Developing an automated iterative

near-term forecasting system for an

ecological study

- Ethan P. White^{1,2,3}, Glenda M. Yenni¹, Shawn D. Taylor⁴, Erica M.
- 5 Christensen¹, Ellen K. Bledsoe⁴, Juniper L. Simonis¹, S. K. Morgan
- $Ernest^{1,3}$
- ⁷ Department of Wildlife Ecology and Conservation, University of Florida, Gainesville,
- 8 FL, United States
- ⁹ Informatics Institute, University of Florida, Gainesville, FL, United States
- ³ Biodiversity Institute, University of Florida, Gainesville, FL, United States
- ⁴ School of Natural Resources and Environment, University of Florida Gainesville, FL,
- 12 United States

13 Abstract

- 1. Most forecasts for the future state of ecological systems are conducted once and
- never updated or assessed. As a result, many available ecological forecasts are not
- based on the most up-to-date data, and the scientific progress of ecological
- forecasting models is slowed by a lack of feedback on how well the forecasts
- perform.

19

2. Iterative near-term ecological forecasting involves repeated daily to annual scale

forecasts of an ecological system as new data becomes available and regular assessment of the resulting forecasts. We demonstrate how automated iterative near-term forecasting systems for ecology can be constructed by building one to conduct monthly forecasts of rodent abundances at the Portal Project, a long-term study with over 40 years of monthly data. This system automates most aspects of the six stages of converting raw data into new forecasts: data collection, data sharing, data manipulation, modeling and forecasting, archiving, and presentation of the forecasts.

- 3. The forecasting system uses R code for working with data, fitting models, making forecasts, and archiving and presenting these forecasts. The resulting pipeline is automated using continuous integration (a software development tool) to run the entire pipeline once a week. The cyberinfrastructure is designed for long-term maintainability and to allow the easy addition of new models. Constructing this forecasting system required a team with expertise ranging from field site experience to software development.
- 4. Automated near-term iterative forecasting systems will allow the science of ecological forecasting to advance more rapidly and provide the most up-to-date forecasts possible for conservation and management. These forecasting systems will also accelerate basic science by allowing new models of natural systems to be quickly implemented and compared to existing models. Using existing technology, and teams with diverse skill sets, it is possible for ecologists to build these systems and use them to advance our understanding of natural systems.
- Key-words: forecasting, prediction, mammals, iterative forecasting, Portal Project

Introduction

```
Forecasting the future state of ecological systems is important for management,
   conservation, and evaluation of how well models capture the processes governing
45
   ecological systems (Clark et al., 2001; Tallis & Kareiva, 2006; Díaz et al., 2015; Dietze,
46
   2017). In 2001, Clark et al. (2001) called for a more central role of forecasting in
   ecology. Since then, an increasing number of ecological forecasts are being published.
48
   Most of these forecasts, however, are made once, published, and never assessed or
   updated. This lack of both regular assessment and active updating has limited the
50
   progress of ecological forecasting and hindered our ability to make useful and reliable
   predictions. The lack of active assessment results in limited information on how much
52
   confidence to place in forecasts and makes it difficult to determine on which forecasting
   methods to build. Without regular updates, forecasts lack the most current data, and the
   longer a forecast remains out of date, the less accurate it becomes (Petchey et al., 2015;
   Dietze et al., 2016). More regular updating and assessment will advance ecological
   forecasting as a field by accelerating the identification of the best models for individual
   forecasts and improving our understanding of how to best design forecasting
58
   approaches for ecology in general. For ecological forecasting to mature as a field, we
59
   need to change how we produce and interact with forecasts, creating a more dynamic
60
   interplay between model development, prediction generation, and incorporation of new
   data and information (Dietze et al., 2016).
62
   With the goal of making ecological forecasting more dynamic and responsive, Dietze et
63
   al (2016) recently called for an increase in iterative near-term forecasting. Iterative
64
   near-term forecasting is defined as making predictions for the near future and repeatedly
65
   updating those predictions through a cycle of evaluation, integration of new data, and
66
   generation of new forecasts. Because forecasts are made 'near-term'—daily to annual
67
   time scales instead of multi-decadal—predictions can be assessed more quickly and
68
   frequently, leading to more rapid model improvements (Dietze et al., 2016; Tredennick
```

```
et al., 2016). Since forecasts are made repeatedly through time, new data can be
   continuously integrated with each iteration (Dietze et al., 2016). By quickly identifying
71
   how models are failing, facilitating rapid testing of improved models, and incorporating
   the most up-to-date data available, iterative near-term forecasting has the potential to
73
   promote rapid improvement in the state of ecological forecasting. In addition to
   yielding improved information for guiding policy and management (Clark et al., 2001;
   Luo et al., 2011; Petchey et al., 2015), this iterative approach will help improve our
   basic understanding of ecological systems (Dietze et al., 2016). For example, alternative
77
   mechanistic models can be compared to determine which model provides the best
78
   forecasts, thus providing insights into the importance of different ecological processes
79
   (Dietze et al., 2016). Iterative near-term forecasting provides the more dynamic
80
   interplay between models, predictions, and data that has been identified as necessary for
   improving ecological forecasting and our understanding of ecological systems more
82
   broadly.
83
   Because iterative near-term forecasting requires a dynamic integration of models,
84
   predictions, and data, Dietze et al (2016) highlight approaches to data management,
85
   model construction and evaluation, and cyberinfrastructure that are necessary to
86
   effectively implement this type of forecasting (Box 1). Data needs to be released
87
   quickly under open licenses (Dietze et al., 2016; Vargas et al., 2017) and structured so
88
   that it can be used easily by a variety of researchers and in multiple modeling
89
   approaches (Borer, Seabloom, Jones, & Schildhauer, 2009; Strasser, Cook, Michener,
90
   Budden, & Koskela, 2011). Models need to be able to deal with uncertainty, in both the
91
   predictors and the predictions, to properly convey uncertainty in the resulting forecasts
92
   (Diniz-Filho et al., 2009). Multiple models should be developed, both to assess which
93
   models are performing best (Dietze et al., 2016) and to facilitate combining models to
   form ensemble predictions which tend to perform better than single models (Araujo &
   New, 2007; Diniz-Filho et al., 2009). Ensuring that data and models are regularly
```

