# Automated iterative forecasting for the

## Portal Project

### **Introduction**

- 4 Forecasting the future state of ecological systems is important for management,
- 5 conservation, and evaluation of our fundamental understanding of ecology (Clark et al.,
- 6 2001; Tallis & Kareiva, 2006; Díaz et al., 2015; Dietze, 2017). Since Clark et al.
- <sup>7</sup> [-clark2001] called for a more central role of forecasting in ecology, an increasing
- 8 number of ecological forecasts are being published. However, most of these forecasts
- are made once, published, and never assessed or updated. Without assessment, we have
- limited information on how much confidence to place in our predictions; without
- regular updates, forecasts lack the most up-to-date information as conditions change
- <sub>12</sub> (Dietze et al., 2016). This lack of both regular assessment and active updating has
- limited the progress of ecological forecasting and hindered our ability to make useful
- and reliable predictions. For ecological forecasting to mature as a field, we need to
- 15 change how we produce and interact with forecasts, creating a more dynamic interplay
- between model development, prediction generation, and incorporation of new data and
- information (Dietze et al., 2016).
- With the goal of making ecological forecasting more dynamic and responsive, Dietze et
- al [-dietze2018] recently called for an increase in iterative near-term forecasting.
- 20 Iterative near-term forecasting means making forecasts for the near future and making
- 21 these forecasts repeatedly through a cycle of forecast evaluation, integration of updated
- data, and generation of new forecasts. This approach to forecasting has a number of
- 23 advantages. Because forecasts are made 'near-term'—daily to annual forecasting

```
instead of multi-decadal—predictions can be assessed more quickly and frequently,
   leading to more rapid model improvements (Dietze et al., 2016; Tredennick et al., 2016).
25
   Because the forecasts are made repeatedly through time, new data can be integrated with
   each new forecast cycle. This iterative approach to forecasting allows any changes in
   the state of the system that have occurred since the previous forecast to be incorporated
28
   and accounted for (Dietze et al., 2016). Iterative near-term forecasting has the potential
29
   to promote rapid improvement in the state of ecological forecasting by quickly
30
   identifying how models are failing, facilitating rapid testing of improved models, and
31
   incorporating updated data so models run with the most up-to-date information on the
32
   system available. While use of iterative near-term forecasting is often contextualized as
33
   a management tool, this approach to model testing can also be used to improve our
34
   basic understanding of ecological systems. For example, alternative mechanistic models
35
   can be competed to see which model provides the best forecasts for near-term dynamics,
36
   thus providing insights into the relative importance of different processes driving
37
   dynamics of ecological systems (Dietze et al., 2016). Whether deployed for basic or
38
   applied uses, iterative near-term forecasting incorporates a more dynamic interplay
39
   between models, predictions, and data that is clearly needed to improve ecological
40
   forecasting and our understanding of ecological systems more broadly.
   Because iterative near-term forecasting requires a dynamic interplay of models,
   predictions, and data, Dietze et al [-dietze2018] highlight approaches to data
43
   management, model construction and evaluation, and cyberinfrastructure that are
44
   necessary to effectively implement this type of forecasting (Box 1). Data to be used for
45
   iterative near-term forecasting needs to be widely accessible, which requires data to be
46
   released quickly under open licenses (Dietze et al., 2016; Vargas et al., 2017) and
   structured so that it can be used easily by a variety of researchers and in multiple
   modeling approaches (Borer, Seabloom, Jones, & Schildhauer, 2009; Strasser, Cook,
   Michener, Budden, & Koskela, 2011). Models need to be able to deal with uncertainty,
```

- in both the predictors and the predictions, to properly convey uncertainty in the
- resulting forecasts. Multiple models should be compared to assess which models are
- performing best and to allow for combining models to form ensemble predictions.
- 54 Ensuring that data and models are regularly updated and new forecasts are made
- requires cyberinfrastructure to automate data processing, model fitting, prediction,
- model evaluation, forecast visualization, and archiving. In combination, these
- 57 approaches should allow forecasts to be easily rerun and evaluated as new data becomes
- <sub>58</sub> available (Box 1; Dietze et al., 2016).
- 59 While iterative near-term forecasting is an important next step in the evolution of
- ecological forecasting, the requirements outlined by Dietze et al (Box 1) are not trivial
- to implement; few of their recommendations are in widespread use in ecology today.
- We examined what it would entail to operationalize Dietze et al's recommendations by
- constructing our own iterative near-term forecasting pipeline for an on-going long-term
- 64 (~40 year) ecological study that collects high-frequency data on desert rodent
- abundances. We constructed our forecasting pipeline with the goal of being able to
- 66 forecast rodent abundances and evaluate our predictions on a monthly basis. In this
- paper, we discuss our approach for creating this iterative near-term forecasting pipeline,
- the challenges we encountered, the tools we used, and the lessons we learned that may
- 69 help others to create their own iterative forecasting systems.

