
3. Is the source code of the program available?
4. What operating systems (OSs) are supported?

5. What is the main output file format?
6. Is it a specialist or a generalist program?
7. Does the program consider uncertainty?
8. Is a manual available? If yes, how many pages?
9. Is there a support for users?
10. Is there a mailing/discussion list?

These questions were defined before investigating the programs; however, the way they were addressed was adjusted during the study. Considering the large number of programs found that meet the above criteria, it was not practically possible to run and test all of them. The answers to questions 1 and 3–7 were searched by reading the documentation or the general presentation of the program (e.g., section “About” of a web page). Questions 2 and 8–10 were answered by looking at the web pages of the program. Further information to answer questions 1, 3, and 8 were found by inspecting the downloaded programs. Questions 2 and 3 are not independent and are related to the distribution licence of the programs. However, the licence under which a computer program is distributed is a complex issue as illustrated by the many existing free licences (e.g., https://en.wikipedia.org/wiki/Free_and_open-source_software). Furthermore, a program can be published under several licences or its licencing status can change through time (e.g., <https://www.r-project.org/Licenses/>). Although this is clearly an important issue, it was out of the scope of the present study which considered only the availability of source code. Questions 3 and 4 were connected since some programs are distributed simply as source code and not as compiled executables for one or several specific OSs, so ‘source code’ was a separate

category when answering question 4. In order to be more specific, if any form of source or computer code was available, then the program was considered as 'open source' (question 3), whereas if a program was packaged only with its source code, then it was considered as 'source code' (question 4). Thus, a program could be 'open source' while not being distributed as 'source code' (whereas a program classified as 'source code' is necessarily 'open source'). The distinction between these two categories stems from the fact 'source code' programs are often independent of the OS. In order to answer question 6, the programs that model a specific system (e.g., diffusion of pollutants) or consider a specific geographical area were classified as specialist. Programs that consider or model a system which can be considered generic (e.g., a biological population, a watershed) were classified as generalist. Question 6 stems from the importance of being able to use the outputs of a program for further downstream analyses with other program(s), for instance, for uncertainty assessment, or graphical display. Question 7 was answered 'Yes' if the documentation mentioned uncertainty explicitly, or the approach described in the documentation was probabilistic.

All data analyses and graphics presented below were done with R version 3.6.0 (R Core Team, 2019); the R code is available in the Supplementary Information.

3. Results

A large number of Web pages and resources were found. A substantial number of programs were described "in development" or "coming soon". Other programs were listed on some Web pages but could not be located or downloaded. These "orphaned" or "lost" programs were not counted precisely. In the end of the search, 106 computer programs were found and examined (Table S1).

The majority of the programs selected for this study (59 or 56%) were distributed by a US federal agency (main domain of the web site URL ending with .gov, .mil, or .us). These included 24 programs by the Environmental Protection Agency (EPA), 15 by the US Forest Service (USFS), 11 by the US Army Corps of Engineers (USACE), three by the US Department of Agriculture (USDA), and three by the US Geological Service (USGS). Almost all programs were distributed on dedicated web pages: only two were distributed on GitHub and two others on R-Forge.

One hundred and two programs (96%) were available free, some of them after registration, three were available as commercial products, and one was available as a free demo version.

For 34 programs (32%), it was not possible to find the computer programming language or platform used for implementation. For 24 programs (23%), a standard compiled language C or Fortran (or one of their variants or dialects: F77, F90, C++, or C#) was used (Fig. 1). Eleven programs were implemented in Excel, six in R, six in Python, six as ArGIS modules, four in Java, one in Julia, and one in Delphi. Six programs were modules of commercial programs (e.g., SAS, Matlab). Finally, seven programs were available as Web forms through Internet and not available for download.

Forty-six programs (43%) were available as open-source, 33 (31%) were distributed only as compiled applications and their sources were not available, one was available as open-source subject to collaboration, and four were commercially distributed. The open-source status of the remaining 22 programs (21%) could not be determined (Fig. 2).