processing, model fitting, prediction, model evaluation, forecast visualization, and archiving. In combination, these approaches should allow forecasts to be easily rerun and evaluated as new data becomes available (Box 1; Dietze et al., 2016). While iterative near-term forecasting is an important next step in the evolution of 101 ecological forecasting, the requirements outlined by Dietze et al (Box 1) are not trivial 102 to implement, and few of their recommendations are in widespread use in ecology today. 103 We explored 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 ecological study that collects high-frequency data on desert rodent abundances (J. 106 Brown, 1998; S. M. Ernest, Brown, Thibault, White, & Goheen, 2008). We constructed 107 an automated forecasting pipeline with the goal of being able to forecast rodent 108 abundances and evaluate our predictions on a monthly basis. In this paper, we discuss 109 our approach for creating this iterative near-term forecasting pipeline, the challenges we 110 encountered, the tools we used, and the lessons we learned so that others can create 111 their own iterative forecasting systems. 112

updated and new forecasts are made requires cyberinfrastructure to automate data

113 System Background

Iterative forecasting is most effective with frequently collected data, since it 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 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 climatic factors such as air temperature and precipitation (daily) (J. Brown, 1998; S. Ernest, Valone, & Brown, 2009; S. M. Ernest et al., 2016).

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 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. This information on rodent

populations is high-frequency, uses consistent trapping methodology, and has an

extended time-series (470 monthly samples and counting), making this study an ideal

case for near-term iterative forecasting.

Implementing an automated iterative forecasting system

Implementation of iterative forecasting requires the regular rebuilding of models with 131 new raw data as it becomes available and the presentation of those forecasts in usable 132 forms; in our case, this occurs monthly. Rebuilding models in an efficient and 133 maintainable way relies on developing an automated pipeline to handle the six stages of 134 converting raw data into new forecasts: data collection, data sharing, data manipulation, 135 modeling and forecasting, archiving, and presention of the forecasts (Figure 1a). To 136 implement the pipeline outlined in Figure 1a, we used a "continuous analysis" 137 framework (sensu Beaulieu-Jones & Greene, 2017) that automatically processes the 138 most up-to-date data, refits the models, makes new forecasts, archives the forecasts, and 139 updates a website with analysis of current and previous forecasts. In this section we 140 describe our approach to streamlining and automating the multiple components of the forecasting pipeline and the tools and infrastructure we employed to execute each component.

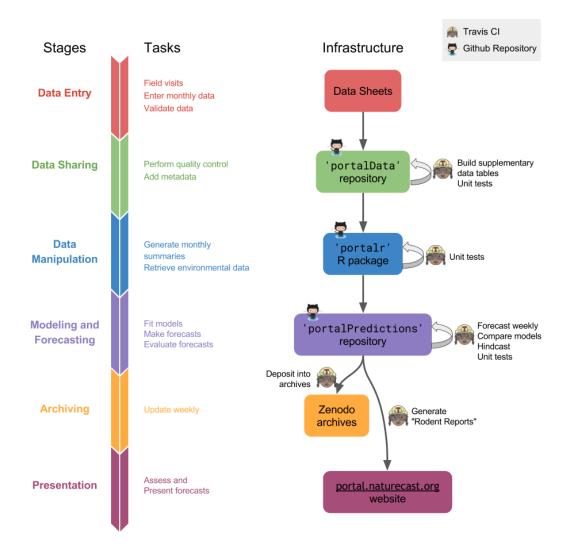


Figure 1: Figure 1. a) Stages of the forecasting pipeline. To go from raw data to forecast presentation involves a number of stages, each of which requires unique tasks, tools and infrastructure. The stages are interdependent, with outputs from one stage forming the inputs for the subsequent stage. Tasks in all stages are run using code written in R. b) Continuous integration system. Each box denotes the core infrastructure used for each stage of the forecasting pipeline. Continuous integration (denoted by the Travis icon, a woman wearing safety glasses and hardhat) triggers the code involved in events that link the stages of the pipeline, such as using the output from the forecasting stage (purple box) to create an updated website (rose box). Travis also runs tasks within a stage, such as testing code and adding weather data (icons on arrows originating and ending on the same box).