## System Background

- 71 Iterative forecasting requires data that is collected repeatedly, and it benefits most from
- data that is collected frequently, as this provides more opportunities for updating model
- results and assessing (and potentially improving) model performance (Box 1; Dietze et
- al., 2016). The Portal Project is a long-term ecological study situated in the Chihuahuan
- <sub>75</sub> Desert (2 km north and 6.5 km east of Portal, Arizona, US). Researchers have been

continuously collecting data at the site since 1977, including data on the abundance of rodent and plant species (monthly and twice yearly, respectively) and climactic factors such as air temperature and precipitation (daily). The site consists of 24 50m x 50m experimental plots. Each plot contains 49 permanently marked trapping stations laid out in a 7 x 7 grid, and all plots are trapped with Sherman live traps for one night each 80 month. For all rodents caught during a trapping session, information on species identity, size, and reproductive condition is collected, and new individuals are given identification tags. We use the data from the control plots at this site, where rodent 83 populations are not experimentally manipulated. This data on rodent populations is 84 high-frequency, uses consistent trapping methodology, and has an extended time-series 85 (469 monthly samples and counting), making this study an ideal case for near-term 86 iterative forecasting.

## 88 Implementing an automated iterative forecasting system

Implementation of iterative forecasting requires the regular rebuilding of models with new raw data as it becomes available and the presentation of those forecasts in usable 90 forms; in our case, this occurs monthly. Doing this in an efficient and maintainable way 91 relies on developing an automated pipeline to handle the six stages of converting raw 92 data into new forecasts: data collection, data sharing, data manipulation, modeling and 93 forecasting, archiving, and presentation of the forecasts (Figure 1). To implement the 94 pipeline outlined in Figure 1, we used a "continuous analysis" framework (sensu 95 Beaulieu-Jones & Greene, 2017) that automatically processes the most up-to-date data, refits the models, makes new forecasts, archives the forecasts, and updates a website with analysis of current and previous forecasts. In this section we describe our approach to streamlining and automating the multiple components of the forecasting pipeline and the tools and infrastructure we employed to execute each stage of the pipeline.

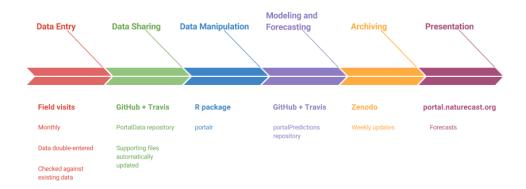


Figure 1: Figure 1. Stages of the forecasting pipeline. To go from raw data to forecast presentation involves a number of stages, each of which required unique tasks, tools and infrastructure. While each stage has unique tasks associated with it, the stages of our pipeline are also interdependent. Our pipeline is primarily a linear structure where outputs from one stage form the inputs for the subsequent stage

#### 101 Continuous Analysis Framework

A core component of iterative near-term forecasting is the regular rerunning of the 102 forecasting pipeline. This can be conducted manually—with a human making sure all 103 code is run and all tables and files are updated—or automatically by having the 104 computer conduct those tasks. We chose to have the computer run our pipeline and 105 employed "continuous analysis" (sensu Beaulieu-Jones & Greene, 2017) to drive the 106 automation of both the full pipeline and a number of its individual components. 107 Continuous analysis uses a set of tools originally designed for software development 108 called "continuous integration" (CI). CI combines computing environments for running 109 code with monitoring systems to identify changes in data or code. Essentially, CI is a 110 computer helper whose job is to watch the pipeline and, when it sees a change in the code or data, it runs all the tasks needed to ensure that the forecasting pipeline runs from beginning to end. This is useful for iterative near-term forecasting because it does

not rely on humans to remember to create forecasts when new models or data are added. These tools are common in the area of software development where they are used to automate software testing and integrate work by multiple software developers working on the same software. However, these tools can be used for any computational task that needs to be regularly repeated or run after changes to code or data (Beaulieu-Jones & Greene, 2017). Because of the widespread use of CI in software development, several 119 CI services already exist. Our forecasting pipeline currently runs on a publicly available 120 continuous integration service (Travis CI; https://travis-ci.org/) that is free for open 121 source projects (up to a limited amount of computing time); alternative services that can 122 be used to run code on local or cloud-based computational infrastructure are available, 123 such as Drone (http://try.drone.io/) (Beaulieu-Jones & Greene, 2017). As detailed 124 below, we use CI to quality check data, test code using "unit tests" (Wilson et al., 2014), 125 build models, make forecasts, and publicly present and archive the results (Figure 2). 126 In addition to automatically running software pipelines, the other key component of 127 "continuous analysis" is making sure that the pipelines will continue to run even as 128 software dependencies change (Beaulieu-Jones & Greene, 2017). Many of us have 129 experienced the frustrations that can occur when software updates (e.g., changes in R 130 package versions) create errors in previously functional code. We experienced this issue 131 when a package one of our models relies on, tscount [liboschik2015], was 132 temporarily removed from CRAN (the R package repository) and, therefore, could not 133 be installed in the usual way. This broke our forecasting pipeline because we could no 134 longer run models that used that package. To minimize issues with changes in software 135 dependencies, we follow Beaulieu and Green's (2017) recommendation to use software 136 containers. Software containers are standalone packages that contain copies of everything you need to run some piece of software. Once created, a software container is basically a time capsule, it contains all the software dependencies in the exact state used to develop and run the software. If those dependencies change (or disappear) in the