For the analysis of OSs, the programs coded in Excel or in Java were considered as source code because a wide range of office applications can run Excel spreadsheets on most OSs, and there are many Java environments on most OSs as well. The vast majority of programs were available as applications

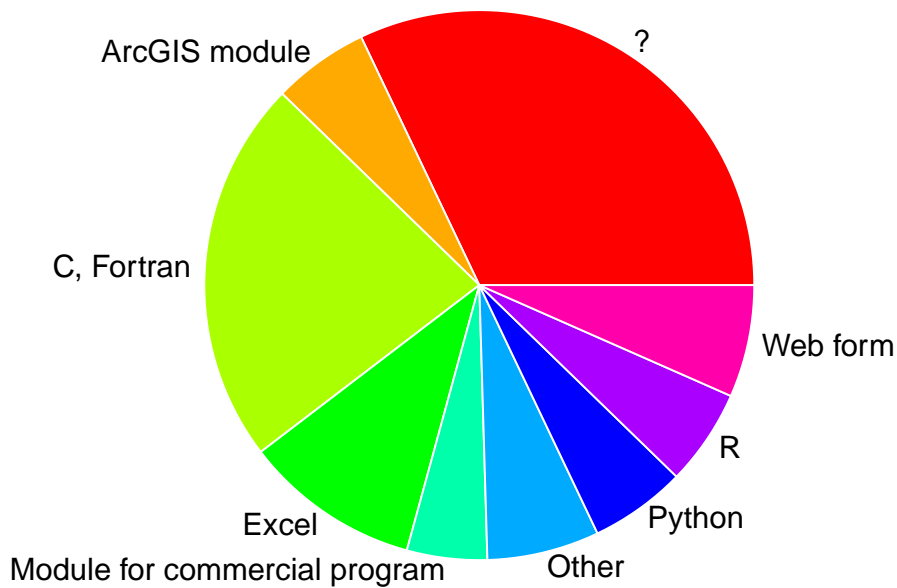


Figure 1: Frequencies of computer language implementation of 106 computer programs for ecosystem prediction.

running under Windows (73 or 69%), or even only for this OS (55 or 52%; Fig. 3). Twenty-nine (27%) programs were distributed as source-code, and exclusively in this form for 22 of them (mainly as Excel code and secondarily as R programs which are OS-independent). Only one program was available only for Linux, and none of them were distributed as MacOS application. Additionally, one program run under 16-bit MS-DOS, and the running OS of two programs was not found.

A majority of programs (47 or 44%) output their results as text files, either only (37 or 35%) or in association with other formats (GIS or HDF5; Fig. 4). Six programs output their results in various file formats (labelled as “many” on Fig. 4). Seventeen programs (16%) did not output files, 13 output Excel files, and two output results in files that cannot be interfaced with other software (PDF reports or private format). Finally, the output format could not be determined for 13 programs (12%).

