Synthetic datasets for global ecology in a data-rich world

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work in progress

- 4 Ecologists are tasked with providing information on issues at the global scale. Notable examples include, in addition to the
- 5 global biodiversity crisis (???), predicting the consequences of the loss of trophic structure Estes et al. (2011), rapid shifts
- 6 in species distributions (???), and . Most of these pressing topics require to be addressed (i) at the global scale and (ii)
- through the integration of several types of data (Thuiller et al. 2013). Because of these requirements, new sampling is not a
- viable solution: there is no funding structure to finance it, and there are time and scale constraints involved that make it
- 9 unrealistic.
- Thankfully, developments in the recent years means that ecologists can now leverage existing data, and use them to build
- new datasets (henceforth synthetic datasets) suitable for the questions at hand. There are several parallel advances that
- make this approach possible. First, the volume of data on ecological systems that are available *openly* increases on a daily
- basis. This includes point-occurence data, as in e.g. GBIF, ITIS, but also taxonomic knowledge (through NCBI or EOL),
- and trait and interactions data. A vast treasure trove of ecological information is now available without having to contact
- and secure authorization from every contributor individually. Second, this data is available in a *programmatic* way. As
- opposed to manual collection, identification, and curation of datasets, most of these services implement web API that allow
- to query them, either once or on a regular basis, to retrieve records with the desired properties. This ensures that the process
- is repeatable, testable, transparent, and error-proof. Finally, most of the heavy-lifting for these tasks can be done through a
- burgeoning ecosystem of packages and software, that take care of handling query formatting, data retrieval, etc., and expose
- 20 simple interfaces to researchers.
- 21 To us, this opens no less than a new area of research for ecologists interested in asking questions at large spatial and
- organizational scales we live in a data-rich world, and a very large amount of these data can now easily be collected,
- 23 reducing the need for additional costly and time-consuming sampling. More importantly, this allows rapid evaluation of
- scenarios. In this contribution, building on a real-life example, we (i) outline the basic approach, (ii) identify technical
- bottlenecks, (iii) discuss ethical considerations, and (iv) provide clear recommendations moving forward.

26 An illustrative case-study

- Food-web data, that is the determination of trophic interactions among species, are difficult to collect. The usual approach
- is to assemble literature data, expert knowledge, and additional information coming from field work, either as observation
- 29 of direct feeding events, or through the analysis of gut content. Because of these technical constraints, food-web data are
- most often assembled in a single location. This impedes our ability to address the variation of their structure in space,
- which may both translate the action of macro-ecological mechanisms, as well as hold key to our ability to predict the spatial
- variation of ecological properties.
- In this case study, we are interested in predicting the structure of the pine-marsh food web worldwide. One example of this
- system has been described in detail by (???). We will show how coupling these data with additional interactions reported
- in the literature, as well as species occurrence data, allows building a predictive model that describes the spatial variation of
- 36 this system.

7 Interactions data

- Data from the pine-marsh food web were take from **REF**, as made available in the IWDB database (URL). Marshes, as
- almost all wetlands, are critically endangered and home to a host of endemic biodiversity (Fensham et al. 2011; Minckley,
- Turner, and Weinstein 2013). They represent a prime example of ecosystems for which data-based prediction can be used
- 41 to generate scenarios at a temporal scale relevant for conservation decisions, and faster than what sampling could allow.
- The original food web (105 nodes, including vague denominations like *Unidentified detritus* or *Terrestrial invertebrates*),
- were cleaned in the following way. First, all nodes were aggregated to the genus level. Due to high level of structure in
- 44 trophic interactions emerging from taxonomic rank alone (Eklof et al. 2011), aggregating to the genus level has the double
- 45 advantage of (i) removing ambiguities on the identification of species and (ii) allowing to integrate data when any two
- 46 species from given genera interact. Second, all nodes that were not identified (Unidentified or Unknown in the original
- data). The cleaned network documented 227 interactions, between 80 genera. Using the name checking functions from the
- taxize package (S. A. Chamberlain and Szöcs 2013) revealed that all of these genus names were valid.
- ⁴⁹ Because the original foodweb was sampled *locally*, there is the possibility that interactions between genera are not reported.
- 50 To circumvent this, we queried the GLOBI database (Poelen, Simons, and Mungall 2014) for each genus name, and
- retrieved all *feeding* interactions. For all *new* genera retrieved through this method, we retrieved their interactions with
- 52 genera already in the network. This network has 789 genera, and a total of 9328 interactions.