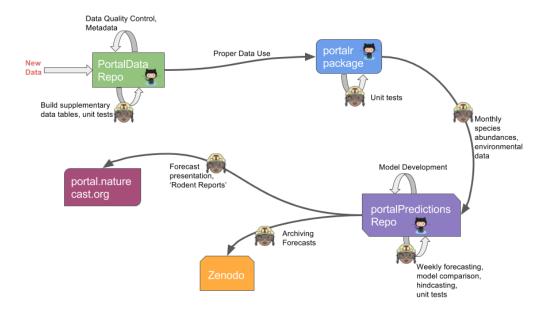


Figure 2: Figure 2. Continuous integration system. Each box denotes the core infrastructure used for each stage of the forecasting pipeline denoted in Figure 1. Continuous integration, denoted here with the Travis icon (a girl wearing safety glasses and hardhat), plugs into our pipeline at every stage. Travis triggers the code involved in major events that involve integration across stages of the pipeline, such as taking the output from the forecasting stage (purple box) to create an updated presentation (rose box). Travis also runs tasks within a stage, such as conducting tests to make sure code changes have not introduced errors (icons on arrows originating and ending on the same box)

wider world, they still exist, unchanged, in your container. We use an existing platform, Docker, to store an exact image of the complete software environment for running the forecasts. Docker also allows a specified set of packages to be used consistently across different computer and server environments. Using containers allows us to update to new package versions after testing and making any necessary changes to the data 145 processing and analysis code. We use a container created by the Rocker project which is 146 a Docker image with many important R packages (i.e. tidyverse) pre-installed (Boettiger & Eddelbuettel, 2017). We use add our code and dependencies to this existing Rocker 148 image to create a software container for our forecasting pipeline. In combination, the 149 automated running of the pipeline (continuous integration) and the guarantee it will not 150 stop working unexpectedly due to software dependencies (via a software container) 151 allows continuous analysis to serve as the glue that connects all stages of the forecasting 152 pipeline. 153

## **Data Collection, Entry, and Processing**

164

165

Iterative forecasting benefits from frequently updated data on the state of the system so that state changes can be quickly incorporated into new forecasts (Dietze et al., 2016). Frequent data collection and rapid entry and processing of data are both important for 157 providing the most up-to-date data for forecasting. Since our data is collected monthly, 158 ensuring that the models have access to the newest data requires a data latency period of 159 less than 1 month from collection to availability for modeling. To accomplish this, we 160 automated components of the data processing and quality assurance/quality control 16 (QA/QC) process to reduce the time needed to add new data to the database (Figures 1 162 and 2). 163 New data is double-entered into Excel using the "data validation" feature. The two

control (QC) checks written in R using the testthat R package (Wickham, 2011) are

versions are then compared in an R script to control for errors in data entry. Quality

run on the data to test for validity and consistency both within the new data (e.g. sexual characteristics of an animal match M/F designation) and between the new and archived data (e.g. species and sex are consistent for recaptures of the same animal based on tag number). The local use of the QC scripts to flag problematic data greatly reduces the time spent error-checking and ensures that the quality of data is consistent. The data is 17 then submitted to a GitHub-based data repository. GitHub is a software development 172 tool for managing computer code development, but we have also found it useful for data management. Changes to data can be tracked through version control, and additions and 174 changes to the data can be monitored through pull requests (notifications that someone 175 has a modified version of the data to contribute). QA/QC checks are automatically rerun 176 on the submitted data using continuous integration to ensure that these checks have been 177 run and that no avoidable errors reach the official version of the dataset. 178 We also automated the updating of supplementary data tables, including information on 179 weather and trapping history, that were previously updated manually. As soon as new 180 field data is merged into the repository, continuous integration updates all 181 supplementary files. Weather data is automatically fetched from our cellular-connected 182 weather station, cleaned, and appended to the weather data table. Supplementary data 183 tables related to trapping history are updated based on the data added to the main data 184 tables. Using CI for this ensures that all supplementary data tables are always 185 up-to-date with the core data.

## **Data Sharing**

186

The Portal Project has a long history of making its data publicly available, which means 188 that anyone can use it for forecasting or other projects. Historically the publication of 189 the data was conducted through data papers, the most common approach in ecology; 190 however, this approach caused years of data latency. Recently, the project has switched 191 to posting data directly to a public GitHub repository with a CC0 license (Figure 1).