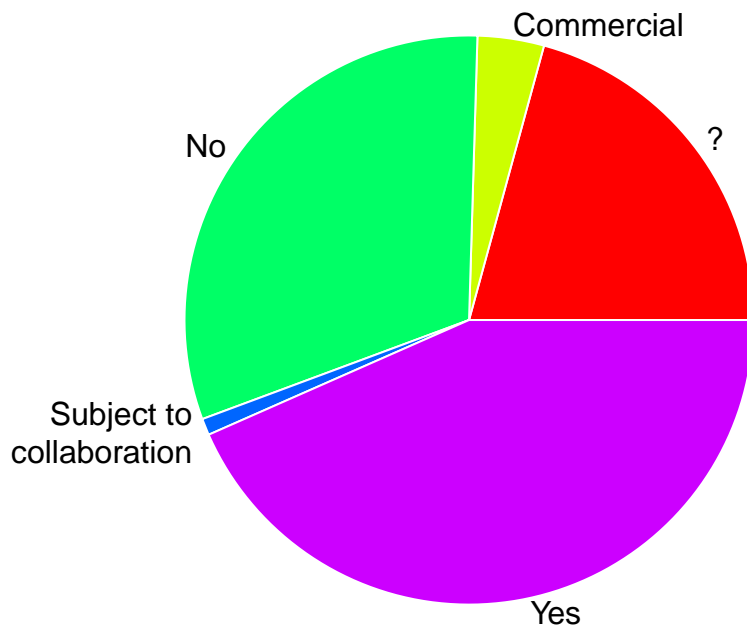


Figure 2: Frequencies of open-source features of 106 computer programs for ecosystem prediction.

The vast majority of the programs (71 or 67%) were specialist. There seemed to be an association between this variable and the programming language used: programs coded in Excel or as Web forms were all specialist, whereas the generalist ones were more represented among the programs implements in C/Fortran, R, or under a commercial platform (Fig. 5). No association with other variables were apparent.

Uncertainty was a feature in 60 (57%) programs, while this could not be found in six of the 106 (6%). There was a very significant association between this variable and whether a program is specialist or generalist: among the 35 generalist programs, 30 took uncertainty into account, whereas 30 specialist programs did out of 71 (Fisher's exact test: $P < 0.0001$; this test excluded the six programs where handling of uncertainty was unknown). There was also an association with the programming language: programs taking uncertainty into

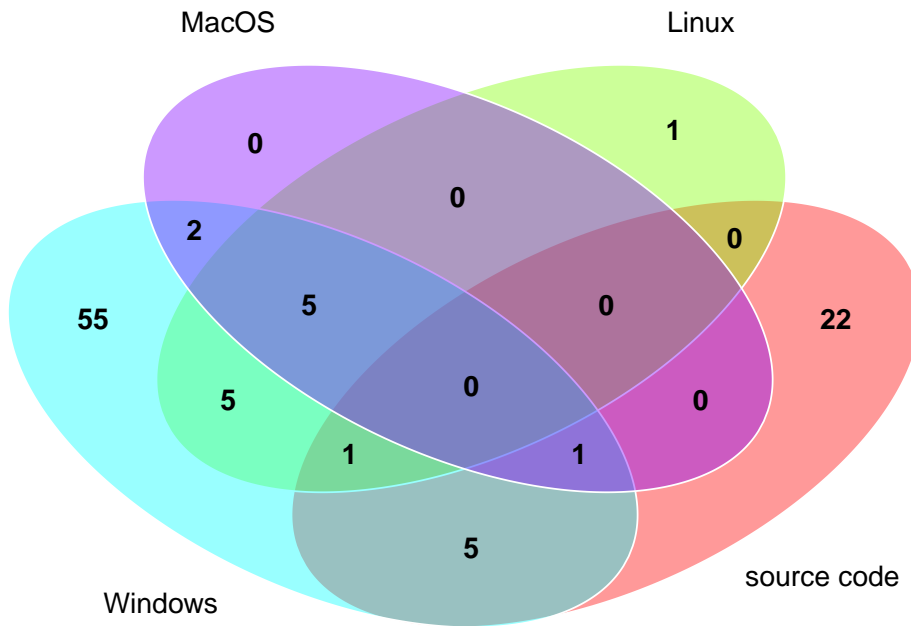


Figure 3: Venn diagram of the supported operating systems for 96 programs (the ten excluded programs from this diagram are: seven Web forms, one MS-DOS program, and two with unknown OS).