53 Occurrence data and filtering

- For each genera, we downloaded the known occurrences from GBIF and BISON. This yielded 64763 point-presence records. Because the goal is, ultimately, to do spatial modeling of the structure of the network, we removed genera for which less than 100 occurrences were known. This seems like a stringent filter, yet it enables to (i) maintain sufficient predictive powers for SDMs, and (ii) only work on the genera for which we have "high-quality" data. Genera with less than 100 records were removed from the occurrence data and from the metanetwork. The final metanetwork has 4271 interactions between 188 genera. Given the curated publicly available data, it represents the current best description of feeding interactions between species of this ecosystem. A visual depiction of the network is given in *Fig. 1*.
- In itself, the fact that filtering for genera with over 100 records reduced the sample size from 739 genera to 188 indicates how crucial it is that observations are reported in public databases. The type of analysis we present here, although cost-effective and enabling rapid evaluation of different scenarios, is only as good as the underlying data. Since most modelling tools require a minimal sample size in order to achieve acceptable accuracy, a concerted efforts by the community and funding agencies to ensure that the minimal amount of data is deposited upon publication or acquisition is needed.

Species Distribution Model

For each species in this subset of data, we retrieved the nineteen bioclim variables (Hijmans et al. 2005), with a resolution of 5 arc-minutes. This enabled us to build climatic envelope models for each species; these models tend to be more conservative than alternate modeling strategies, in that they predict smaller range sizes (Hijmans and Graham 2006), but perform well overall on presence-only data (Elith et al. 2006). The output of these models is, for species i, the probability of an observation P(i) within each pixel. We appreciate that this is a coarse analysis, but its purpose is only to highlight how the different data can be combined. A discussion of the limitations of this approach is given below.

73 Assembly

For each of the 4271 interactions in the metanetwork, we measured the probability of it being observed in each pixel as being the joint probability of observing both species: $P(L_{ij}) \propto P(i)P(j)$. This resulted in 4271 LDMs ("link distribution models"). Based on these informations, we generated the following illustrations. First, a map of species richness (*Fig. 2A*) and number of interactions (*Fig. 2B*). Second, a map of *connectance* (*Fig. 2C*), which is the number of interactions divided by the squared species richness. Finally, a scatterplot of connectance as a function of latitude (*Fig. 2D*), which reveals a systematic macroecological trend. Interestingly, this last panel shows a strong response to this system to the fact that the tropics, in the Africa, are surrounded by desertic areas in which the species studied here are not predicted to occur given the climatic variables.

82 Opportunities

Hypothesis testing for large-scale systems is inherently limited by the availability of suitable datasets. Perhaps as a result,
macro-ecology has been guided by a search for patterns that are very broad both in scale and nature (???), as opposed to the
testing of pre-established hypothesis. While it is obvious that collecting data at scales that are large enough to be relevant is
an insurmountable effort (both because of the monetary, time, and human costs needed), we suggest that macroecologists
should build on existing databases, and aggregate them in a way that allows direct testing of proposals stemming from

89 Challenges

90 Attribution stacking and intellectual paternity:

The merging of large databases is already asking the question of proper attribution of data paternity. Namely, there are two core issues that need community consultation in order to be resolved. First, what is the proper mode of attribution when a very large volume of data is aggregated? Second, what should be the intellectual property of the synthetic dataset? Currently, citations (whether to articles or datasets) are only counted when they are part of the main text. This example relies on well over a thousand references, and it makes no sense to expect that these will be given in the main text. One intermediate solution would be to collate these references in a supplement, but it is unclear that these would be counted, and therefore contribute to the impact of each individual dataset. This is a problem that we think can only be solved by publishers; proper attribution and credit is key to provide incentives to data release. As citations is currently the currency of scientific impact, publishers have a responsibility not only to ensure that data are available (which many already do), but that they are recognized. The synthetic dataset, on the other, can reasonnably be understood as a novel product; there is technical and intellectual effort involved in producing it, and although it is a derivative work, we would encourage authors to deposit it anew.