This immediate posting reduces that data latency to less than one month and, therefore, makes meaningful iterative near-term forecasting possible for not only our group but other interested parties as well.

#### 96 Data Manipulation

Once data is available, it needs to be processed into a form appropriate for modeling 197 (Figure 1). In many ecological datasets, this requires not only simple data manipulation 198 but also a good understanding of the dataset to allow data to be aggregated 199 appropriately. These data manipulation steps are often conducted using custom one-off 200 code to convert the data into the desired form (Morris & White, 2013), but this approach 201 has several limitations. First, each researcher must develop their own data manipulation 202 code, which is inefficient and can result in different decisions by different researchers 203 about the details of data cleaning and aggregation. Subtle differences in data processing 204 decisions have lead to confusion when reproducing results for the Portal data in the past. 205 Second, this kind of code is rarely robust to changes in data structure and location. Based on our experience developing and maintaining the Data Retriever (Morris & 20 White, 2013; Senyondo et al., 2017), these kinds of changes are common. Finally, this kind of code is generally poorly tested, which can lead to errors based on mistakes in 209 data manipulation. To avoid these issues for the Portal Project data, the Portal team has 210 been developing an R package (portalR; http://github.com/weecology/portalr) for 211 acquiring the data and handling common data cleaning and aggregation tasks. As a 212 result, our modeling and forecasting code only needs to install this package and run the 213 data manipulation and summary functions to get the appropriate data (Figure 2). The 214 package undergoes thorough automated unit tests to ensure that data manipulations are 215 achieving the desired results. Having data manipulation code maintained in a separate 216 package that focuses on consistently providing properly summarized forms of the most 217 recent data has made maintaining the forecasting code itself much more straightforward.

#### Modeling and Forecasting

Ideally, iterative near-term forecasting involves regularly refitting a variety of different models (Figure 1). New models should be easy to incorporate to allow for iterative improvements to the general modeling structure and approach. We use CI to refit the 222 models and make new forecasts each time the modeling code changes and when new 223 data becomes available (Figure 2). We use a plugin infrastructure to allow new models to be easily added to the system. Each model is a script that takes in standardized inputs and returns standardized outputs (Figure 3). All models are run by the main forecasting 226 code at each update, and the standardized outputs are combined to store the results of 22 the different models' forecasts. A weighted ensemble model is then added with weights 228 based on how well individual models fit the training data. This plugin infrastructure 229 allows flexibility in all aspects of the modeling process, making it easier to explore new 230 modeling approaches, and allows new models that fit the data well to immediately 231 improve the ensemble forecast. 232 To allow flexibility in what the models predict, we designed a forecast output format 233 that allows us to store relatively generic forecasts. Each forecast output file contains the 234 date being forecast, the collection date of the data used for fitting the models, the date 235 the forecast was made, the state variable being forecast (e.g., rodent biomass, the 236 abundance of a species), and the forecast value and associated uncertainty of that 237 forecast (Figure 3). This allows a variety of different forecasts to be stored in a common 238 format and may serve as a useful starting point for developing a standard for storing 239 ecological forecasts more generally. Forecasts are currently evaluated using root mean square error (RMSE) to evaluate 241 point forecasts and coverage to evaluate uncertainty. We plan to add additional metrics 242 in the future. In addition to evaluating the actual forecasts, we also use hindcasting 243 (forecasting on already collected data) to gain additional insight into the methods that 244 work best for forecasting this system. For example a model is fit using rodent

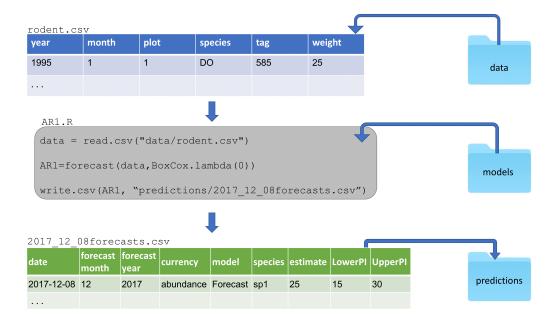


Figure 3: Figure 3. Demonstration of plugin infrastructure where each model script (represented here as AR1.R) uses data provided by the core forecasting code (represented here as rodent.csv) and returns its forecasts in a predefined structure that is consistent across models (represented here as 2017\_12\_08forecasts.csv) to allow cross-model evaluations.

observations up to June 2005, then used to make a forecast 12 months out to May 2006.
The observations of that 12 month period can immediately be used to evaluate the
model. Hindcasting can be conducted using all months from the beginning of the study,
thus allowing model comparison of large numbers of hindcasts and giving insight into
which models make the best forecasts. It can also be used to quickly evaluate new
models instead of waiting for an adequate amount of data to accumulate.