Continuous Analysis Framework

A core aspect of iterative near-term forecasting is the regular rerunning of the forecasting pipeline. We employed "continuous analysis" (sensu Beaulieu-Jones & Greene, 2017) to drive the automation of both the full pipeline and a number of its 147 individual components. Continuous analysis uses a set of tools originally designed for software development called "continuous integration" (CI). CI combines computing environments for running code with monitoring systems to identify changes in data or code. Essentially, CI is a computer helper who watches the pipeline and, when it sees a 15 change in the code or data, runs all the computer scripts needed to ensure that the 152 forecasting pipeline runs from beginning to end. This is useful for iterative near-term 153 forecasting because it does not rely on humans to create new forecasts whenever new 154 models or data are added. These tools are common in the area of software development, 155 where they are used to automate software testing and integrate work by multiple 156 developers working on the same code base. However, these tools can be used for any 157 computational task that needs to be regularly repeated or run after changes to code or 158 data (Beaulieu-Jones & Greene, 2017). Our forecasting pipeline currently runs on a 159 publicly available continuous integration service (Travis CI; https://travis-ci.org/) that is 160 free for open source projects (up to a limited amount of computing time). Because of the 161 widespread use of CI in software development, alternative services that can run code on 162 local or cloud-based computational infrastructure also exist (Beaulieu-Jones & Greene, 163 2017). We use CI to quality check data, test code using "unit tests" (Wilson et al., 2014), 164 build models, make forecasts, and publicly present and archive the results (Figure 1b). 165 In addition to automatically running software pipelines, the other key component of 166 "continuous analysis" is making sure that the pipelines will continue to run even as 167 software dependencies change (Beaulieu-Jones & Greene, 2017). Many of us have 168 experienced the frustrations that can occur when software updates (e.g., changes in R 169 package versions) create errors in previously functional code. We experienced this issue

when the tscount package (Liboschik, Fokianos, & Fried, 2015), used by one of our forecasting models, was temporarily removed from CRAN (the R package repository) 172 and could not be installed in the usual way. This broke our forecasting pipeline, as we could no longer run models that used that package. To make our pipeline robust to changes in external software dependencies, we follow Beaulieu and Greene's (2017) 175 recommendation to use software containers. Software containers are standalone 176 packages that contain copies of everything needed to run a given piece of software, 177 including the operating system. Once created, a software container is basically a time 178 capsule, containing all the software dependencies in the exact state used to develop and 179 run the software. If those dependencies change (or disappear) in the wider world, they 180 still exist, unchanged, in the container. We use an existing platform, Docker (Merkel, 181 2014), to store an exact image of the complete software environment for running the 182 forecasts. Docker also allows a specified set of packages to be used consistently across 183 different computer and server environments. Using containers allows us to control 184 transitions to new package versions, implementing them only after we have tested them 185 and made any necessary changes to the data processing and analysis code. We use a 186 container created by the Rocker project, which is a Docker image with many important 187 R packages (i.e. tidyverse) pre-installed (Boettiger & Eddelbuettel, 2017). We add our 188 code and dependencies to this existing Rocker image to create a software container for our forecasting pipeline. In combination, the automated running of the pipeline (continuous integration) and the guarantee it will not stop working unexpectedly due to software dependencies (via a software container) allows continuous analysis to serve as 192 the glue that connects all stages of the forecasting pipeline. 193

Data Collection, Entry, and Processing

195 Iterative forecasting benefits from frequently updated data so that state changes can be 196 quickly incorporated into new forecasts (Dietze et al., 2016). Both frequent data

collection and rapid processing are important for providing timely forecasts. Since we collect data monthly, ensuring that the models have access to the newest data requires a 198 data latency period of less than 1 month from collection to availability for modeling. To accomplish this, we automated components of the data processing and quality 200 assurance/quality control (QA/QC) process to reduce the time needed to add new data 20 to the database (Figure 1). 202 New data are double-entered into Microsoft Excel using the "data validation" feature. 203 The two versions are then compared using an R script to control for errors in data entry. Quality control (QC) checks using the testthat R package (Wickham, 2011) are run 205 on the data to test for validity and consistency both within the new data and between the 206 new and archived data. The local use of the QC scripts to flag problematic data greatly 207 reduces the time spent error-checking and ensures that the quality of data is consistent. 208 The cleaned data are then uploaded to the GitHub-based PortalData repository 209 (https://github.com/weecology/PortalData). GitHub (https://github.com/) is a software 210 development tool for managing computer code development, but we have also found it 211 useful for data management. On GitHub, changes to data can be tracked through the Git 212 version control system which logs all changes made to any files in the repository, giving 213 us a record of exactly of when specific lines of data were changed or added. All updates 214 to data are processed through "pull requests," which are notifications that someone has a modified version of the data to contribute. QA/QC checks are automatically run on the submitted data using continuous integration to ensure that no avoidable errors reach the 217 official version of the dataset. We also automated the updating of supplementary data tables, including information on 219 weather and trapping history, that were previously updated manually. As soon as new field data is merged into the repository, continuous integration updates all 22 supplementary files. Weather data is automatically fetched from our cellular-connected 222 weather station, cleaned, and appended to the weather data table. Supplementary data