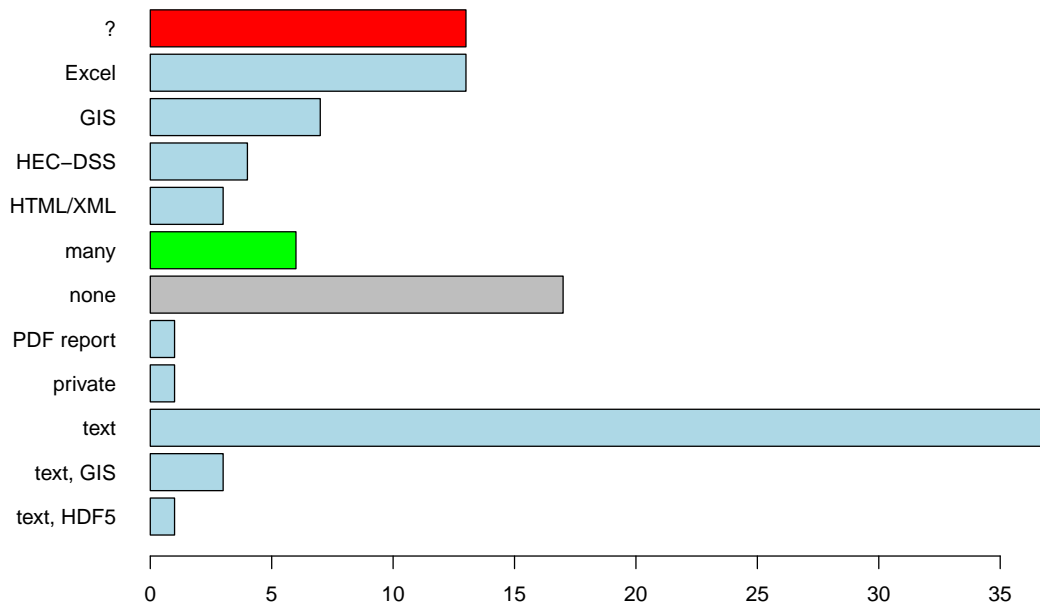


Figure 4: Formats of the output files.

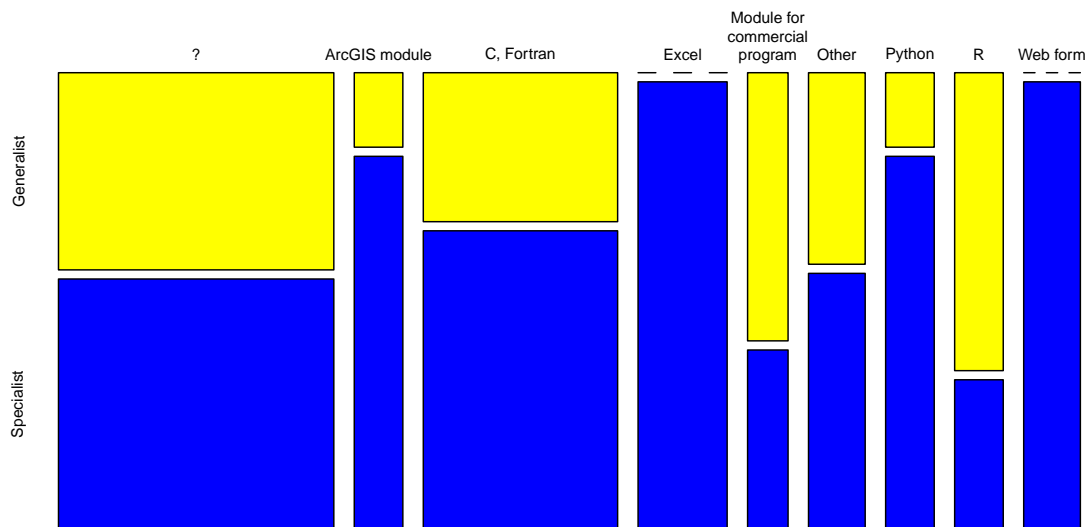


Figure 5: Mosaic plot of the contingency between whether a program is specialist or generalist and its programming language implementation. The widths of the rectangles are proportional to the frequencies of the different categories.

account were implemented in C/Fortran, R (all four of them) or with commercial programs (also all four of them; Fig. 6). On the other hand, programs in Python, Excel, or available as Web forms did not mostly consider uncertainty.