## 252 Archiving

Publicly archiving forecasts before new data is collected allows the field to assess,
compare, and build on forecasts made by different groups (McGill, 2012; Tredennick et
al., 2016; Dietze, 2017; J. Harris David, Taylor, & White, 2018)(Figure 1). This
archiving serves as a form of pre-registration for model predictions, helping facilitate
unbiased interpretation of model performance. We explored three major repositories for

archiving our forecasts: FigShare, Zenodo, and Open Science Framework. While all three repositories allowed for easy manual submissions (i.e., a human uploading files 259 after each forecast), automating this process was substantially more difficult. Various combinations of repositories, APIs and associated R packages had issues with: 1) integrating authorization with continuous integration; 2) automatically making archived 262 files public; 3) adding new files to an existing location; or 4) automatically permanently 263 archiving the files. Our eventual solution was to leverage the GitHub-Zenodo 264 integration (https://guides.github.com/activities/citable-code/) and automatically push 265 forecasts to the GitHub repository from the CI server. The GitHub-Zenodo integration is 266 designed to automatically create versioned archives of GitHub repositories. There is an 267 existing one-time process for linking our forecasting repository on GitHub with Zenodo. 268 Once this link is created, each time a new forecast is created, our pipeline adds the new 269 forecasts to the GitHub repository and uses the GitHub API to create a new "release" of 270 our repository. This triggers the Zenodo-GitHub integration, which automatically 27 archives the resulting forecasts and the code that generated them under a top-level DOI that refers to all archived forecasts (https://doi.org/10.5281/zenodo.833438). Through 273 this process, we automatically archive every forecast made with a documented history 274 of the archive. While this approach is functional because everything in the repository is archived when a new forecast is made, these archives are complicated, making it more complicated than necessary to find and access the forecasting results.

#### 278 Presentation

In addition to archiving the results of each forecast, we present them on a website that
displays monthly rodent forecasts, model evaluation metrics, monthly reports, and
information about the study site (Figure 4; http://portal.naturecast.org). The website
includes a graphical presentation of the most recent month's forecasts (including
uncertainty) and compares the latest data to the previous forecasts. Information on the

# Portal Forecast Total Abundance Forecast

This is the forecast for next month's sampling of rodents at Portal.

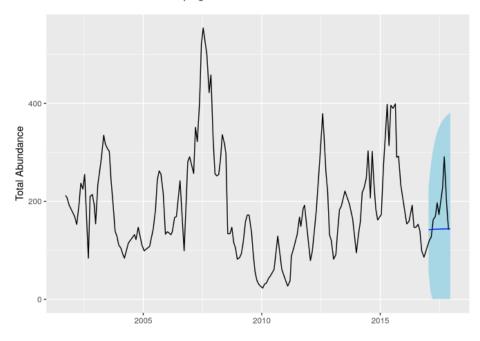


Figure 4: Figure 4. Screen capture of the homepage of the Portal Forecasting website; http://portal.naturecast.org. This site contains information on the most current forecasts, evaluation of forecast performance, and general information about the species being forecast.

the species and the field site targeted to a general audience are also included. The site is built using Rmarkdown (Allaire et al., 2017), which naturally integrates into the pipeline, and is automatically updated after each forecast. The knitr R package (Xie, 2015) compiles the code into HTML, which is then published using Github Pages (https://pages.github.com/). The files for the website are stored in a subdirectory of the forecasting repository. As a result, the website is also archived automatically as part of the forecast archiving.

## Discussion

automated iterative forecasting system (Figures 1 and 2) to support repeated forecasting 293 of an ecological system. Our forecasting system automatically acquires and processes 294 the newest data, refits the models, makes new forecasts, publicly archives those 295 forecasts, and presents both the current forecast and information on how previous 296 forecasts performed. Every week our forecasting system generates a new set of forecasts with no human intervention, except for the entry of new field data. This 298 ensures that forecasts based on the most recent data are always available and allows us 299 to rapidly assess the performance of multiple forecasting models for a number of 300 different states of the system, including the abundances of individual species and 30 community-level variables such as total abundance. To create this iterative near-term forecasting system, we used R to process data and conduct analyses, and we leveraged already existing services (i.e. GitHub, Travis, Docker) for more complicated cyberinfrastructure tasks. Thus, our approach to developing iterative near-term 305 forecasting infrastructure provides an example for how short-term ecological 306 forecasting systems can be initially developed. We designed this forecasting system with the goal of making it relatively easy to build, maintain, and extend. We used existing technology for both running the pipeline and building individual components, which allowed the system to be built relatively cheaply in terms of both time and money. This included the use of tools like Docker for 31 reproducibility, the Travis CI continuous integration system for automatically running 312 the pipeline, Rmarkdown and knitr for generating the website, and the already 313 existing integration between Github and Zenodo to archive the forecasts. By using this 314 "continuous analysis" approach (Beaulieu-Jones & Greene, 2017), where analyses are 315 automatically rerun when changes are made to data, models, or associated code, we 316 have reduced the time required by scientists to run and maintain the forecasting pipeline.