tables related to trapping history are updated based on the data added to the main data tables. Using CI for this ensures that all supplementary data tables are always up-to-date with the core data.

227 Data Sharing

The Portal Project has a long history of making its data publicly available so that anyone 228 can use it for forecasting or other projects. Historically, the publication of the data was 229 conducted through data papers (S. Ernest et al., 2009, S. M. Ernest et al. (2016)), the 230 most common approach in ecology; this approach, however, caused years of data 23 latency. With the recent switch to posting data directly to a public GitHub repository 232 (Figure 1) with a CC0 waiver (i.e. no restrictions on data use; 233 https://creativecommons.org/publicdomain/zero/1.0/), data latency for everyone has 234 been reduced to less than one month, making meaningful iterative near-term forecasting 235 possible for not only our group but other interested parties, as well.

237 Data Manipulation

Once data is available, it must be processed into a form appropriate for modeling
(Figure 1). For many ecological datasets, this requires not only simple data
manipulation but also a good understanding of the data to facilitate appropriate
aggregation. Data manipulation steps are often conducted using custom one-off code to
convert the raw data into the desired form (Morris & White, 2013), but this approach
has several limitations. First, each researcher must develop and maintain their own data
manipulation code, which is inefficient and can result in different researchers producing
different versions of the data for the same task. Subtle differences in data processing
decisions have led to confusion when reproducing results for the Portal data in the past.
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 & 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 data manipulation. To avoid these issues for the Portal Project data, the Portal team has been developing an R package (portalr; http://github.com/weecology/portalr) for 252 acquiring the data and handling common data cleaning and aggregation tasks. As a 253 result, our modeling and forecasting code only needs to install this package and run the data manipulation and summary functions to get the appropriate data (Figure 1b). The 255 package undergoes thorough automated unit testing to ensure that data manipulations 256 are achieving the desired results. Having data manipulation code maintained in a 257 separate package that focuses on consistently providing properly summarized forms of 258 the most recent data has made maintaining the forecasting code itself much more 259 straightforward. 260

Modeling and Forecasting

Iterative near-term forecasting involves regularly refitting a variety of different models (Figure 1). Ideally, 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 264 models and make new forecasts each time the modeling code changes and when new 265 data become available (Figure 1b). We use a plugin infrastructure to allow new models 266 to be easily added to the system. This approach treats each model as an interchangable 26 black box; all models have access to the same input data and generate the same structure 268 for model outputs (Figure 2). During each run of the forecasting code, all existing 269 models are run and the standardized outputs are combined into a single file to store the 270 results of the different models' forecasts. A weighted ensemble model is then added 27 with weights based on how well individual models fit the training data. This plugin 272 infrastructure makes it easy to add and compare very different types of models, from the basic time-series approaches currently implemented to the more complex state-space and machine learning models we hope to implement in the future. As long as a model script can load the provided data and produce the appropriate output, it will be run and its results incorporated into the rest of the forecasting system.

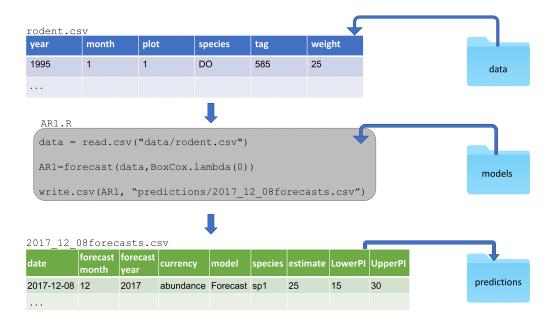


Figure 2: Figure 2. Demonstration of plugin infrastructure. All model scripts (represented here by the example AR1.R) are housed in a single folder. Each model script uses data provided by the core forecasting code (represented here by rodent.csv) and returns its forecast outputs in a predefined structure that is consistent across models (represented here by the example 2017_12_08forecasts.csv). Outputs from all models run on a particular date are combined into the same file (i.e. 2017_12_08forecasts.csv) to allow cross-model evaluations. Model output files are housed in a folder containing all forecast outputs from all previous dates to facilitate archiving and forecast assessment.