A manual in PDF format was available for 71 programs (67%), in HTML for 18 (17%), as an on-line wiki for three, and no manual or documentation was found for 12 of them (11%; Fig. 7). The mean number of pages of the manuals in PDF format was 234 (SD = 346, median = 104, min = 6, max = 2262). Most of the available documentation was recent: 55 (52%) were dated after January 1, 2016, and six were produced in 2020 (Fig. 8). The oldest manual was dated September 1994, and six manuals were dated before 2001.

Support to users was offered on the Web pages for 76 (72%) of the programs, non-free support was proposed for one program, and no apparent support was observed for the remaining 29 programs. A mailing list was found for 20 programs (19%). There was no apparent association between these two variables and the previously analysed ones.

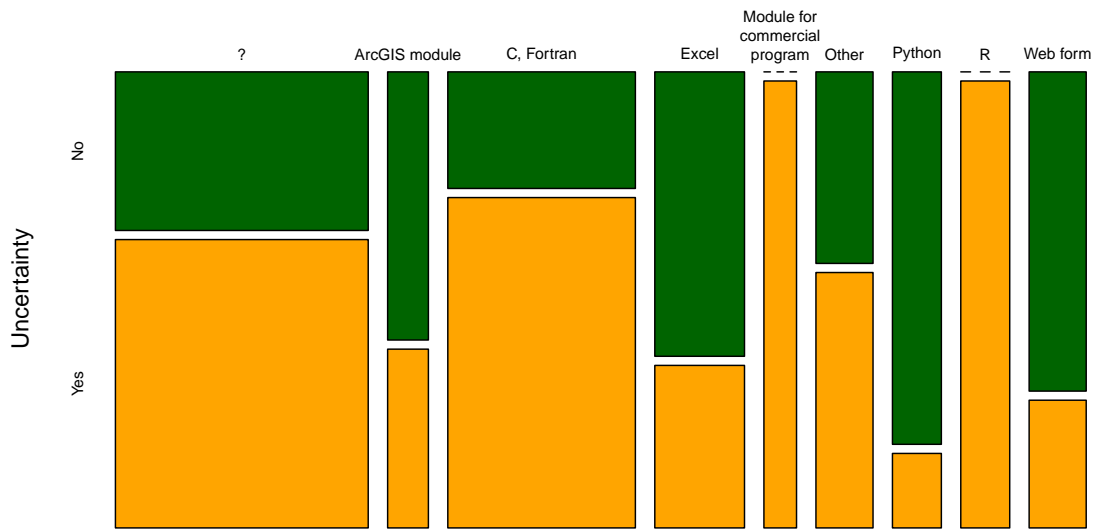


Figure 6: Mosaic plot of the contingency between whether a program considers uncertainty and its programming language implementation. The widths of the rectangles are proportional to the frequencies of the different categories.