Following the recommendations of Dietze et al [-dietze2018], we developed an

To make the system extensible so that new models could be easily incorporated, we use a plugin-based infrastructure so that adding a new model to the system is as easy as adding a single file to the 'models' folder in our repository (Figure 3). This should substantially lower the barriers to other scientists contributing models to this forecasting effort. We also automatically archive the resulting forecasts publicly so that, as new data 322 is collected, the performance of these forecasts can be assessed by both us and other 323 researchers. This serves as a form of "pre-registration" by providing a quantitative record of the forecast before the data being predicted were collected. 325 While building this system was facilitated by the use of existing technological solutions, there were still a number of challenges in making existing tools work for automated 32 iterative forecasting. Continuous integration is designed primarily for running 328 automated tests on software, not for running a coordinated forecasting pipeline. As a 329 result, extra effort was sometimes necessary to figure out how to get these systems to 330 work properly in non-standard situations, like running code that was not part of a 331 software package. In addition, hosted continuous integration solutions, like Travis, 332 provide only limited computational resources. As the number and complexity of the 333 models we fit has grown, we have had to continually invest effort in reducing our total 334 compute time so we can stay within these limits. Finally, we found no satisfactory 335 existing solution for archiving our results. All approaches we tried had limitations when 336 it came to automatically generating publicly versioned archives of forecasts on a 337 repeated basis. Overall, we found existing technology to be sufficient to the task, but it 338 required greater expertise and a greater investment of time than is ideal. Tool 339 development to reduce the effort required for scientists to set up their own short-term forecasting systems would clearly be useful, but our efforts show that it is still currently possible for scientists using existing tools to develop initial iterative systems as a method for both advancing scientific understanding and developing proof of concept forecasting systems. By developing these systems so that they already produce

automated iterative forecasts, it will be easier to convert these systems into fully operationalized forecasting systems that are relied on for decision making (Dietze et al., 2016, other paper by operationalization co-authors). Because of the breadth of expertise needed to set up our forecasting pipeline, our effort required a team with diverse skills and perspectives, ranging from software 349 development to field site expertise. It is rare to find such breadth within a single 350 research group, and our system was developed as a collaboration between the lab collecting the data and a computational ecology lab. When teams have a breadth of expertise, communication can be challenging. We found a shared base of knowledge 353 related to both the field research and fundamental computational skills was important 354 for the success of the group. Everyone on the team had received training in fundamental 355 data management and computing skills through a combination of university courses, 356 Software and Data Carpentry workshops (Teal et al., 2015), and informal lab training 357 efforts. In addition, everyone was broadly familiar with the study site and methods of 358 data collection, and most team members had participated in field work at the site on 359 multiple occasions. This provided a shared set of knowledge and vocabulary that 360 actively facilitated interdisciplinary interactions. Given the current state of existing 36 tools for forecasting, forecasting teams will need people with significant experience in 362 working with continuous integration and APIs, which means interdisciplinary teams will generally be required for creating these pipelines until tool development improves. We developed this infrastructure for automatically making iterative forecasts with the 365 goals of making accurate forecasts for this well-studied system, learning what methods 366 work well for ecological forecasting more generally, and improving our understanding 36 of the processes driving ecological dynamics. The most obvious application of 368 automated iterative ecological forecasting is for speeding up development of forecasting 369 models by providing the most recent data available to models and by quickly iterating to 370 improve the models used for forecasting. By learning what works best for forecasting in

this and other ecological systems, we will better understand what the best approaches are for ecological forecasting more generally. By designing the pipeline so that it can forecast many different aspects of the ecological community, we also hope to learn about what aspects of ecology are more forecastable. Finally, automated forecasting infrastructures like this one also provide a core foundation for faster scientific inquiry more broadly because new models can quickly be applied to data and compared to 37 existing models. The forecasting infrastructure does the time-consuming work of data processing, data integration, and model assessment, allowing new research to focus on 379 the models being developed and the inferences about the system that can be drawn from 380 them (Dietze et al., 2016). We plan to use this pipeline to drive future research into 381 understanding the processes that govern the dynamics of individual populations and the 382 community as a whole. By regularly running different models for population and 383 community dynamics, a near-term iterative pipeline such as ours should also make it 384 possible to rapidly detect changes in how the system is operating, which should allow 385 the rapid identification of ecological transitions or even possibly allow them to be 386 prevented (??? example). By building an automated iterative near-term forecasting 387 infrastructure we can improve our ability to forecast natural systems, our understanding 388 of the biology driving ecological dynamics, and detect or even predict changes in 389 system state that are important for conservation and management.

## 391 Acknowledgements

This research was supported by the National Science Foundation through grant 1622425 to S.K.M. Ernest and by the Gordon and Betty Moore Foundation's Data-Driven Discovery Initiative through grant GBMF4563 to E.P. White. We thank all of the graduate students, postdocs, and volunteers who have collected the Portal Project over the last 40 years and the developers of all of the software and tools that made this

397 project possible.