In addition to flexibility in what model structures can be supported, we also wanted to support flexibility in what the models predict. Allowing models to make forecasts for system properties ranging from individual species' population abundances to total community biomass facilitates exploration of differences in forecastability across different aspects of ecological systems. We designed a forecast output format to support this. Each forecast output file contains the date being forecast, the collection date of the data used for fitting the models, the model name, the date the forecast was made, the state variable being forecast (e.g., rodent biomass, the abundance of a species), and the

forecast value and associated uncertainty of that forecast (Figure 2). This allows us to store a variety of different forecasts in a common format and may serve as a useful 28 starting point for developing a standard for storing ecological forecasts more generally. Forecasts are currently evaluated using root mean square error (RMSE) to evaluate 289 point forecasts and coverage to evaluate uncertainty. We plan to add additional metrics 290 in the future. In addition to evaluating the actual forecasts, we also use hindcasting (forecasting on already collected data; Jolliffe & Stephenson, 2003) to gain additional 292 insight into the methods that work best for forecasting this system. For example, a model is fit using rodent observations up to June 2005, then used to make a forecast 12 294 months out to May 2006. The observations of that 12-month period can immediately be 295 used to evaluate the model. Since hindcasting is conducted using data that has already 296 been collected, it allows model comparisons to be conducted on large numbers of 297 hindcasts and provides insight into which models make the best forecasts without 298 needing to wait for new data to be collected (Harris, Taylor, & White, 2018). It can also 299 be used to quickly evaluate new models instead of waiting for an adequate amount of 300 data to accumulate. 301

302 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; Dietze et al.,

2016; Tredennick et al., 2016; Harris et al., 2018) (Figure 1). Archiving serves as a

form of pre-registration for model predictions because the forecasts cannot be modified

once the data to assess them has been collected. This helps facilitate an unbiased

interpretation of model performance. To serve this role, archives should be publicly

accessible and be a permanent record that cannot be changed or deleted. This second

criterion means that GitHub is not sufficient for archival purposes because repositories

can be changed or deleted (Bergman, 2012; White, 2015). We explored three major

repositories for archiving forecasts: FigShare (https://figshare.com/), Zenodo (https://zenodo.org/), and Open Science Framework (https://osf.io/). While all three repositories allowed for easy manual submissions (i.e., a human uploading files after each forecast), automating this process was substantially more difficult. Various combinations of repositories, APIs (i.e., interfaces for automatically interacting with the 316 archiving websites), and associated R packages had issues with: 1) integrating 317 authorization with continuous integration; 2) automatically making archived files public; 3) adding new files to an existing location; or 4) automatically permanently archiving 319 the files. Our eventual solution was to leverage the GitHub-Zenodo integration 320 (https://guides.github.com/activities/citable-code/) and automatically push forecasts to a 321 GitHub repository from the CI server and release them via the GitHub API. The 322 GitHub-Zenodo integration is designed to automatically create versioned archives of 323 GitHub repositories. We created a repository for storing forecasts 324 (https://github.com/weecology/forecasts) and linked this repository with Zenodo (a 325 one-time manual process). Each time a new forecast is created, our pipeline adds the new forecasts to the GitHub repository and uses the GitHub API to create a new "release" for that repository. This triggers the GitHub-Zenodo integration, which 328 automatically archives the resulting forecasts under a top-level DOI that refers to all 329 archived forecasts (https://doi.org/10.5281/zenodo.839580). Through this process, we 330 automatically archive every forecast made with a documented time-stamp. In addition, we also archive the full state of the modeling and forecasting repository (https://doi.org/10.5281/zenodo.833438). This ensures that every forecast is fully 333 reproducible since the exact code used to generate every forecast is preserved. Early 334 forecasts from this system are archived in the modeling and forecasting code archive, not in the newer repository 'forecasts'.

337 Presentation

Each month, we present our forecasts on a website that displays monthly rodent forecasts, model evaluation metrics, monthly reports, and information about the study 339 site (Figure 3; http://portal.naturecast.org). The website includes a graphical 340 presentation of the most recent month's forecasts (including uncertainty) and compares the latest data to the previous forecasts. Information on the species and the field site 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 345 Github Pages (https://pages.github.com/). The files for the website are stored in a 346 subdirectory of the forecasting repository. As a result, the website is also archived automatically as part of archiving the forecast results. 348

Discussion

Following the recommendations of Dietze et al (2016), we developed an automated 350 iterative forecasting system (Figure 1) to support repeated forecasting of an ecological 35 system. Our forecasting system automatically acquires and processes the newest data, 352 refits the models, makes new forecasts, publicly archives those forecasts, and presents 353 both the current forecast and information on how previous forecasts performed. Every 354 week, the forecasting system generates a new set of forecasts with no human 355 intervention, except for the entry of new field data. Our forecasting system ensures that 356 forecasts based on the most recent data are always available and is designed to allow 35 rapid assessment of the performance of multiple forecasting models for a number of 358 different states of the system, including the abundances of individual species and 359 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 leveraged