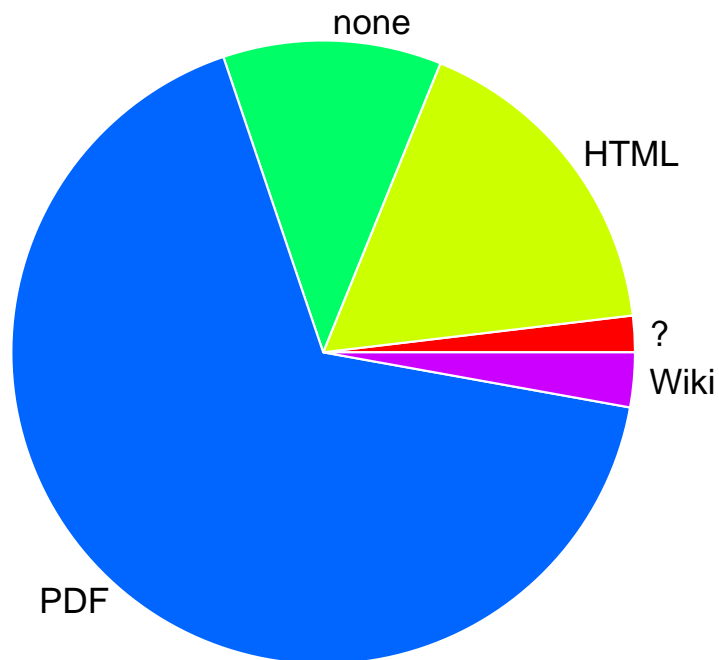


Figure 7: Frequencies of the format of the documentation associated with 106 computer programs for ecosystem prediction.

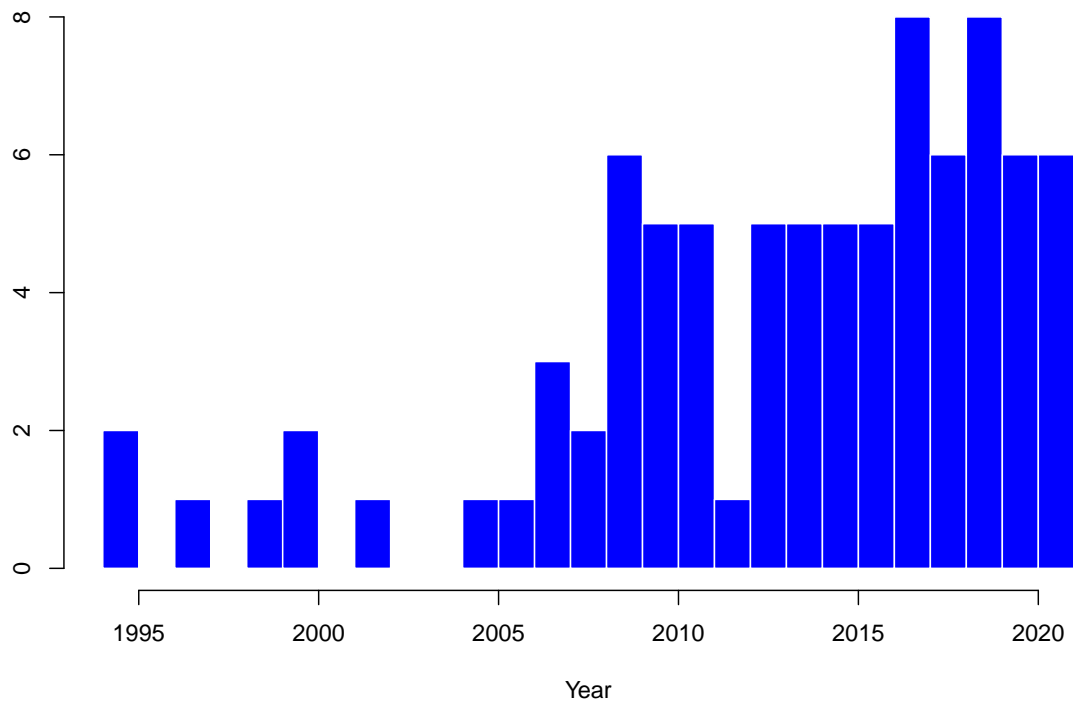


Figure 8: Histogram of the dates of the manuals associated with 85 computer programs for ecosystem prediction.

4. Discussion

The present study leads to draw an overall positive picture of software for ecosystem prediction: a remarkable diversity of free programs are available, their associated documentations are generally of good quality (sometimes very extensive), and a good percentage (43%) are also distributed open-source.

Another significantly positive feature is that a majority of programs output their results in file formats which are easily read by other software, considering that Excel files can be open by many other programs (see for instance the R-package ‘readxl’; Wickham and Bryan, 2019).