## Box 1. Key practices for automated iterative near-term

## ses ecological forecasting

- 400 A list of some of the key practices developed by Dietze et al [-dietze2018] for
- facilitating iterative near-term ecological forecasting and discussion of why these
- 402 practices are important.

#### 403 Data

#### **1. Frequent data collection**

- Frequent data collection allows models to be regularly updated and forecasts to be
- frequently evaluated (Dietze et al., 2016). Depending on the system being studied, this
- frequency could range from sub-daily to annual, but typically the more frequently the
- data is collected the better.

#### **2. Rapid data release under open licenses**

- Data should be released as quickly as possible (low latency) under open licenses so that
- forecasts can be made frequently and data can be accessed by a community of
- forecasters (Dietze et al., 2016; Vargas et al., 2017).

#### 3. Best practices in data structure

- 414 To reduce the time and effort needed to incorporate this data into models, best practices
- in data structure need to be employed for managing and storing collected data to ensure
- it is easy to integrate into other systems (interoperability) (Borer et al., 2009; Strasser et
- al., 2011; White et al., 2013).

#### 418 Models

#### 419 **4. Focus on uncertainty**

- 420 Understanding the uncertainty of forecasts is crucial to interpreting the forecasts and
- understanding their utility. Models used for forecasting should be probabilistic to
- properly quantify uncertainty and to convey how this uncertainty increases through time.
- Evaluation of forecast models should include assessment of how accurately they
- quantify uncertainty as well as point estimates. This can be done using "proper and
- local" scores (Hooten & Hobbs, 2015).

#### **5.** Compare forecasts to simple baselines

- 427 Understanding how much information is present in a forecast requires comparing its
- accuracy to simple baselines to see if the models yield improvements over the naive
- expectation that the system is static (J. Harris David et al., 2018).

#### 430 6. Compare and combine multiple modeling approaches

- To quickly learn about the best approaches to forecasting different aspects of ecology,
- 432 multiple modeling approaches should be compared for forecasting tasks (J. Harris
- David et al., 2018). Different modeling approaches should also be combined into
- ensemble models, which are known to outperform single models for many forecasting
- and prediction tasks (Weigel, Liniger, & Appenzeller, 2008).

## 436 Cyberinfrastructure

- 437 In addition to improvements in data and models, iterative near-term forecasting requires
- improved infrastructure and approaches to support continuous model development and
- iterative forecasting (Dietze et al., 2016).

#### 7. Best practices in software development

- Best practices should be followed in the development of scientific software and
- modeling to make it easier to maintain, integrate into pipelines, and build on by other
- researchers. Key best practices include using open licenses, good documentation,
- version control, and cross-platform support (Wilson et al., 2014; Hampton et al., 2015).

#### 8. Support easy inclusion of new models

- To facilitate the comparison and ensembling of different modeling approaches, code for
- fitting models and making forecasts should be easily extensible, allowing models
- developed by different groups to be easily integrated into a single framework (Dietze et
- al., 2016).

#### 9. Automated end-to-end reproducibility

- 451 Iteratively making forecasts requires that acquiring the newest data, refitting the models,
- and making new forecasts is simple. Ideally, this should be done automatically without
- requiring human intervention. Therefore, the process of making forecasts should
- emphasize end-to-end reproducibility, including data, models, and evaluation (Stodden
- & Miguez, 2014), to allow the forecasts to be easily rerun as new data becomes
- available (Dietze et al., 2016). Ideally, the entire forecasting pipeline will be rerun
- automatically as new data becomes available.

#### **10. Publicly archive forecasts**

- Forecasts should be openly archived to demonstrate that the forecasts were made
- without knowledge of the outcomes (i.e., as a form of pre-registration sensu) and to
- allow the community to assess and compare the performance of different forecasting
- approaches both now and in the future (McGill, 2012; Dietze et al., 2016; Tredennick et
- al., 2016; J. Harris David et al., 2018). Ideally, the forecasts and evaluation of their
- performance should be automatically posted publicly in a manner that is understandable
- by both interested scientists and other stakeholders.