Portal Forecast Total Abundance Forecast

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

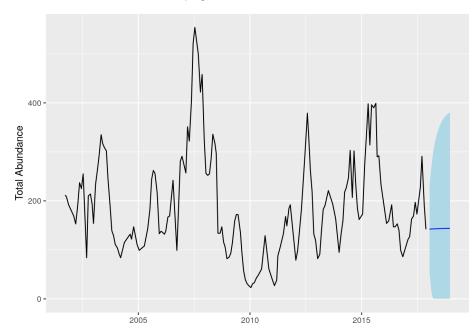


Figure 3: Figure 3. Screen capture of the homepage of the Portal Forecasting website (http://portal.naturecast.org). This site contains information on the most current forecasts, evaluation of forecast performance, and general information about the species being forecast.

existing tools and services (i.e. GitHub, Travis, Docker) for more complicated cyberinfrastructure tasks. Thus, our approach to developing iterative near-term 363 forecasting infrastructure provides an example for how short-term ecological forecasting systems can be 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 us to build the system relatively cheaply in terms of both time and money. This included the use of tools like Docker for reproducibility, Travis CI continuous integration for automatically running the pipeline, Rmarkdown and knitr for generating the website, and the already existing integration 37 between Github and Zenodo to archive the forecasts. By using this "continuous analysis" 372 approach (Beaulieu-Jones & Greene, 2017), where analyses are automatically rerun 373 when changes are made to data, models, or associated code, we have reduced the time 374 required by scientists to run and maintain the forecasting pipeline. To make the system 375 extensible so that new models could be easily incorporated, we used a plugin-based 376 infrastructure so that adding a new model to the system is as easy as adding a single file 377 to the 'models' folder in our repository (Figure 2). This should substantially lower the 378 barriers to other scientists contributing models to this forecasting effort. We also 379 automatically archive the resulting forecasts publicly so that the performance of these 380 forecasts can be assessed by both us and other researchers as new data is collected. This 38 serves as a form of pre-registration by providing a quantitative record of the forecast 382 before the data being predicted were collected. 383 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 385 iterative forecasting. Continuous integration is designed primarily for running 386 automated tests on software, not for running a coordinated forecasting pipeline. As a 387

result, extra effort was sometimes necessary to figure out how to get these systems to

work properly in non-standard situations, like running code that was not part of a software package. In addition, hosted continuous integration solutions, like Travis, 390 provide only limited computational resources. As the number and complexity of the models we fit has grown, we have had to continually invest effort in reducing our total 392 compute time so we can stay within these limits. Finally, we found no satisfactory 393 existing solution for archiving our results. All approaches we tried had limitations when 394 it came to automatically generating publicly-versioned archives of forecasts on a repeated basis, and our eventual solution was difficult to configure to such a degree that 396 it will remain an impediment for most researchers. Overall, we found existing 397 technology to be sufficient to the task of creating an iterative forecasting pipeline, but it 398 required greater expertise and a greater investment of time than is ideal. Additional tool 399 development to reduce the effort required for scientists to set up their own short-term 400 forecasting systems would clearly be useful. Our efforts, however, show that it is 40 possible to use existing tools to develop initial iterative systems as a method for both 402 advancing scientific understanding and developing proof of concept forecasting systems. 403 Because of the breadth of expertise needed to set up our forecasting pipeline, our effort 404 required a team with diverse skills and perspectives, ranging from software 405 development to field site expertise. It is rare to find such breadth within a single 406 research group, and our system was developed as a collaboration between the lab 407 collecting the data and a computational ecology lab. When teams have a breadth of 408 expertise, communication can be challenging (Winowiecki et al., 2011). We found a 409 shared base of knowledge related to both the field research and fundamental 410 computational skills was important for the success of the group. The two labs are part of a joint interdisciplinary ecology group that has a mission of breaking down barriers between field and computational/theoretical ecologists (http://weecology.org). Everyone on the team had received training in fundamental data management and computing skills through a combination of university courses, Software and Data Carpentry

workshops (Teal et al., 2015), and informal lab training efforts. In addition, everyone was broadly familiar with the study site and methods of data collection, and most team members had participated in field work at the site on multiple occasions. This provided a shared set of knowledge and vocabulary that actively facilitated interdisciplinary interactions. Given the current state of tools for forecasting, forecasting teams will need 420 people with significant experience in working with continuous integration and APIs. 42 This means interdisciplinary teams will generally be required for creating these pipelines until tool development improves. To improve the success of these diverse 423 groups, we believe efforts at providing 'team science' training to scientists interested in 424 forecasting will be beneficial for the success of iterative forecasting attempts for the 425 foreseeable future (Read et al., 2016). 426 We developed infrastructure for automatically making iterative forecasts with the goals 427 of making accurate forecasts for this well-studied system, learning what methods work 428 well for ecological forecasting more generally, and improving our understanding of the 429 processes driving ecological dynamics. The most obvious application of automated 430 iterative ecological forecasting is for speeding up development of forecasting models by 431 using the most recent data available and by quickly iterating to improve the models used 432 for forecasting. By learning what works best for forecasting in this and other ecological 433 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 435 different aspects of the ecological community, we also hope to learn about what aspects 436 of ecology are more forecastable. Finally, automated forecasting infrastructures like this 437 one also provide a core foundation for faster scientific inquiry because new models can 438 quickly be applied to data and compared to existing models. The forecasting 439 infrastructure does the time-consuming work of data processing, data integration, and model assessment, allowing new research to focus on the models being developed and the inferences about the system that can be drawn from them (Dietze et al., 2016). We