Remarkably, US federal agencies took a major part of the programs considered here. This highlights several points. First, this emphasises the importance of public agencies in making available to the public the research work on ecosystems and biodiversity. Second, a substantial number of these programs were published before 2000, so that they constitute an important

archive for researchers and students. Even if the distributed programs are only available as executables running on “vintage” OS, the associated documentation, often containing the model description, details on the algorithms, and references to the literature, is a very useful source of information. Third, most of these programs are distributed as Windows executables which explain, at least partly, the predominance of this OS.

Uncertainty was considered in a majority of programs (57%). Unfortunately, it was not possible to assess for the present study whether uncertainty is correctly implemented in these programs. For instance, some manuals state that uncertainty can be taken into account by changing the input parameters of the program. This is a crude approach which could be useful in some situations (e.g., if the predictions are not changed substantially by the different input parameter values) but that could lead to difficulties in interpreting the results if the predictions differ with respect to the input parameter values. A more rigorous approach would be to weigh the outputs by the likelihood of the input values. There is a vast literature on this topic, especially oriented towards the use of Bayesian methods (Hoeting et al., 1999; Clyde and George, 2004). Uncertainty is a difficult topic that often requires computationally intensive methods and/or sophisticated statistical techniques (Draper, 1995; Evans and Swartz, 1995; Efron and Hastie, 2016). Even if some of these methods are complicated to implement, weighting outputs by the likelihood of the input values seems as a bare minimum to take uncertainty into account. From a practical point of view, it is important for programs to include the possibility to save their outputs in a format which can be read and write by the vast majority of software (typically text). Parallel computing will also certainly attract more attention in the future in order to implement such intensive computing tasks. Interestingly, parallel programming is available in the major languages observed in this study (C, C++, Fortran, R, Python).

It is interesting to note that the programs considering uncertainty were preferentially implemented in compiled languages (C/Fortran) or in a statistical language (R). This highlights the need to use a performing computer language to implement uncertainty. Moreover, these languages are widely used, free, and efficient implementations (e.g., the GCC compilers) are available to all users. It appears therefore that considering uncertainty in a program devoted to ecosystem prediction has several beneficial effects: it not only increases its usefulness and relevance for prediction but it also increases its likelihood to use an efficient, open source implementation.

Open source is not yet a prominent feature of software for ecosystem prediction. However, the above observations are encouraging: the programs that take uncertainty into account are more likely to be implemented in a language commonly associated with open source. Interestingly, a number of programs (7) distributed for Windows are also available as source code. This emphasises that open source is independent of the OS. On the other hand, the software for ecosystem prediction clearly lag behind other scientific fields in terms of code sharing: only two programs are currently distributed on GitHub, a platform for code sharing used by dozens of thousands of developers and currently hosting more than 100 million repositories. Quite illustrative of this symptom, none of the R packages reviewed here are distributed on the Comprehensive R Archive Network (CRAN) which is the standard Internet repository of R packages. The more than 15,000 packages currently on CRAN are checked daily to ensure that they can be installed and run correctly on most common operating systems (currently: Linux, Windows, MacOS X, and Solaris). It is regrettable that the computer programs for ecosystem prediction do not currently benefit of this free service.

Open source is not only about the price of the software, it also makes possible to develop code in a more transparent and efficient manner with two

major side-effects: scalability and integration. The latter feature is of particular importance for ecosystem prediction. Indeed, predicting future ecosystem trajectories, or some of its characteristics such as ecosystem services, often requires the integration of different components (Titeux et al., 2016; Di Minin et al., 2017). Open software makes integration of different components much easier than closed systems (Wheeler, 2015). In this perspective, the integration of spatial data, for instance land use and land cover data, is a predominant feature or many studies attempting to predict changes in ecosystems or biodiversity (Titeux et al., 2016; Bonnot et al., 2017; Chaplin-Kramer et al., 2017).