## References

- Allaire, J., Cheng, J., Xie, Y., McPherson, J., Chang, W., Allen, J., ... Arslan, R. (2017).
- 468 Rmarkdown: Dynamic documents for r. Retrieved from
- https://CRAN.R-project.org/package=rmarkdown
- Beaulieu-Jones, B. K., & Greene, C. S. (2017). Reproducibility of computational
- workflows is automated using continuous analysis. *Nature Biotechnology*, 35(4),
- 472 342–346.
- Boettiger, C., & Eddelbuettel, D. (2017). An introduction to rocker: Docker containers
- 474 for r. *arXiv Preprint arXiv:1710.03675*.
- Borer, E. T., Seabloom, E. W., Jones, M. B., & Schildhauer, M. (2009). Some simple
- guidelines for effective data management. The Bulletin of the Ecological Society of
- 477 America, 90(2), 205–214.
- <sup>478</sup> Clark, J. S., Carpenter, S. R., Barber, M., Collins, S., Dobson, A., Foley, J. A., ... others.
- (2001). Ecological forecasts: An emerging imperative. Science, 293(5530), 657–660.
- Dietze, M. C. (2017). Ecological forecasting. Princeton University Press.
- Dietze, M. C., Fox, A., Betancourt, J. L., Hooten, M. B., Jarnevich, C. S., Keitt, T. H.,
- 482 ... others. (2016). Iterative ecological forecasting: Needs, opportunities, and
- challenges. Proceedings of the National Academy of Sciences.
- Díaz, S., Demissew, S., Carabias, J., Joly, C., Lonsdale, M., Ash, N., ... others. (2015).
- The ipbes conceptual framework—connecting nature and people. Current Opinion in
- 486 Environmental Sustainability, 14, 1–16.
- Hampton, S. E., Anderson, S. S., Bagby, S. C., Gries, C., Han, X., Hart, E. M., ...
- others. (2015). The tao of open science for ecology. *Ecosphere*, 6(7), 1–13.
- 489 Harris, J., David, Taylor, S. D., & White, E. P. (2018). Forecasting biodiversity in

- breeding birds using best practices. *PeerJ*.
- Hooten, M. B., & Hobbs, N. (2015). A guide to bayesian model selection for ecologists.
- 492 Ecological Monographs, 85(1), 3–28.
- 493 McGill, B. J. (2012). Ecologists need to do a better job of prediction part ii partly
- cloudy and a 20% chance of extinction (or the 6 p's of good prediction). Retrieved from
- https://dynamicecology.wordpress.com/2013/01/09/
- ecologists-need-to-do-a-better-job-of-prediction-part-ii-mechanism-vs-pattern/
- 497 Morris, B. D., & White, E. P. (2013). The ecodata retriever: Improving access to
- existing ecological data. *PloS One*, 8(6), e65848.
- Senyondo, H., Morris, B. D., Goel, A., Zhang, A., Narasimha, A., Negi, S., ... White,
- E. P. (2017). Retriever: Data retrieval tool. *The Journal of Open Source Software*, 2(19),
- 501 451. doi:10.21105/joss.00451
- 502 Stodden, V., & Miguez, S. (2014). Best practices for computational science: Software
- infrastructure and environments for reproducible and extensible research. *Journal of*
- 504 Open Research Software, 2(1).
- 505 Strasser, C., Cook, R., Michener, W., Budden, A., & Koskela, R. (2011). Promoting data
- stewardship through best practices. In *Proceedings of the environmental information*
- management conference 2011 (eim 2011). Oak Ridge National Laboratory (ORNL).
- Tallis, H. M., & Kareiva, P. (2006). Shaping global environmental decisions using
- socio-ecological models. *Trends in Ecology & Evolution*, 21(10), 562–568.
- Teal, T. K., Cranston, K. A., Lapp, H., White, E., Wilson, G., Ram, K., & Pawlik, A.
- 511 (2015). Data carpentry: Workshops to increase data literacy for researchers.
- 512 International Journal of Digital Curation, 10(1), 135–143.
- Tredennick, A. T., Hooten, M. B., Aldridge, C. L., Homer, C. G., Kleinhesselink, A. R.,
- & Adler, P. B. (2016). Forecasting climate change impacts on plant populations over

- large spatial extents. *Ecosphere*, 7(10).
- Vargas, R., Alcaraz-Segura, D., Birdsey, R., Brunsell, N. A., Cruz-Gaistardo, C. O.,
- Jong, B. de, ... others. (2017). Enhancing interoperability to facilitate implementation
- of redd+: Case study of mexico. Carbon Management, 8(1), 57–65.
- <sup>519</sup> Weigel, A. P., Liniger, M., & Appenzeller, C. (2008). Can multi-model combination
- really enhance the prediction skill of probabilistic ensemble forecasts? *Quarterly*
- Journal of the Royal Meteorological Society, 134(630), 241–260.
- White, E. P., Baldridge, E., Brym, Z. T., Locey, K. J., McGlinn, D. J., & Supp, S. R.
- 523 (2013). Nine simple ways to make it easier to (re) use your data. *Ideas in Ecology and*
- Evolution, 6(2).
- Wickham, H. (2011). Testthat: Get started with testing. *The R Journal*, 3, 5–10.
- 526 Retrieved from
- http://journal.r-project.org/archive/2011-1/RJournal\_2011-1\_Wickham.pdf
- <sup>528</sup> Wilson, G., Aruliah, D. A., Brown, C. T., Hong, N. P. C., Davis, M., Guy, R. T., ...
- others. (2014). Best practices for scientific computing. *PLoS Biology*, 12(1), e1001745.
- Xie, Y. (2015). Dynamic documents with r and knitr (Vol. 29). CRC Press.