plan to use this pipeline to drive future research into understanding the processes that
govern the dynamics of individual populations and the community as a whole. By
regularly running different models for population and community dynamics, a near-term
iterative pipeline such as ours should also make it possible to rapidly detect changes in
how the system is operating, which should allow the rapid identification of ecological
transitions or even possibly allow them to be prevented (Pace et al., 2017). By building
an automated iterative near-term forecasting infrastructure, we can improve our ability
to forecast natural systems, understand the biology driving ecological dynamics, and
detect or even predict changes in system state that are important for conservation and
management.

453 Acknowledgements

We thank Henry Senyondo for help with continuous integration and Hao Ye for
discussions and feedback on the manuscript. 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 the software and tools that made this project possible. 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.

Data Accessibility

The data used in this study is from the Portal Project and is openly available (CC0) on
GitHub (https://github.com/weecology/PortalData). Code for reproducing all analyses is
available on GitHub (https://github.com/weecology/portalPredictions) and archived on
Zenodo (White et al., 2018b). Forecasts made by this system are all archived to Zenodo

466 (White et al., 2018a).

Box 1. Key practices for automated iterative near-term

ecological forecasting

- A list of some of the key practices developed by Dietze et al (2016) for facilitating
- iterative near-term ecological forecasting and discussion of why these practices are
- 471 important.

472 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

- To reduce the time and effort needed to incorporate data into models, best practices in
- data structure should 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).

487 Models

88 4. Focus on uncertainty

- 489 Understanding the uncertainty of forecasts is crucial to interpreting 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
- 492 forecast models should include assessment of how accurately they quantify uncertainty
- as well as point estimates (Hooten & Hobbs, 2015).

5. Compare forecasts to simple baselines

- 495 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 (Harris et al., 2018).

6. Compare and combine multiple modeling approaches

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

503 Cyberinfrastructure

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

507 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 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, to allow models developed by different groups to be integrated into a single framework (Dietze et al., 2016).

9. Automated end-to-end reproducibility

Each forecast iteration involves acquiring new data, refitting the models, and making
new forecasts. 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).

523 10. Publicly archive forecasts

Forecasts should be openly archived to demonstrate that the forecasts were made
without knowledge of the outcomes 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; Harris et al., 2018). Ideally, the
forecasts and evaluation of their performance should be automatically posted publicly in
a manner that is understandable by both scientists and the broader stakeholder
community.

References

Allaire, J., Cheng, J., Xie, Y., McPherson, J., Chang, W., Allen, J., ... Arslan, R. (2017). *Rmarkdown: Dynamic documents for r*. Retrieved from

- https://CRAN.R-project.org/package=rmarkdown
- Araujo, M. B., & New, M. (2007). Ensemble forecasts of species distributions. Trends
- *in Ecology and Evolution*, 22(1), 42–47.
- Beaulieu-Jones, B. K., & Greene, C. S. (2017). Reproducibility of computational
- workflows is automated using continuous analysis. *Nature Biotechnology*, 35(4),
- 539 342-346.
- Bergman, C. (2012). On the preservation of published bioinformatics code on github.
- Retrieved from https://caseybergman.wordpress.com/2012/11/08/
- on-the-preservation-of-published-bioinformatics-code-on-github/
- Boettiger, C., & Eddelbuettel, D. (2017). An introduction to rocker: Docker containers
- 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
- 547 *America*, 90(2), 205–214.
- Brown, J. (1998). The desert granivory experiments at portal. *Experimental Ecology*.
- oxford University Press, Oxford, UK, 71–95.
- ⁵⁵⁰ Clark, J. S., Carpenter, S. R., Barber, M., Collins, S., Dobson, A., Foley, J. A., ... others.
- 551 (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.,
- ... others. (2016). Iterative ecological forecasting: Needs, opportunities, and
- challenges. *Proceedings of the National Academy of Sciences*.
- Diniz-Filho, J. A. F., Bini, L. M., Rangel, T. F., Loyola, R. D., Hof, C., Nogues-Bravo,
- 557 D., & Araujo, M. B. (2009). Partitioning and mapping uncertainties in ensembles of