103 Computational literacy:

This approach hardly qualifies as *big data*; nevertheless, it relies on the management and integration of a large volume of
heterogeneous information, both qualitatively larger than the current "norm". The first challenge is being able to *manage*this data; it requires data management skills that are not usually needed when the scale of the dataset is small, and (failible
though this process may be) data can reasonably be inspected manually. The second challenge is being able to *manipulate*these data; even within the context of this simple use-case, the data do not fit in the memory of R (arguably the most
commonly known and used software in ecology) without some adjustments. Once these issues were overcome, running the
analysis involved a few hours worth of computation time. It is now worth asking whether our total reliance on this tool

(as opposed to more performing yet equally user-friendly languages as python or julia) is going to pay off in the long term. Since it makes very little doubt that computational approaches are going to become increasingly common in ecology (Hampton et al. 2013), and are identified by the community as both in-demand skills and not receiving enough attention in current ecological curricula (Barraquand et al. 2014), it seems that efforts should be allocated to raise the computational literacy of ecologists, and recognize that there is value in the diversity of tools one can use to carry out more demanding studies.

Standards and best practices:

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In conducting this analysis, we noticed that a common issue was the identification of species and genera. All of these 118 datasets were deposited by people, and are prone to failure. Using tools such as taxize (S. A. Chamberlain and Szöcs 119 2013) allows to resolve a few of the uncertainties. Yet this has to be done every time the data are queried, and requires 120 the end user to make educated guesses as to what the "true" identity of the species is. These limitations can be overcome, on two conditions. Database maintainers should implement automated curation of the data they have the stewardship of, 122 and identify potential mistakes and correct them upstream, so that users download high-quality, high-reliability data. Data contributors should rely more extensively on biodiversity identifiers (such as TSN, GBIF, NCBI Taxonomy ID, ...), to 124 make sure that even when there are typos in the species name, they can be matched across datasets. Constructing this dataset highlighted a fundamental issue: the rate-limiting step is not the availability of tools or platforms, but rather the 126 adoption of standars and publication of data in a way that conforms to them. 127

Propagation of error:

There are some caveats to using synthetic datasets. First, the extent to which each component dataset is adequately sampled is unknown. This can create gaps in the information that is available *in fine*. Second, because it is unlikely that all component datasets were acquired using reconcilable standards and protocol, it is likely that the quantitative information needs be discarded, and therefore the conservative position is to do qualitative analyses only. Although these have to be kept in mind, we do not think they should prevent use and evaluation of the approach we suggest. For one thing, at large spatial and organizational scales, coarse-grained analyses are still able to pick up qualitative differences in community structure. Second, most emergent properties are relatively insensitive to fine-scale error; for example, Gravel et al. (2013) show that even though a simple statistical model of food web structure mispredicts some individual interactions, it produces communities with realistic emergent properties. Which level of error is acceptable needs to be determined for each application, but we argue that for broad-scale description of community-level measures, the use of synthetic datasets is a cost and time-effective approach.

140 Recommendations

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1. Publish data (even the small one!)

Ideally, authors should release their analysis *pipeline* in addition to the data and explanation of the steps. The pipeline can take the form of a makefile (which allows to generate the results, from the raw data, without human intervention), or be all of the relevant code that allows to re-generate the figures and results. For example, we have released all of the R code that was used to generate the figures at **XXX**. Sharing the analysis pipeline has several advantages. First, it is a first steps towards ensuring the quality of analyses, since reviewers can (and should reasonably be expected to) look at the source code. Second, it provides a *template* for future analyses – instead of re-developping the pipeline from scratch, authors can re-use (and acknowledge) the previous codebase and build on it. Finally, it helps identifying areas of future improvement. The development of software should primarily aim to make the work of researchers easier. Looking at commonalities in the analytical pipelines for which no ready-made solutions exists will be a great way to influence priorities in software development.

3. Pay attention to standard when releasing data

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