Newman et al. (2017) reviewed 101 papers on decision support systems and found that most effort has been placed on assessing areas of risk and economic consequences of direct losses, whereas less effort has been placed on assessing risk-reduction options. These authors listed a series of recommendations for future research. Although, they did not mention explicitly the development of better software, this is clearly an area that deserves to be considered as carefully as others. As rightly stated by these authors, impacts of natural hazards are likely to increase significantly in the future, so that more rigorous predictions of environmental changes are becoming more and more crucial.

Zasada et al. (2017b) performed a review of 60 European projects aiming at developing decision support systems, and found that 88% of them were available after two years and only 61% after eight years. Furthermore, only 50% of these tools are being updated after the end of the project. Interestingly, only a small portion of these tools (3.4%) were available as downloadable programs, and a minority (31%) were integrated with other tools. No mention of either “source code” or “open source” is made in this study.

5. Conclusion and Recommendations

The present study agrees with some statements from IPBES, notably: “There are large gaps in the availability of data for constructing and testing scenarios and models, and significant barriers to data sharing remain.” (IPBES, 2016, p. xxvii). Such statements clearly call for significant improvements of the ‘software ecosystem’ for ecosystem prediction. In addition to the recommendations from IPBES, I wish to formulate a few recommendations.

1. Open source: this feature is coming into wider acceptance in many scientific fields, including ecosystem prediction. However, open source should be considered in the wider context of portability so that software can be installed and run on as many computing platforms as possible. In this perspective, the computer languages R, C, and Fortran (and the dialects of these last two) appear as best choices to implement software for ecosystem and biodiversity prediction. There are free implementations for all common OSs of these languages. Furthermore, they make possible high-performance computing, and there already exist a wide range of tools in these languages to handle the data commonly encountered in ecosystem modelling (see for instance the package `rgdal` for reading GIS data in a wide range of formats Bivand et al., 2018).
2. Uncertainty: there is need to have more rigorous implementation of uncertainty in ecosystem predictive modelling. The statement that “different input parameter values” can be tested is not generally a valid approach, and should be avoided. Statistical techniques such as weighted integration should be considered more widely.
3. Output file formats: greater care should be taken on output formats. Even if using the standard text output files, a number of difficulties may be encountered, typically related to encoding, text layout, or file sizes. For

GIS data, an open binary format (e.g., GeoTIFF or netCDF for more complex data structures) should be preferred to simple text files.

The main criterion for guiding decisions in an open-source software development project should always be quality over quantity. Releasing a lot of computer code that it is not operational, that has not been tested or documented is very likely to be a waste of resources.

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Supplementary Information

Table S1: URLs of the 106 programs.

database.csv: database of the 106 computer programs.

script.R: R code used for data analyses and graphics.

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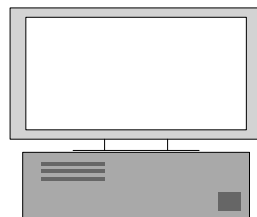
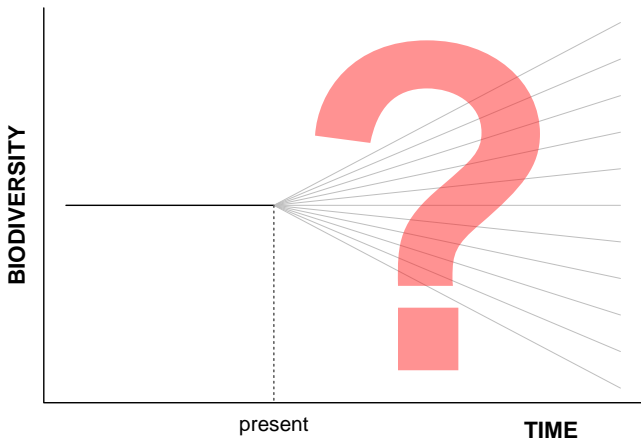
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