- forecasts of species turnover under climate change. *Ecography*, 32(6), 897–906.
- 559 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
- 561 Environmental Sustainability, 14, 1–16.
- ⁵⁶² Ernest, S. M., Brown, J. H., Thibault, K. M., White, E. P., & Goheen, J. R. (2008). Zero
- sum, the niche, and metacommunities: Long-term dynamics of community assembly.
- 564 *The American Naturalist*, 172(6), E257–E269.
- Ernest, S. M., Yenni, G. M., Allington, G., Christensen, E. M., Geluso, K., Goheen, J.
- R., ... others. (2016). Long-term monitoring and experimental manipulation of a
- chihuahuan desert ecosystem near portal, arizona (1977–2013). Ecology, 97(4),
- 568 1082-1082.
- Ernest, S., Valone, T. J., & Brown, J. H. (2009). Long-term monitoring and
- experimental manipulation of a chihuahuan desert ecosystem near portal, arizona, usa.
- 571 Ecology, 90(6), 1708–1708.
- 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.
- Harris, D. J., 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.
- 577 Ecological Monographs, 85(1), 3–28.
- Jolliffe, I. T., & Stephenson, D. B. (Eds.). (2003). Forecast verification: a practitioner's
- guide in atmospheric science. John Wiley; Sons, Ltd. Retrieved from
- http://linkinghub.elsevier.com/retrieve/pii/S0169207005001214
- Liboschik, T., Fokianos, K., & Fried, R. (2015). Tscount: An r package for analysis of
- count time series following generalized linear models. Universitätsbibliothek

- 583 Dortmund.
- 584 Luo, Y., Ogle, K., Tucker, C., Fei, S., Gao, C., LaDeau, S., ... Schimel, D. S. (2011).
- Ecological forecasting and data assimilation in a data-rich era. *Ecological Applications*,
- 586 *21*(5), 1429–1442.
- 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/
- Merkel, D. (2014). Docker: Lightweight linux containers for consistent development
- and deployment. *Linux J.*, 2014(239). Retrieved from
- 593 http://dl.acm.org/citation.cfm?id=2600239.2600241
- Morris, B. D., & White, E. P. (2013). The ecodata retriever: Improving access to
- existing ecological data. *PloS One*, 8(6), e65848.
- Pace, M. L., Batt, R. D., Buelo, C. D., Carpenter, S. R., Cole, J. J., Kurtzweil, J. T., &
- Wilkinson, G. M. (2017). Reversal of a cyanobacterial bloom in response to early
- warnings. Proceedings of the National Academy of Sciences, 114(2), 352–357.
- Petchey, O. L., Pontarp, M., Massie, T. M., Kéfi, S., Ozgul, A., Weilenmann, M., ...
- others. (2015). The ecological forecast horizon, and examples of its uses and
- determinants. *Ecology Letters*, 18(7), 597–611.
- Read, E. K., O'Rourke, M., Hong, G., Hanson, P., Winslow, L. A., Crowley, S., ...
- Weathers, K. (2016). Building the team for team science. *Ecosphere*, 7(3).
- 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),
- 606 451. doi:10.21105/joss.00451
- Stodden, V., & Miguez, S. (2014). Best practices for computational science: Software

- 608 infrastructure and environments for reproducible and extensible research. Journal of
- 609 Open Research Software, 2(1).
- 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.
- 616 (2015). Data carpentry: Workshops to increase data literacy for researchers.
- 617 International Journal of Digital Curation, 10(1), 135–143.
- ⁶¹⁸ 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.
- 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. (2015). Some thoughts on best publishing practices for scientific software.
- 628 *Ideas in Ecology and Evolution*, 8(1).
- White, E. P., Baldridge, E., Brym, Z. T., Locey, K. J., McGlinn, D. J., & Supp, S. R.
- 630 (2013). Nine simple ways to make it easier to (re) use your data. *Ideas in Ecology and*
- Evolution, 6(2).
- White, E. P., Bledsoe, E. K., Christensen, E. M., Harris, D. J., Simonis, J. L., Taylor, S.

- 633 D., ... Ernest, S. K. M. (2018a, February). Weecology/forecasts: 2018-02-17.
- 634 doi:10.5281/zenodo.839580
- White, E. P., Yenni, G. M., Taylor, C., Shawn D and, Bledsoe, E. K., Simonis, J. L., &
- Ernest, S. K. M. (2018b, February). Weecology/portalPredictions 2018-02-16.
- 637 doi:10.5281/zenodo.833438
- Wickham, H. (2011). Testthat: Get started with testing. *The R Journal*, 3, 5–10.
- 639 Retrieved from
- http://journal.r-project.org/archive/2011-1/RJournal_2011-1_Wickham.pdf
- 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.
- 643 Winowiecki, L., Smukler, S., Shirley, K., Remans, R., Peltier, G., Lothes, E., ...
- Alkema, L. (2011). Tools for enhancing interdisciplinary communication.
- Sustainability: Science, Practice and Policy, 7(1), 74–80.
- Kie, Y. (2015). Dynamic documents with r and knitr (Vol. 29). CRC Press.